



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 12:40 PM EST

PDB ID : 6L87  
BMRB ID : 27677  
Title : Solution structure of the tandem PWWP-ARID domains of human RBBP1  
Authors : Gong, W.B.; Perrett, S.; Feng, Y.G.  
Deposited on : 2019-11-05

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

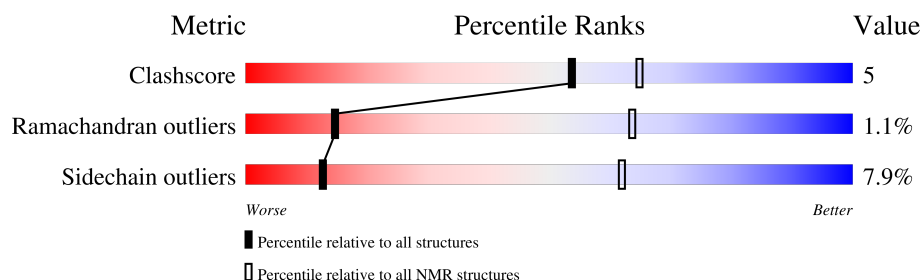
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 86%.

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	229	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:103, A:117-A:212 (198)	1.06	7

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 6, 7, 11, 17, 18
2	1, 8, 13, 16, 19, 20
3	3, 12, 14, 15
4	9, 10

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3730 atoms, of which 1856 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called AT-rich interactive domain-containing protein 4A.

Mol	Chain	Residues	Atoms						Trace
1	A	229	Total	C	H	N	O	S	0
			3730	1193	1856	320	354	7	

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	LYS	ASP	See sequence details	UNP P29374
A	110	LYS	GLU	See sequence details	UNP P29374
A	?	-	ASP	deletion	UNP P29374
A	?	-	GLY	deletion	UNP P29374
A	?	-	PRO	deletion	UNP P29374
A	?	-	ALA	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	ASN	deletion	UNP P29374
A	?	-	ASP	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	LYS	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	LYS	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	ALA	deletion	UNP P29374
A	?	-	LYS	deletion	UNP P29374
A	?	-	LYS	deletion	UNP P29374
A	?	-	THR	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	VAL	deletion	UNP P29374
A	?	-	PRO	deletion	UNP P29374
A	112	LYS	GLU	See sequence details	UNP P29374
A	222	LEU	-	expression tag	UNP P29374
A	223	GLU	-	expression tag	UNP P29374
A	224	HIS	-	expression tag	UNP P29374
A	225	HIS	-	expression tag	UNP P29374
A	226	HIS	-	expression tag	UNP P29374

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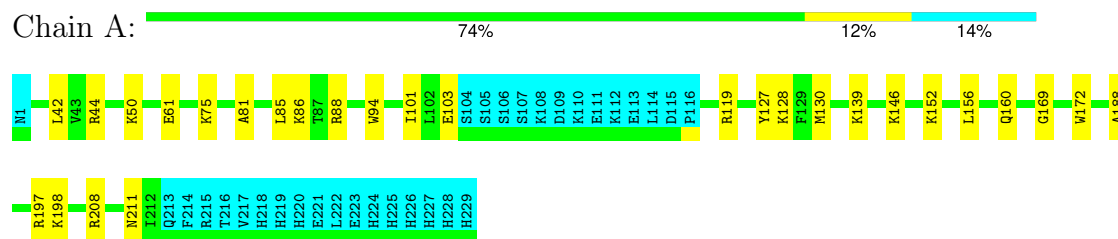
Chain	Residue	Modelled	Actual	Comment	Reference
A	227	HIS	-	expression tag	UNP P29374
A	228	HIS	-	expression tag	UNP P29374
A	229	HIS	-	expression tag	UNP P29374

## 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: AT-rich interactive domain-containing protein 4A

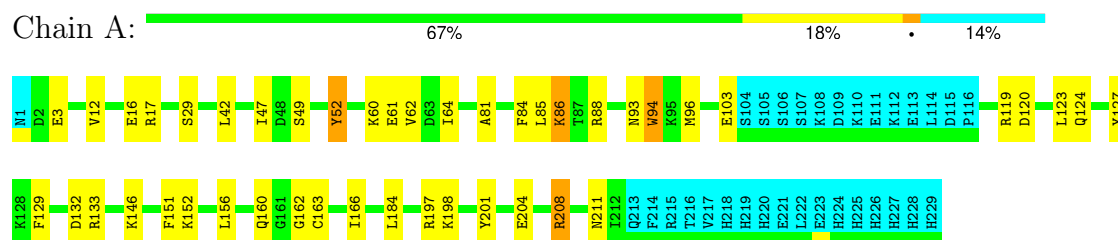


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

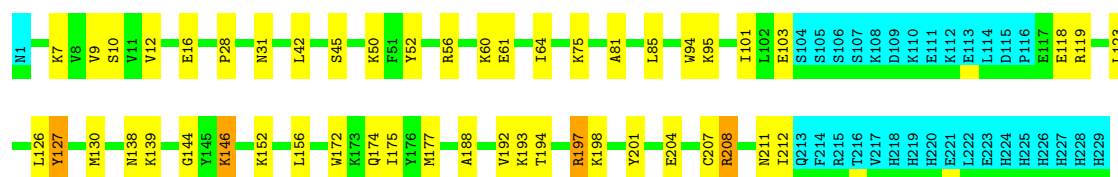
- Molecule 1: AT-rich interactive domain-containing protein 4A



#### 4.2.2 Score per residue for model 2

- Molecule 1: AT-rich interactive domain-containing protein 4A

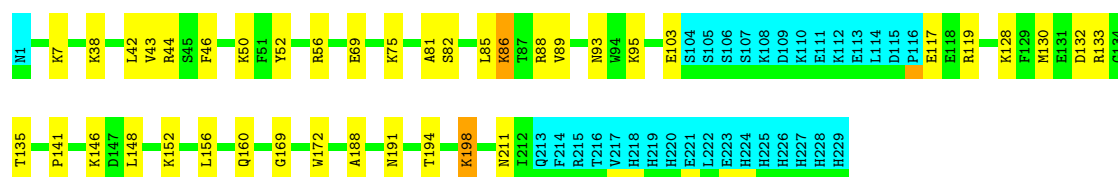




#### 4.2.3 Score per residue for model 3

- Molecule 1: AT-rich interactive domain-containing protein 4A

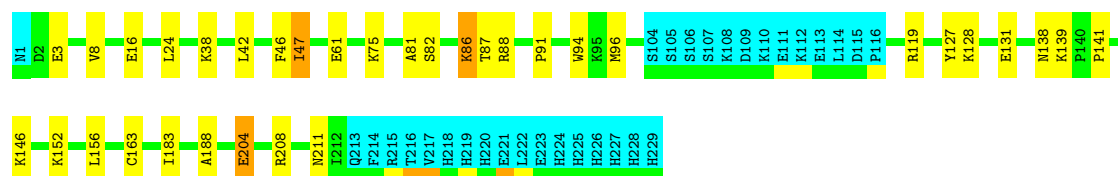
Chain A: 69% 17% 14%



#### 4.2.4 Score per residue for model 4

- Molecule 1: AT-rich interactive domain-containing protein 4A

Chain A: 72% 14% 14%



#### 4.2.5 Score per residue for model 5

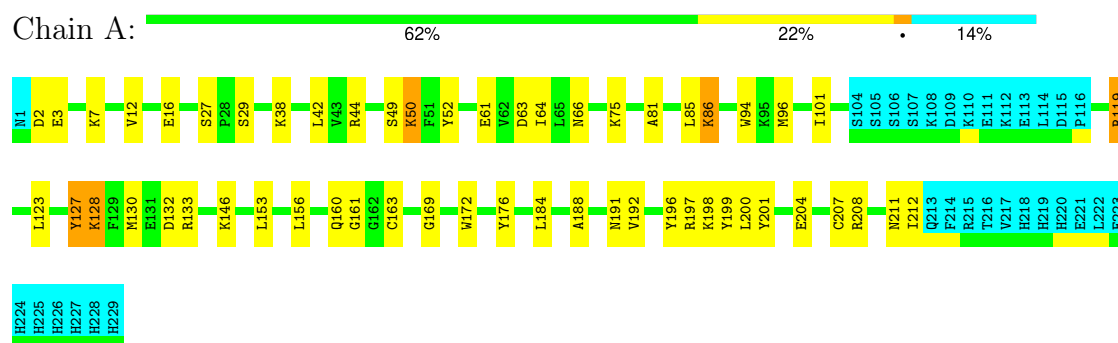
- Molecule 1: AT-rich interactive domain-containing protein 4A

Chain A: 71% 12% 14%



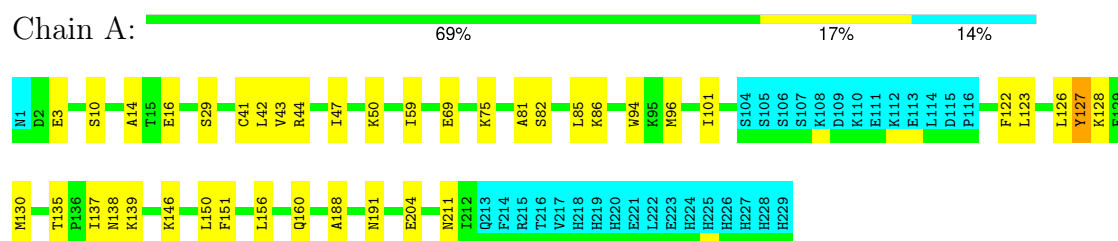
#### 4.2.6 Score per residue for model 6

- Molecule 1: AT-rich interactive domain-containing protein 4A



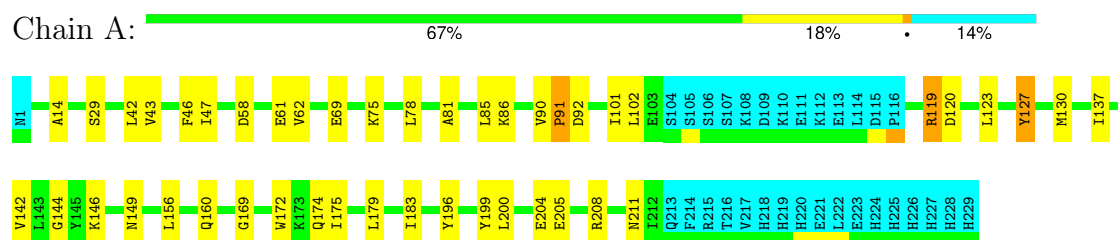
#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: AT-rich interactive domain-containing protein 4A



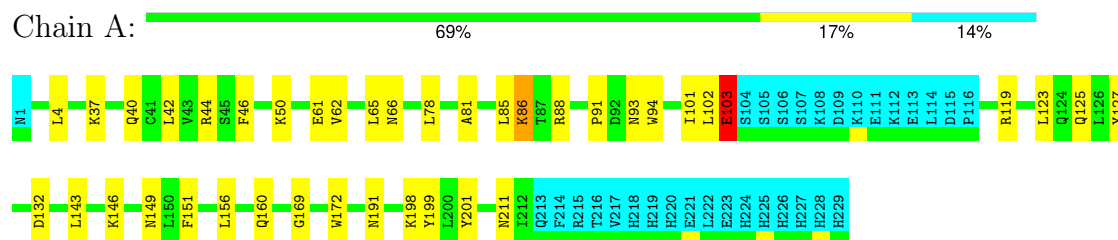
#### 4.2.8 Score per residue for model 8

- Molecule 1: AT-rich interactive domain-containing protein 4A



#### 4.2.9 Score per residue for model 9

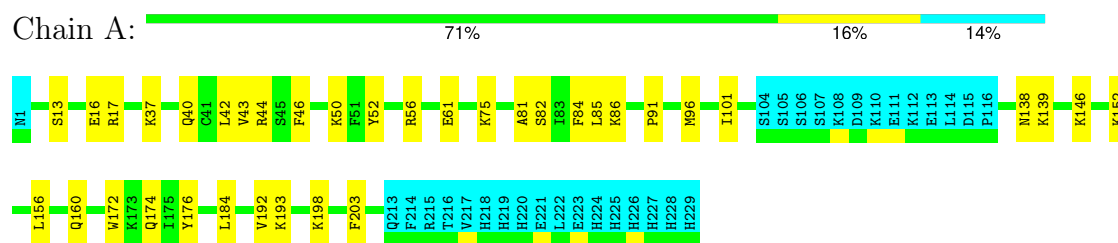
- Molecule 1: AT-rich interactive domain-containing protein 4A





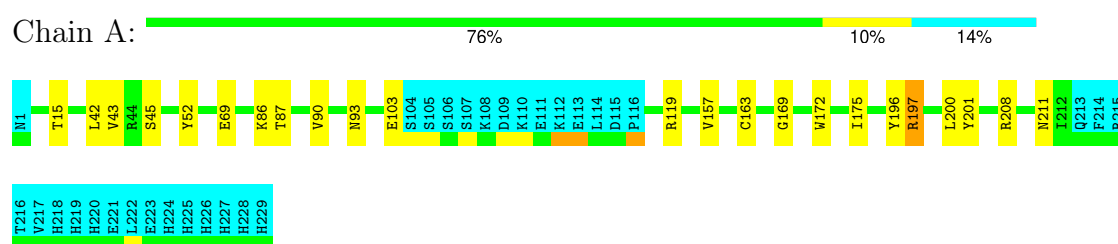
### 4.2.10 Score per residue for model 10

- Molecule 1: AT-rich interactive domain-containing protein 4A



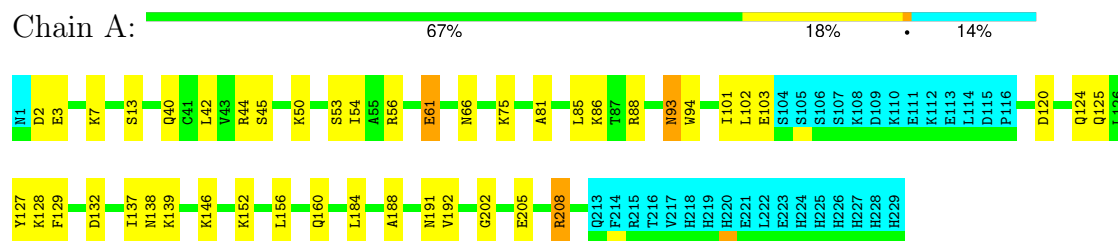
### 4.2.11 Score per residue for model 11

- Molecule 1: AT-rich interactive domain-containing protein 4A



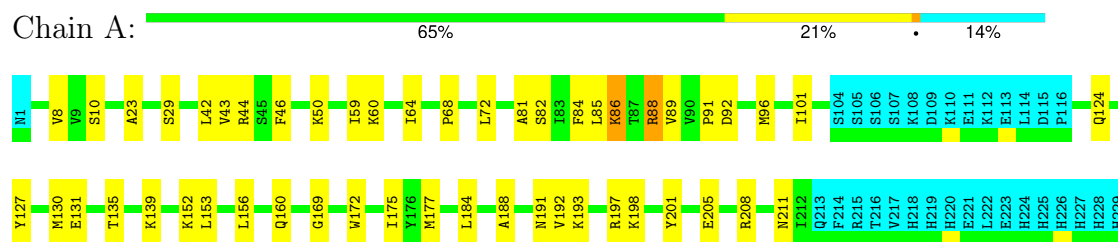
### 4.2.12 Score per residue for model 12

- Molecule 1: AT-rich interactive domain-containing protein 4A



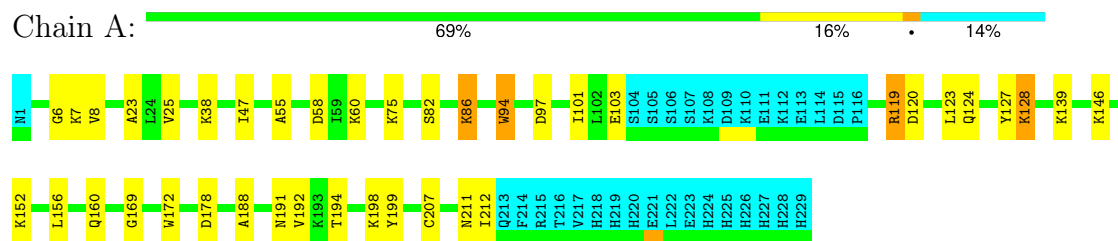
### 4.2.13 Score per residue for model 13

- Molecule 1: AT-rich interactive domain-containing protein 4A



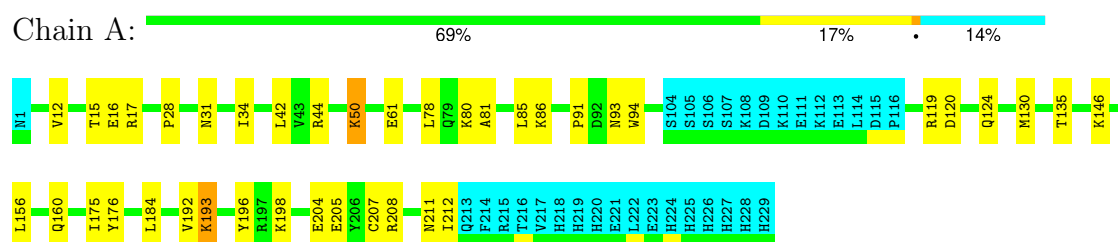
#### 4.2.14 Score per residue for model 14

- Molecule 1: AT-rich interactive domain-containing protein 4A



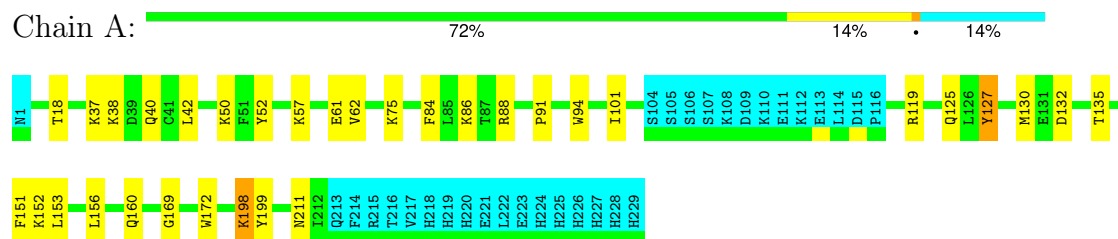
#### 4.2.15 Score per residue for model 15

- Molecule 1: AT-rich interactive domain-containing protein 4A



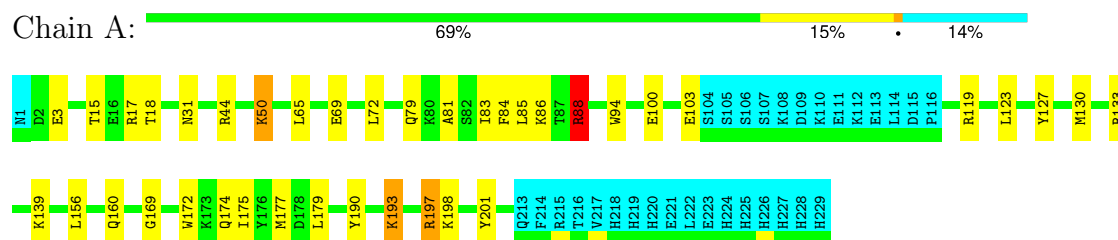
#### 4.2.16 Score per residue for model 16

- Molecule 1: AT-rich interactive domain-containing protein 4A



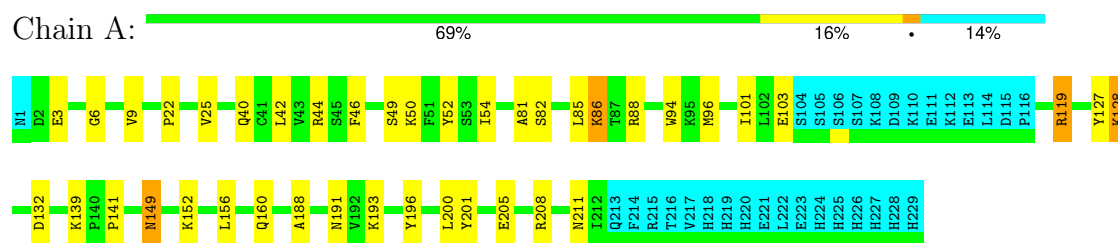
#### 4.2.17 Score per residue for model 17

- Molecule 1: AT-rich interactive domain-containing protein 4A



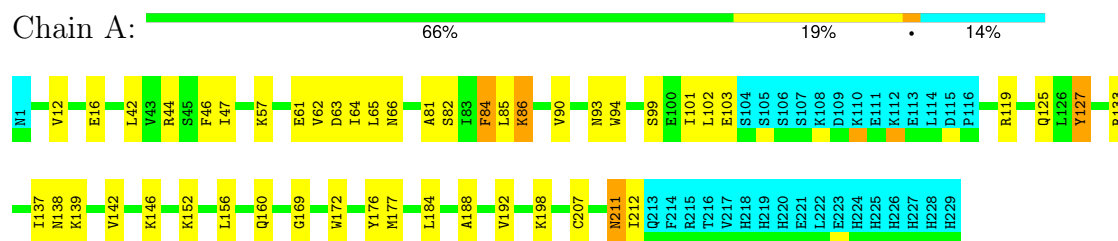
### 4.2.18 Score per residue for model 18

- Molecule 1: AT-rich interactive domain-containing protein 4A



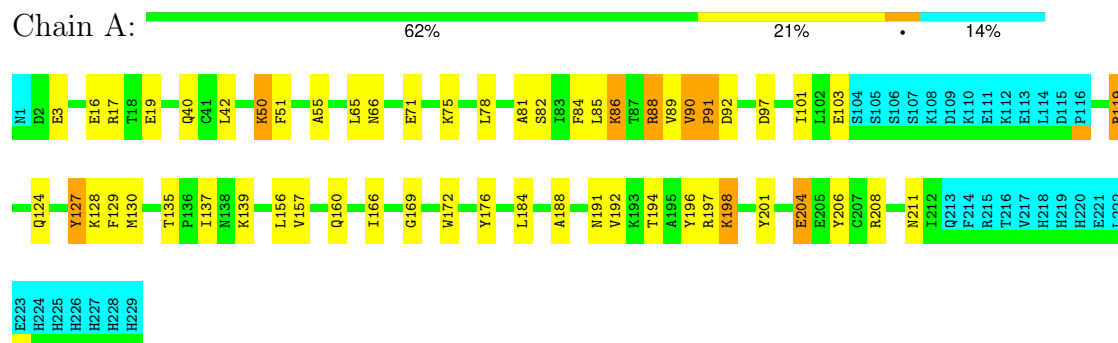
### 4.2.19 Score per residue for model 19

- Molecule 1: AT-rich interactive domain-containing protein 4A



### 4.2.20 Score per residue for model 20

- Molecule 1: AT-rich interactive domain-containing protein 4A



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2611
Number of shifts mapped to atoms	2611
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

## 6 Model quality [i](#)

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.8
All	All	0	18

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	119	ARG	Sidechain	6
1	A	197	ARG	Sidechain	3
1	A	44	ARG	Sidechain	3
1	A	17	ARG	Sidechain	2
1	A	88	ARG	Sidechain	2
1	A	133	ARG	Sidechain	1
1	A	56	ARG	Sidechain	1

### 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	1604	1610	1609	16±4
All	All	32080	32200	32180	324

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:MET:SD	1:A:133:ARG:HD3	0.64	2.32	5	2
1:A:81:ALA:O	1:A:85:LEU:HG	0.62	1.93	19	15
1:A:169:GLY:HA2	1:A:172:TRP:CE3	0.61	2.30	5	12
1:A:156:LEU:O	1:A:160:GLN:HG2	0.61	1.96	17	15
1:A:204:GLU:O	1:A:208:ARG:HG2	0.60	1.96	6	2
1:A:46:PHE:CE1	1:A:81:ALA:HA	0.59	2.32	13	3
1:A:130:MET:HG3	1:A:135:THR:O	0.59	1.97	7	5
1:A:197:ARG:O	1:A:201:TYR:HB3	0.58	1.98	1	3
1:A:119:ARG:HG3	1:A:120:ASP:N	0.58	2.11	14	2
1:A:84:PHE:O	1:A:88:ARG:HG2	0.57	1.99	16	2
1:A:197:ARG:O	1:A:201:TYR:HB2	0.57	1.99	13	3
1:A:101:ILE:HG21	1:A:123:LEU:HB3	0.56	1.78	9	1
1:A:119:ARG:O	1:A:123:LEU:HG	0.56	2.00	1	4
1:A:152:LYS:O	1:A:156:LEU:HG	0.56	2.00	3	9
1:A:82:SER:O	1:A:86:LYS:HG3	0.56	2.01	10	9
1:A:101:ILE:HG23	1:A:127:TYR:CE2	0.55	2.37	7	4
1:A:188:ALA:O	1:A:192:VAL:HG23	0.55	2.02	14	3
1:A:188:ALA:HA	1:A:191:ASN:ND2	0.55	2.16	12	8
1:A:84:PHE:CE2	1:A:88:ARG:HD2	0.54	2.37	1	1
1:A:163:CYS:SG	1:A:204:GLU:HG3	0.54	2.42	1	1
1:A:193:LYS:O	1:A:197:ARG:HB2	0.54	2.03	2	2
1:A:44:ARG:HG3	1:A:50:LYS:O	0.53	2.02	7	5
1:A:10:SER:O	1:A:59:ILE:HA	0.53	2.03	13	2
1:A:90:VAL:HB	1:A:91:PRO:HD2	0.53	1.80	20	2
1:A:119:ARG:HA	1:A:151:PHE:CD1	0.53	2.38	1	1
1:A:130:MET:SD	1:A:199:TYR:HA	0.53	2.44	8	2
1:A:129:PHE:CE1	1:A:202:GLY:HA3	0.52	2.40	12	1
1:A:86:LYS:O	1:A:93:ASN:HB3	0.52	2.05	1	2
1:A:46:PHE:CE2	1:A:81:ALA:HA	0.52	2.40	18	3
1:A:172:TRP:CZ3	1:A:193:LYS:HA	0.52	2.40	10	1
1:A:198:LYS:HE3	1:A:199:TYR:CZ	0.51	2.40	14	1
1:A:196:TYR:CD1	1:A:200:LEU:HD12	0.51	2.40	8	1
1:A:127:TYR:CE1	1:A:137:ILE:HG13	0.51	2.39	12	1
1:A:101:ILE:HG23	1:A:127:TYR:CE1	0.51	2.41	12	6
1:A:127:TYR:CZ	1:A:137:ILE:HG21	0.51	2.40	7	1
1:A:204:GLU:O	1:A:208:ARG:HG3	0.50	2.06	2	3
1:A:99:SER:O	1:A:103:GLU:HA	0.50	2.06	19	1
1:A:46:PHE:HB2	1:A:84:PHE:CE1	0.50	2.41	19	2
1:A:64:ILE:HD12	1:A:64:ILE:H	0.50	1.66	2	3
1:A:123:LEU:O	1:A:127:TYR:HB2	0.50	2.06	7	1
1:A:96:MET:SD	1:A:101:ILE:HD11	0.50	2.46	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:ILE:HG23	1:A:127:TYR:CD1	0.49	2.42	16	3
1:A:122:PHE:O	1:A:126:LEU:HG	0.49	2.07	7	1
1:A:37:LYS:HD2	1:A:40:GLN:NE2	0.49	2.22	16	1
1:A:86:LYS:HD2	1:A:87:THR:N	0.48	2.22	4	1
1:A:198:LYS:HE2	1:A:199:TYR:CZ	0.48	2.42	9	1
1:A:6:GLY:HA2	1:A:25:VAL:O	0.48	2.08	18	2
1:A:119:ARG:HH11	1:A:119:ARG:HG3	0.48	1.69	18	1
1:A:176:TYR:CE2	1:A:188:ALA:HB1	0.48	2.44	19	1
1:A:120:ASP:O	1:A:124:GLN:HG2	0.48	2.09	15	1
1:A:193:LYS:HA	1:A:196:TYR:CE1	0.48	2.44	15	1
1:A:196:TYR:CD2	1:A:200:LEU:HD12	0.48	2.43	6	1
1:A:194:THR:O	1:A:198:LYS:HG2	0.48	2.09	20	3
1:A:120:ASP:O	1:A:124:GLN:HG3	0.47	2.09	12	1
1:A:176:TYR:CD2	1:A:192:VAL:HB	0.47	2.44	20	2
1:A:50:LYS:HE3	1:A:50:LYS:N	0.47	2.24	17	1
1:A:163:CYS:SG	1:A:208:ARG:HB3	0.47	2.49	11	1
1:A:196:TYR:HA	1:A:200:LEU:HD23	0.47	1.85	11	2
1:A:40:GLN:HG3	1:A:54:ILE:O	0.47	2.09	5	2
1:A:12:VAL:HB	1:A:16:GLU:O	0.47	2.10	2	3
1:A:205:GLU:OE2	1:A:208:ARG:HD3	0.47	2.09	15	1
1:A:71:GLU:OE2	1:A:75:LYS:HE2	0.47	2.10	20	1
1:A:96:MET:SD	1:A:128:LYS:HG2	0.47	2.49	4	1
1:A:87:THR:HA	1:A:93:ASN:O	0.47	2.10	11	1
1:A:44:ARG:NH2	1:A:132:ASP:HB2	0.47	2.25	18	1
1:A:88:ARG:O	1:A:94:TRP:HB3	0.47	2.09	18	1
1:A:101:ILE:HG23	1:A:127:TYR:CZ	0.47	2.45	18	1
1:A:90:VAL:HG21	1:A:93:ASN:HB2	0.47	1.87	19	1
1:A:84:PHE:HA	1:A:88:ARG:NH2	0.47	2.24	20	1
1:A:102:LEU:O	1:A:103:GLU:HB2	0.47	2.10	9	1
1:A:127:TYR:CE2	1:A:137:ILE:HG13	0.47	2.44	20	1
1:A:207:CYS:HA	1:A:212:ILE:HD12	0.46	1.88	14	4
1:A:88:ARG:HA	1:A:94:TRP:CD1	0.46	2.45	1	1
1:A:172:TRP:CE3	1:A:175:ILE:HD11	0.46	2.44	2	1
1:A:81:ALA:O	1:A:85:LEU:HD13	0.46	2.11	17	1
1:A:46:PHE:CZ	1:A:81:ALA:HA	0.46	2.45	9	2
1:A:156:LEU:HB3	1:A:175:ILE:HG22	0.46	1.86	8	3
1:A:141:PRO:HB2	1:A:148:LEU:O	0.46	2.11	3	1
1:A:31:ASN:ND2	1:A:34:ILE:HB	0.46	2.25	15	1
1:A:130:MET:HG2	1:A:135:THR:O	0.46	2.10	3	1
1:A:28:PRO:HA	1:A:31:ASN:OD1	0.46	2.11	15	2
1:A:12:VAL:HG13	1:A:16:GLU:O	0.46	2.10	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LYS:HD3	1:A:40:GLN:NE2	0.46	2.27	9	1
1:A:91:PRO:HA	1:A:94:TRP:O	0.46	2.10	15	1
1:A:43:VAL:HB	1:A:52:TYR:CE1	0.45	2.46	3	1
1:A:41:CYS:SG	1:A:59:ILE:HD12	0.45	2.51	7	1
1:A:205:GLU:OE2	1:A:208:ARG:HD2	0.45	2.11	18	2
1:A:144:GLY:O	1:A:146:LYS:HD3	0.45	2.11	8	1
1:A:50:LYS:HD2	1:A:51:PHE:N	0.45	2.26	20	1
1:A:64:ILE:HG21	1:A:81:ALA:CB	0.45	2.42	1	1
1:A:55:ALA:HB3	1:A:58:ASP:OD2	0.45	2.11	14	1
1:A:10:SER:HB2	1:A:60:LYS:HB2	0.45	1.88	13	1
1:A:156:LEU:O	1:A:160:GLN:HG3	0.44	2.12	19	1
1:A:157:VAL:HG21	1:A:196:TYR:CE1	0.44	2.48	20	1
1:A:144:GLY:O	1:A:146:LYS:HD2	0.44	2.13	5	1
1:A:40:GLN:NE2	1:A:53:SER:HB2	0.44	2.28	12	1
1:A:127:TYR:O	1:A:131:GLU:HG3	0.44	2.13	13	1
1:A:89:VAL:O	1:A:90:VAL:HG22	0.44	2.12	20	1
1:A:176:TYR:CD1	1:A:192:VAL:HB	0.44	2.48	19	3
1:A:17:ARG:HD2	1:A:17:ARG:N	0.44	2.28	10	1
1:A:96:MET:HB3	1:A:124:GLN:OE1	0.44	2.13	1	1
1:A:188:ALA:O	1:A:192:VAL:HG12	0.44	2.13	2	1
1:A:96:MET:CE	1:A:128:LYS:HE2	0.44	2.42	18	1
1:A:45:SER:HB2	1:A:52:TYR:OH	0.43	2.12	2	2
1:A:183:ILE:O	1:A:188:ALA:HB2	0.43	2.13	4	1
1:A:9:VAL:O	1:A:22:PRO:HA	0.43	2.14	18	1
1:A:128:LYS:HD3	1:A:129:PHE:N	0.43	2.28	20	1
1:A:4:LEU:H	1:A:4:LEU:HD23	0.43	1.73	9	1
1:A:152:LYS:O	1:A:156:LEU:HD13	0.43	2.13	16	2
1:A:75:LYS:N	1:A:75:LYS:HD2	0.43	2.28	12	4
1:A:119:ARG:HB3	1:A:151:PHE:CG	0.43	2.48	16	1
1:A:126:LEU:HB3	1:A:130:MET:HE2	0.43	1.89	2	1
1:A:44:ARG:NH1	1:A:132:ASP:HA	0.43	2.28	12	1
1:A:68:PRO:O	1:A:72:LEU:HG	0.43	2.13	13	1
1:A:94:TRP:CZ2	1:A:125:GLN:HA	0.43	2.48	19	1
1:A:157:VAL:HG21	1:A:196:TYR:CE2	0.43	2.49	11	1
1:A:198:LYS:NZ	1:A:198:LYS:HB2	0.43	2.28	16	1
1:A:175:ILE:O	1:A:179:LEU:HD23	0.43	2.14	17	1
1:A:49:SER:HB2	1:A:52:TYR:CE1	0.43	2.49	6	1
1:A:44:ARG:HD2	1:A:132:ASP:OD1	0.43	2.13	9	1
1:A:44:ARG:HG2	1:A:45:SER:N	0.43	2.29	12	1
1:A:40:GLN:HA	1:A:55:ALA:HA	0.43	1.91	20	1
1:A:8:VAL:HA	1:A:23:ALA:O	0.43	2.13	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:GLN:HA	1:A:125:GLN:OE1	0.43	2.14	16	1
1:A:8:VAL:HG12	1:A:24:LEU:HD23	0.42	1.92	4	1
1:A:130:MET:CE	1:A:137:ILE:HD11	0.42	2.44	8	1
1:A:207:CYS:HA	1:A:212:ILE:HD13	0.42	1.90	2	1
1:A:130:MET:O	1:A:133:ARG:HG2	0.42	2.14	3	1
1:A:91:PRO:HA	1:A:94:TRP:CZ3	0.42	2.49	4	1
1:A:153:LEU:HD21	1:A:175:ILE:HD12	0.42	1.92	13	1
1:A:64:ILE:HB	1:A:85:LEU:CD1	0.42	2.44	19	1
1:A:29:SER:HB2	1:A:205:GLU:OE1	0.42	2.15	8	1
1:A:90:VAL:HG11	1:A:93:ASN:HD22	0.42	1.74	11	1
1:A:119:ARG:O	1:A:123:LEU:HD13	0.42	2.15	8	2
1:A:128:LYS:HE2	1:A:128:LYS:HA	0.42	1.91	14	1
1:A:137:ILE:HG23	1:A:139:LYS:O	0.42	2.13	19	1
1:A:85:LEU:O	1:A:89:VAL:HB	0.42	2.14	3	1
1:A:119:ARG:HA	1:A:151:PHE:CG	0.42	2.50	5	1
1:A:49:SER:HB2	1:A:52:TYR:CE2	0.42	2.50	18	1
1:A:188:ALA:HA	1:A:191:ASN:CG	0.42	2.35	18	1
1:A:129:PHE:HA	1:A:132:ASP:OD2	0.42	2.14	1	1
1:A:47:ILE:HD13	1:A:47:ILE:O	0.42	2.14	4	1
1:A:160:GLN:HB2	1:A:166:ILE:HD11	0.42	1.92	5	1
1:A:120:ASP:O	1:A:124:GLN:HB2	0.42	2.15	5	1
1:A:86:LYS:HD2	1:A:86:LYS:C	0.42	2.35	6	1
1:A:149:ASN:CB	1:A:179:LEU:HD11	0.42	2.44	8	1
1:A:69:GLU:HA	1:A:72:LEU:HG	0.42	1.91	17	1
1:A:52:TYR:HB3	1:A:54:ILE:HG12	0.42	1.92	18	1
1:A:127:TYR:OH	1:A:141:PRO:HD3	0.42	2.14	18	1
1:A:4:LEU:H	1:A:4:LEU:HD12	0.41	1.75	5	1
1:A:93:ASN:HB3	1:A:94:TRP:CE3	0.41	2.50	12	1
1:A:84:PHE:O	1:A:88:ARG:HG3	0.41	2.15	17	1
1:A:190:TYR:O	1:A:193:LYS:HG3	0.41	2.14	17	1
1:A:29:SER:HB2	1:A:205:GLU:OE2	0.41	2.15	13	1
1:A:172:TRP:HA	1:A:175:ILE:HG12	0.41	1.91	2	1
1:A:44:ARG:HD2	1:A:132:ASP:OD2	0.41	2.15	3	1
1:A:37:LYS:HD3	1:A:40:GLN:OE1	0.41	2.15	10	1
1:A:143:LEU:HD11	1:A:191:ASN:HB3	0.41	1.91	9	1
1:A:49:SER:HB2	1:A:52:TYR:CD1	0.41	2.51	1	1
1:A:144:GLY:O	1:A:146:LYS:HG2	0.41	2.16	2	1
1:A:205:GLU:HA	1:A:208:ARG:HG2	0.41	1.93	13	1
1:A:96:MET:SD	1:A:128:LYS:HB2	0.41	2.56	7	2
1:A:88:ARG:HG3	1:A:89:VAL:N	0.41	2.30	13	1
1:A:64:ILE:HG21	1:A:81:ALA:HB3	0.41	1.91	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:LEU:O	1:A:130:MET:HB2	0.41	2.16	7	1
1:A:9:VAL:HB	1:A:60:LYS:O	0.41	2.15	2	1
1:A:130:MET:HG3	1:A:133:ARG:CZ	0.41	2.45	3	1
1:A:27:SER:C	1:A:29:SER:H	0.41	2.19	6	1
1:A:150:LEU:HD12	1:A:151:PHE:N	0.41	2.30	7	1
1:A:79:GLN:O	1:A:83:ILE:HG13	0.41	2.16	17	1
1:A:101:ILE:HG12	1:A:127:TYR:CD1	0.41	2.51	19	1
1:A:166:ILE:HG21	1:A:172:TRP:NE1	0.41	2.30	20	1
1:A:102:LEU:HD12	1:A:123:LEU:HD21	0.41	1.91	8	1
1:A:119:ARG:HB2	1:A:151:PHE:CG	0.41	2.51	9	1
1:A:96:MET:HE1	1:A:127:TYR:HB3	0.41	1.93	13	1
1:A:162:GLY:O	1:A:166:ILE:HG13	0.40	2.16	1	1
1:A:101:ILE:HG12	1:A:127:TYR:CD2	0.40	2.51	6	1
1:A:130:MET:HE3	1:A:199:TYR:HA	0.40	1.93	16	1
1:A:194:THR:O	1:A:198:LYS:HG3	0.40	2.16	3	1
1:A:14:ALA:HA	1:A:58:ASP:OD2	0.40	2.16	8	1
1:A:172:TRP:O	1:A:175:ILE:HG12	0.40	2.17	11	1
1:A:211:ASN:N	1:A:211:ASN:HD22	0.40	2.14	19	1
1:A:63:ASP:HB2	1:A:66:ASN:OD1	0.40	2.15	6	1
1:A:3:GLU:HB3	1:A:61:GLU:HB3	0.40	1.92	12	1
1:A:149:ASN:N	1:A:149:ASN:HD22	0.40	2.14	18	1
1:A:101:ILE:HA	1:A:127:TYR:CZ	0.40	2.51	2	1
1:A:94:TRP:NE1	1:A:124:GLN:HB3	0.40	2.32	14	1
1:A:204:GLU:OE1	1:A:208:ARG:HD3	0.40	2.17	4	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	198/229 (86%)	182±3 (92±2%)	14±3 (7±1%)	2±1 (1±1%)	15	64
All	All	3960/4580 (86%)	3644 (92%)	272 (7%)	44 (1%)	15	64

All 15 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	103	GLU	10
1	A	184	LEU	8
1	A	91	PRO	6
1	A	92	ASP	3
1	A	15	THR	3
1	A	2	ASP	2
1	A	13	SER	2
1	A	88	ARG	2
1	A	97	ASP	2
1	A	141	PRO	1
1	A	101	ILE	1
1	A	212	ILE	1
1	A	14	ALA	1
1	A	183	ILE	1
1	A	90	VAL	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	180/211 (85%)	166±3 (92±2%)	14±3 (8±2%)	13	62
All	All	3600/4220 (85%)	3317 (92%)	283 (8%)	13	62

All 67 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	42	LEU	18
1	A	86	LYS	17
1	A	211	ASN	17
1	A	146	LYS	13
1	A	50	LYS	11
1	A	61	GLU	11
1	A	127	TYR	10
1	A	198	LYS	10
1	A	139	LYS	10
1	A	94	TRP	8
1	A	3	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	47	ILE	6
1	A	138	ASN	6
1	A	75	LYS	6
1	A	62	VAL	5
1	A	7	LYS	5
1	A	177	MET	5
1	A	38	LYS	5
1	A	128	LYS	5
1	A	193	LYS	5
1	A	43	VAL	5
1	A	174	GLN	4
1	A	69	GLU	4
1	A	88	ARG	4
1	A	16	GLU	4
1	A	204	GLU	4
1	A	201	TYR	4
1	A	78	LEU	4
1	A	65	LEU	4
1	A	66	ASN	4
1	A	52	TYR	3
1	A	208	ARG	3
1	A	56	ARG	3
1	A	93	ASN	3
1	A	124	GLN	3
1	A	29	SER	2
1	A	60	LYS	2
1	A	95	LYS	2
1	A	197	ARG	2
1	A	163	CYS	2
1	A	120	ASP	2
1	A	132	ASP	2
1	A	133	ARG	2
1	A	153	LEU	2
1	A	142	VAL	2
1	A	125	GLN	2
1	A	149	ASN	2
1	A	18	THR	2
1	A	57	LYS	2
1	A	17	ARG	2
1	A	10	SER	1
1	A	118	GLU	1
1	A	131	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	156	LEU	1
1	A	119	ARG	1
1	A	103	GLU	1
1	A	203	PHE	1
1	A	178	ASP	1
1	A	80	LYS	1
1	A	160	GLN	1
1	A	31	ASN	1
1	A	100	GLU	1
1	A	40	GLN	1
1	A	63	ASP	1
1	A	84	PHE	1
1	A	19	GLU	1
1	A	206	TYR	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 81% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

Total number of shifts	2611
Number of shifts mapped to atoms	2611
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	216	$-0.62 \pm 0.10$	Should be checked
$^{13}\text{C}_\beta$	206	$0.18 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	210	$-0.17 \pm 0.05$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	201	$0.35 \pm 0.21$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 2394 atoms were assigned a chemical shift out of a possible 2778. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	966/981 (98%)	389/396 (98%)	391/396 (99%)	186/189 (98%)
Sidechain	1345/1574 (85%)	913/1020 (90%)	412/494 (83%)	20/60 (33%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	83/223 (37%)	49/106 (46%)	32/112 (29%)	2/5 (40%)
Overall	2394/2778 (86%)	1351/1522 (89%)	835/1002 (83%)	208/254 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 2611 atoms were assigned a chemical shift out of a possible 3216. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	1052/1134 (93%)	425/457 (93%)	426/458 (93%)	201/219 (92%)
Sidechain	1476/1777 (83%)	1006/1148 (88%)	448/561 (80%)	22/68 (32%)
Aromatic	83/305 (27%)	49/147 (33%)	32/135 (24%)	2/23 (9%)
Overall	2611/3216 (81%)	1480/1752 (84%)	906/1154 (79%)	225/310 (73%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

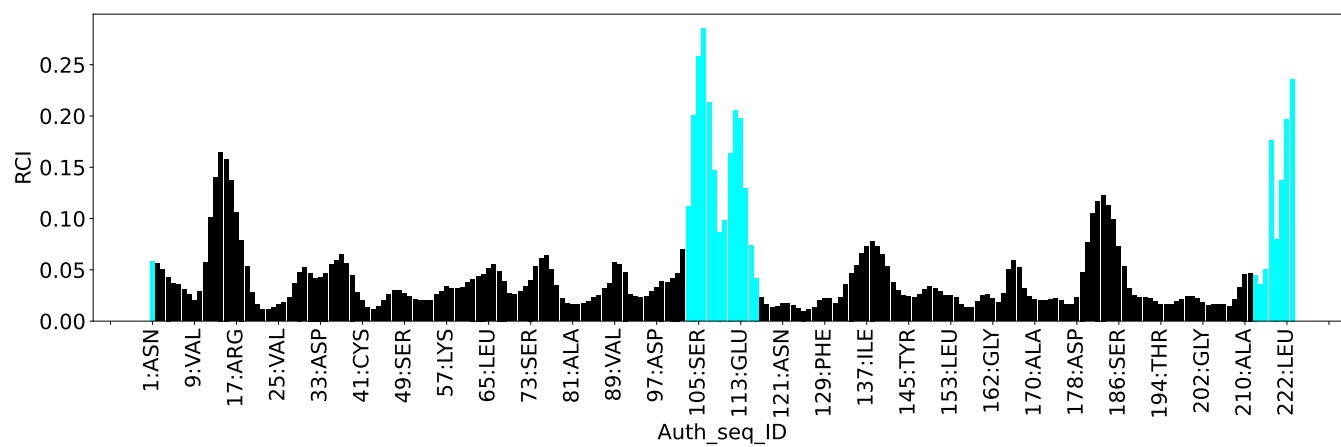
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	203	PHE	CE1	116.70	124.17 – 137.29	-10.7
1	A	193	LYS	HB2	0.24	0.58 – 2.97	-6.4
1	A	172	TRP	HB2	1.32	1.51 – 4.87	-5.5

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

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

Random coil index (RCI) for chain A:





## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	6481
Intra-residue ( $ i-j =0$ )	1847
Sequential ( $ i-j =1$ )	1454
Medium range ( $ i-j >1$ and $ i-j <5$ )	1151
Long range ( $ i-j \geq 5$ )	1961
Inter-chain	0
Hydrogen bond restraints	68
Disulfide bond restraints	0
Total dihedral-angle restraints	323
Number of unmapped restraints	0
Number of restraints per residue	29.7
Number of long range restraints per residue <sup>1</sup>	8.6

<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)	61.0	0.2
0.2-0.5 (Medium)	91.9	0.5
>0.5 (Large)	51.8	1.78

### 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)	7.2	3.68
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

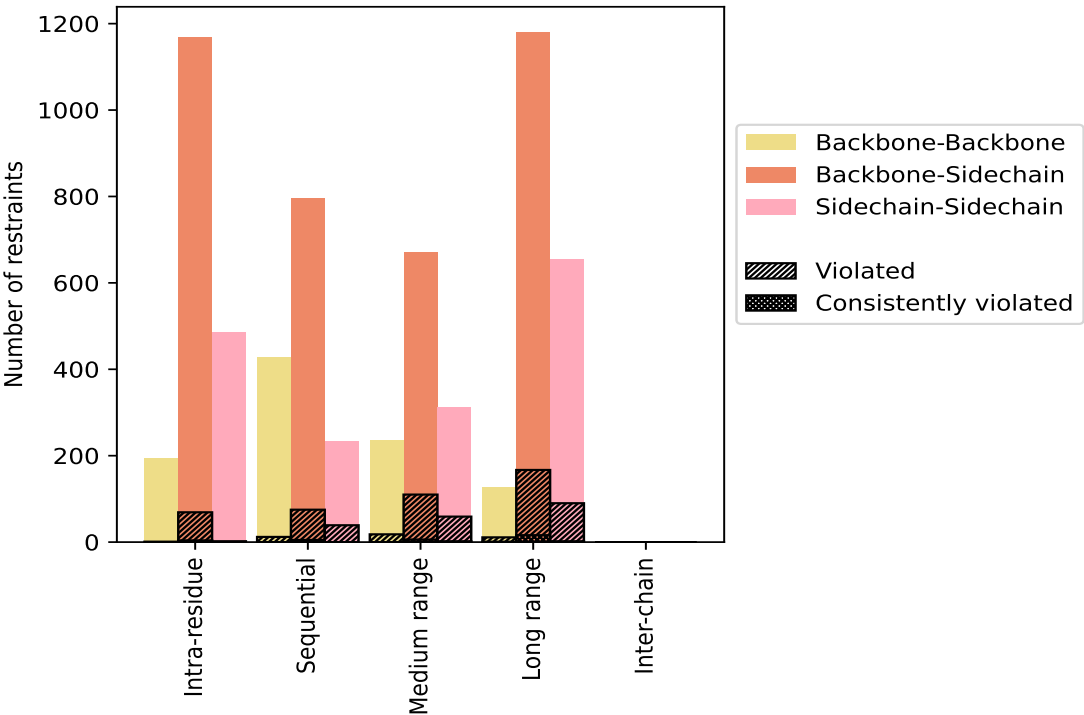
### 9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>1847</b>	<b>28.5</b>	<b>72</b>	<b>3.9</b>	<b>1.1</b>	<b>4</b>	<b>0.2</b>	<b>0.1</b>
Backbone-Backbone	193	3.0	1	0.5	0.0	0	0.0	0.0
Backbone-Sidechain	1169	18.0	69	5.9	1.1	4	0.3	0.1
Sidechain-Sidechain	485	7.5	2	0.4	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>1454</b>	<b>22.4</b>	<b>126</b>	<b>8.7</b>	<b>1.9</b>	<b>5</b>	<b>0.3</b>	<b>0.1</b>
Backbone-Backbone	427	6.6	12	2.8	0.2	0	0.0	0.0
Backbone-Sidechain	795	12.3	75	9.4	1.2	5	0.6	0.1
Sidechain-Sidechain	232	3.6	39	16.8	0.6	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>1151</b>	<b>17.8</b>	<b>184</b>	<b>16.0</b>	<b>2.8</b>	<b>8</b>	<b>0.7</b>	<b>0.1</b>
Backbone-Backbone	236	3.6	18	7.6	0.3	0	0.0	0.0
Backbone-Sidechain	603	9.3	107	17.7	1.7	6	1.0	0.1
Sidechain-Sidechain	312	4.8	59	18.9	0.9	2	0.6	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>1961</b>	<b>30.3</b>	<b>268</b>	<b>13.7</b>	<b>4.1</b>	<b>19</b>	<b>1.0</b>	<b>0.3</b>
Backbone-Backbone	127	2.0	11	8.7	0.2	1	0.8	0.0
Backbone-Sidechain	1180	18.2	167	14.2	2.6	16	1.4	0.2
Sidechain-Sidechain	654	10.1	90	13.8	1.4	2	0.3	0.0
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Hydrogen bond</b>	<b>68</b>	<b>1.0</b>	<b>3</b>	<b>4.4</b>	<b>0.0</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>6481</b>	<b>100.0</b>	<b>653</b>	<b>10.1</b>	<b>10.1</b>	<b>36</b>	<b>0.6</b>	<b>0.6</b>
Backbone-Backbone	983	15.2	42	4.3	0.6	1	0.1	0.0
Backbone-Sidechain	3815	58.9	421	11.0	6.5	31	0.8	0.5
Sidechain-Sidechain	1683	26.0	190	11.3	2.9	4	0.2	0.1

<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	32	53	50	70	0	205	0.39	1.47	0.3	0.28
2	25	53	55	76	0	209	0.39	1.59	0.29	0.29
3	28	63	63	75	0	229	0.37	1.59	0.26	0.3
4	27	56	48	80	0	211	0.36	1.46	0.27	0.26
5	21	47	52	73	0	193	0.38	1.47	0.27	0.29
6	22	54	57	71	0	204	0.38	1.45	0.28	0.29
7	31	53	56	67	0	207	0.36	1.5	0.26	0.28
8	26	49	57	72	0	204	0.38	1.66	0.29	0.27
9	27	57	54	68	0	206	0.36	1.32	0.25	0.29
10	25	55	57	74	0	211	0.36	1.34	0.24	0.28

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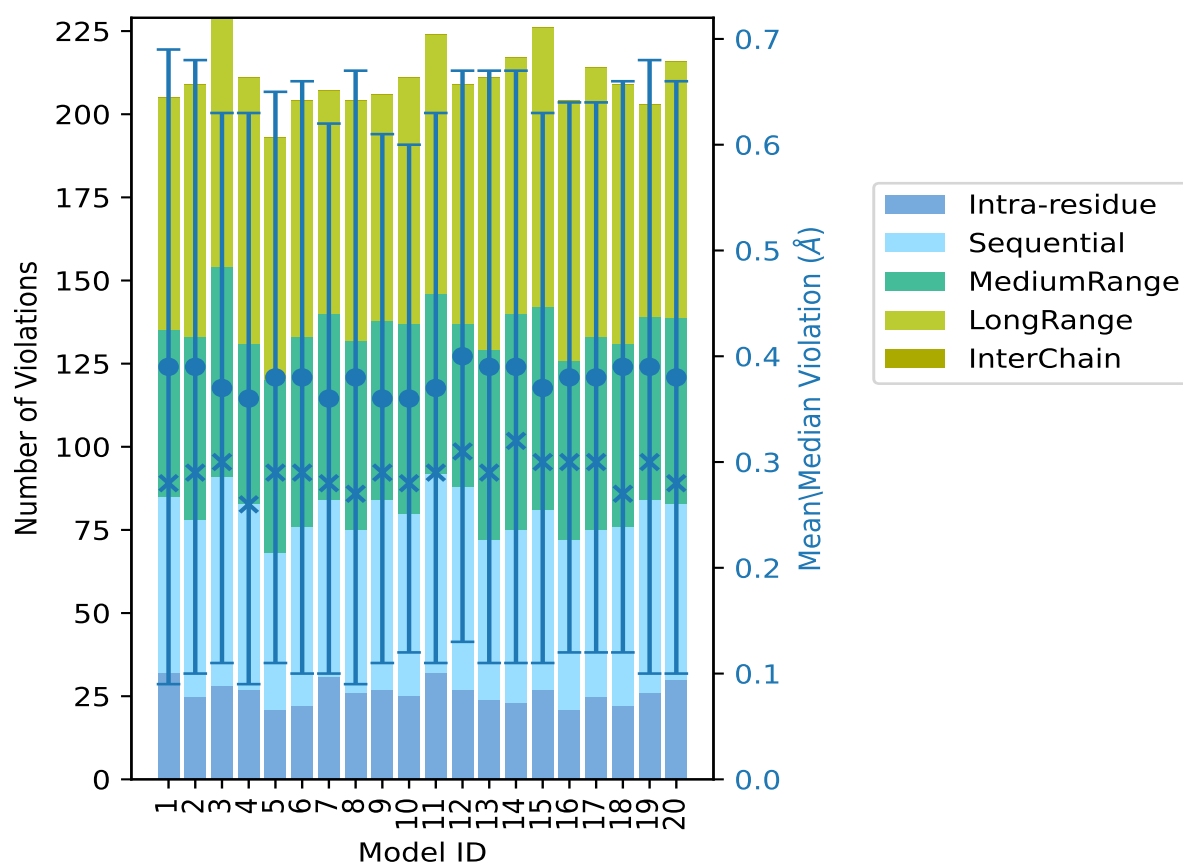
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	32	60	54	78	0	224	0.37	1.47	0.26	0.29
12	27	61	49	72	0	209	0.4	1.42	0.27	0.31
13	24	48	57	82	0	211	0.39	1.37	0.28	0.29
14	23	52	65	77	0	217	0.39	1.57	0.28	0.32
15	27	54	61	84	0	226	0.37	1.56	0.26	0.3
16	21	51	54	78	0	204	0.38	1.39	0.26	0.3
17	25	50	58	81	0	214	0.38	1.42	0.26	0.3
18	22	54	55	78	0	209	0.39	1.38	0.27	0.27
19	26	58	55	64	0	203	0.39	1.78	0.29	0.3
20	30	53	56	77	0	216	0.38	1.64	0.28	0.28

<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 ⓘ



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

### 9.3 Distance violation statistics for the ensemble

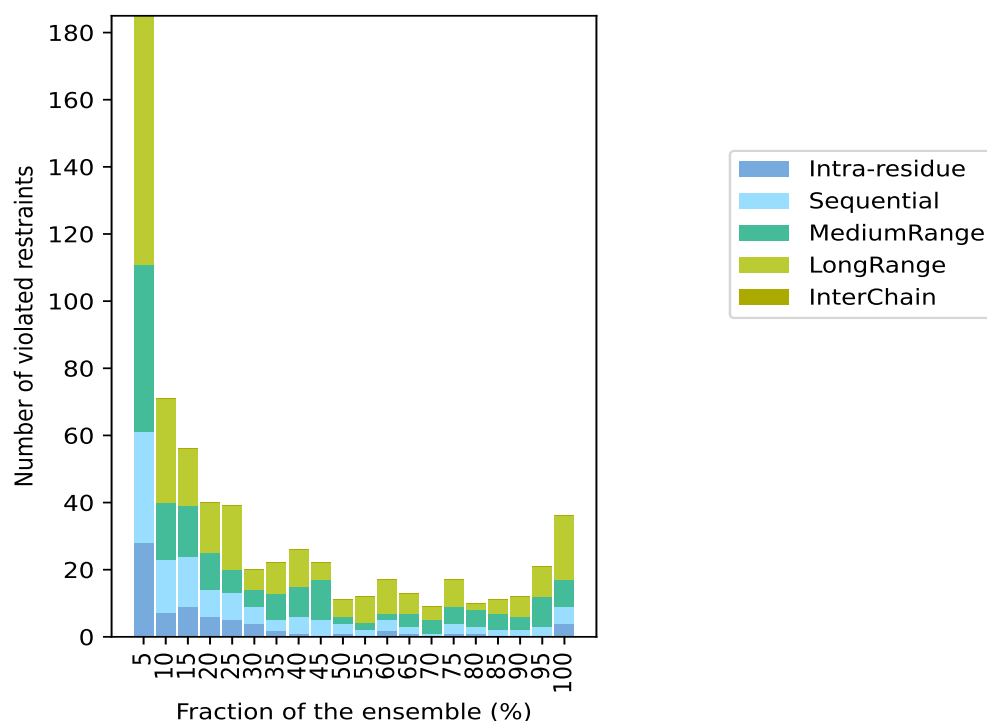
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 5763(IR:1775, SQ:1328, MR:967, LR:1693, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
28	33	50	74	0	185	1	5.0
7	16	17	31	0	71	2	10.0
9	15	15	17	0	56	3	15.0
6	8	11	15	0	40	4	20.0
5	8	7	19	0	39	5	25.0
4	5	5	6	0	20	6	30.0
2	3	8	9	0	22	7	35.0
1	5	9	11	0	26	8	40.0
0	5	12	5	0	22	9	45.0
1	3	2	5	0	11	10	50.0
0	2	2	8	0	12	11	55.0
2	3	2	10	0	17	12	60.0
1	2	4	6	0	13	13	65.0
0	1	4	4	0	9	14	70.0
1	3	5	8	0	17	15	75.0
1	2	5	2	0	10	16	80.0
0	2	5	4	0	11	17	85.0
0	2	4	6	0	12	18	90.0
0	3	9	9	0	21	19	95.0
4	5	8	19	0	36	20	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

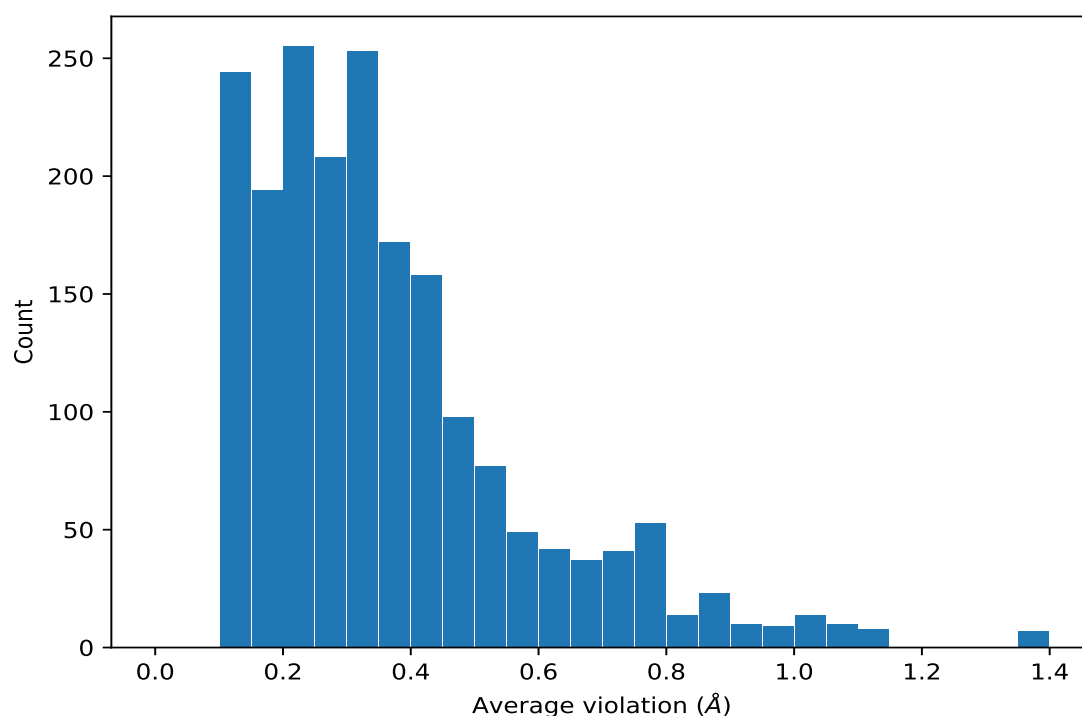
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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)
(1,5734)	1:54:A:ILE:HG21	1:11:A:VAL:H	20	1.35	0.25	1.38
(1,5734)	1:54:A:ILE:HG23	1:60:A:LYS:H	20	1.35	0.25	1.38
(1,5734)	1:54:A:ILE:HG22	1:53:A:SER:H	20	1.35	0.25	1.38
(1,5734)	1:54:A:ILE:HG23	1:53:A:SER:H	20	1.35	0.25	1.38
(1,5734)	1:54:A:ILE:HG22	1:11:A:VAL:H	20	1.35	0.25	1.38
(1,5734)	1:54:A:ILE:HG23	1:11:A:VAL:H	20	1.35	0.25	1.38
(1,5734)	1:54:A:ILE:HG21	1:60:A:LYS:H	20	1.35	0.25	1.38
(1,2538)	1:183:A:ILE:HD12	1:182:A:PRO:HA	20	1.13	0.41	1.34
(1,2538)	1:183:A:ILE:HD11	1:182:A:PRO:HA	20	1.13	0.41	1.34
(1,2538)	1:183:A:ILE:HD13	1:184:A:LEU:HA	20	1.13	0.41	1.34
(1,2538)	1:183:A:ILE:HD11	1:172:A:TRP:HA	20	1.13	0.41	1.34
(1,2538)	1:183:A:ILE:HD11	1:184:A:LEU:HA	20	1.13	0.41	1.34
(1,2538)	1:183:A:ILE:HD13	1:182:A:PRO:HA	20	1.13	0.41	1.34
(1,2538)	1:183:A:ILE:HD12	1:172:A:TRP:HA	20	1.13	0.41	1.34
(1,2538)	1:183:A:ILE:HD12	1:184:A:LEU:HA	20	1.13	0.41	1.34
(1,5787)	1:98:A:ILE:HD13	1:100:A:GLU:H	20	1.08	0.25	1.1

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5787)	1:98:A:ILE:HD12	1:100:A:GLU:H	20	1.08	0.25	1.1
(1,5787)	1:98:A:ILE:HD11	1:100:A:GLU:H	20	1.08	0.25	1.1
(1,5787)	1:98:A:ILE:HD12	1:103:A:GLU:H	20	1.08	0.25	1.1
(1,5787)	1:98:A:ILE:HD11	1:103:A:GLU:H	20	1.08	0.25	1.1
(1,5787)	1:98:A:ILE:HD13	1:103:A:GLU:H	20	1.08	0.25	1.1
(1,167)	1:176:A:TYR:HE1	1:177:A:MET:H	20	1.05	0.15	1.08
(1,167)	1:176:A:TYR:HE2	1:177:A:MET:H	20	1.05	0.15	1.08
(1,167)	1:176:A:TYR:HE1	1:145:A:TYR:H	20	1.05	0.15	1.08
(1,167)	1:176:A:TYR:HE2	1:145:A:TYR:H	20	1.05	0.15	1.08
(1,2543)	1:64:A:ILE:HG12	1:65:A:LEU:HA	20	0.96	0.12	0.97
(1,2543)	1:64:A:ILE:HG13	1:62:A:VAL:HA	20	0.96	0.12	0.97
(1,2543)	1:64:A:ILE:HG12	1:62:A:VAL:HA	20	0.96	0.12	0.97
(1,2843)	1:181:A:ILE:HD12	1:182:A:PRO:HG2	20	0.92	0.29	0.96
(1,2843)	1:181:A:ILE:HD12	1:182:A:PRO:HG3	20	0.92	0.29	0.96
(1,2843)	1:181:A:ILE:HD13	1:182:A:PRO:HG2	20	0.92	0.29	0.96
(1,2843)	1:181:A:ILE:HD13	1:182:A:PRO:HG3	20	0.92	0.29	0.96
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB2	20	0.92	0.29	0.96
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB3	20	0.92	0.29	0.96
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB2	20	0.92	0.29	0.96
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB3	20	0.92	0.29	0.96
(1,2843)	1:181:A:ILE:HD11	1:153:A:LEU:HB2	20	0.92	0.29	0.96
(1,2843)	1:181:A:ILE:HD11	1:153:A:LEU:HB3	20	0.92	0.29	0.96
(1,2482)	1:175:A:ILE:HD13	1:174:A:GLN:H	20	0.88	0.14	0.91
(1,2482)	1:175:A:ILE:HD11	1:172:A:TRP:HZ2	20	0.88	0.14	0.91
(1,2482)	1:175:A:ILE:HD11	1:174:A:GLN:H	20	0.88	0.14	0.91
(1,2482)	1:175:A:ILE:HD12	1:174:A:GLN:H	20	0.88	0.14	0.91
(1,2482)	1:175:A:ILE:HD13	1:172:A:TRP:HZ2	20	0.88	0.14	0.91
(1,5678)	1:137:A:ILE:HD13	1:130:A:MET:H	20	0.86	0.21	0.88
(1,5678)	1:137:A:ILE:HD11	1:130:A:MET:H	20	0.86	0.21	0.88
(1,5678)	1:137:A:ILE:HD12	1:130:A:MET:H	20	0.86	0.21	0.88
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD1	20	0.82	0.09	0.84
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD2	20	0.82	0.09	0.84
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD1	20	0.82	0.09	0.84
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD2	20	0.82	0.09	0.84
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD1	20	0.82	0.09	0.84
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD2	20	0.82	0.09	0.84
(1,5558)	1:9:A:VAL:HG12	1:8:A:VAL:H	20	0.79	0.2	0.8
(1,5558)	1:12:A:VAL:HG12	1:17:A:ARG:H	20	0.79	0.2	0.8
(1,5558)	1:9:A:VAL:HG13	1:8:A:VAL:H	20	0.79	0.2	0.8
(1,5558)	1:9:A:VAL:HG11	1:8:A:VAL:H	20	0.79	0.2	0.8
(1,5558)	1:12:A:VAL:HG11	1:17:A:ARG:H	20	0.79	0.2	0.8
(1,2908)	1:137:A:ILE:HD13	1:130:A:MET:H	20	0.76	0.21	0.78

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2908)	1:137:A:ILE:HD11	1:199:A:TYR:H	20	0.76	0.21	0.78
(1,2908)	1:137:A:ILE:HD11	1:130:A:MET:H	20	0.76	0.21	0.78
(1,2908)	1:137:A:ILE:HD12	1:130:A:MET:H	20	0.76	0.21	0.78
(1,2908)	1:137:A:ILE:HD13	1:199:A:TYR:H	20	0.76	0.21	0.78
(1,2908)	1:137:A:ILE:HD12	1:199:A:TYR:H	20	0.76	0.21	0.78
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	20	0.75	0.16	0.78
(1,5665)	1:50:A:LYS:HB2	1:133:A:ARG:H	20	0.75	0.16	0.78
(1,5665)	1:50:A:LYS:HB3	1:133:A:ARG:H	20	0.75	0.16	0.78
(1,5665)	1:200:A:LEU:HB3	1:205:A:GLU:H	20	0.75	0.16	0.78
(1,2848)	1:11:A:VAL:HG21	1:43:A:VAL:H	20	0.74	0.27	0.78
(1,2848)	1:11:A:VAL:HG22	1:43:A:VAL:H	20	0.74	0.27	0.78
(1,2848)	1:11:A:VAL:HG21	1:44:A:ARG:H	20	0.74	0.27	0.78
(1,2848)	1:11:A:VAL:HG23	1:43:A:VAL:H	20	0.74	0.27	0.78
(1,2848)	1:11:A:VAL:HG23	1:44:A:ARG:H	20	0.74	0.27	0.78
(1,2848)	1:11:A:VAL:HG22	1:44:A:ARG:H	20	0.74	0.27	0.78
(1,3016)	1:157:A:VAL:HG21	1:156:A:LEU:HA	20	0.63	0.08	0.65
(1,3016)	1:157:A:VAL:HG23	1:156:A:LEU:HA	20	0.63	0.08	0.65
(1,3016)	1:157:A:VAL:HG11	1:156:A:LEU:HA	20	0.63	0.08	0.65
(1,3016)	1:157:A:VAL:HG12	1:156:A:LEU:HA	20	0.63	0.08	0.65
(1,3016)	1:157:A:VAL:HG22	1:156:A:LEU:HA	20	0.63	0.08	0.65
(1,2536)	1:181:A:ILE:HD11	1:179:A:LEU:HA	20	0.62	0.17	0.62
(1,2536)	1:181:A:ILE:HD12	1:179:A:LEU:HA	20	0.62	0.17	0.62
(1,2536)	1:181:A:ILE:HD13	1:179:A:LEU:HA	20	0.62	0.17	0.62
(1,2429)	1:181:A:ILE:HD13	1:180:A:GLY:H	20	0.56	0.08	0.58
(1,2429)	1:181:A:ILE:HD11	1:180:A:GLY:H	20	0.56	0.08	0.58
(1,2429)	1:181:A:ILE:HD12	1:180:A:GLY:H	20	0.56	0.08	0.58
(1,2429)	1:181:A:ILE:HD13	1:145:A:TYR:H	20	0.56	0.08	0.58
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG12	20	0.54	0.21	0.55
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG13	20	0.54	0.21	0.55
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	20	0.54	0.21	0.55
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	20	0.54	0.21	0.55
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	20	0.52	0.04	0.52
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	20	0.52	0.04	0.52
(1,173)	1:146:A:LYS:H	1:145:A:TYR:HD1	20	0.52	0.04	0.52
(1,173)	1:146:A:LYS:H	1:145:A:TYR:HD2	20	0.52	0.04	0.52
(1,173)	1:191:A:ASN:HD21	1:190:A:TYR:HD1	20	0.52	0.04	0.52
(1,173)	1:191:A:ASN:HD21	1:190:A:TYR:HD2	20	0.52	0.04	0.52
(1,173)	1:191:A:ASN:HD22	1:190:A:TYR:HD1	20	0.52	0.04	0.52
(1,173)	1:191:A:ASN:HD22	1:190:A:TYR:HD2	20	0.52	0.04	0.52
(1,3014)	1:175:A:ILE:HG21	1:156:A:LEU:HA	20	0.49	0.07	0.5
(1,3014)	1:175:A:ILE:HG23	1:156:A:LEU:HA	20	0.49	0.07	0.5
(1,3014)	1:175:A:ILE:HG22	1:156:A:LEU:HA	20	0.49	0.07	0.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	20	0.46	0.05	0.46
(1,3012)	1:173:A:LYS:HB3	1:174:A:GLN:HA	20	0.46	0.09	0.47
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	20	0.46	0.09	0.47
(1,3012)	1:160:A:GLN:HG3	1:156:A:LEU:HA	20	0.46	0.09	0.47
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	20	0.46	0.13	0.42
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD11	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD12	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD13	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD21	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD22	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD23	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD11	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD12	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD13	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD21	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD22	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD23	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG11	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG12	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG13	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG21	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG22	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG23	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG11	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG12	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG13	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG21	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG22	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG23	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG11	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG12	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG13	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG21	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG22	20	0.42	0.12	0.44
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG23	20	0.42	0.12	0.44
(1,2532)	1:183:A:ILE:HG21	1:182:A:PRO:HA	20	0.4	0.09	0.39
(1,2532)	1:183:A:ILE:HG21	1:184:A:LEU:HA	20	0.4	0.09	0.39
(1,2532)	1:183:A:ILE:HG22	1:182:A:PRO:HA	20	0.4	0.09	0.39
(1,2532)	1:183:A:ILE:HG23	1:182:A:PRO:HA	20	0.4	0.09	0.39
(1,2532)	1:183:A:ILE:HG22	1:184:A:LEU:HA	20	0.4	0.09	0.39
(1,2532)	1:183:A:ILE:HG23	1:184:A:LEU:HA	20	0.4	0.09	0.39
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	20	0.39	0.12	0.4

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD11	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD12	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD13	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD21	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD22	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD23	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD11	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD12	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD13	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD21	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD22	20	0.39	0.12	0.4
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD23	20	0.39	0.12	0.4
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	20	0.35	0.14	0.34
(1,5312)	1:20:A:TRP:HE1	1:11:A:VAL:H	20	0.35	0.14	0.34
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	20	0.33	0.08	0.32
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	20	0.33	0.08	0.32
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	20	0.33	0.08	0.32
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	20	0.31	0.1	0.28
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	20	0.31	0.1	0.28
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	20	0.31	0.1	0.28
(1,5139)	1:80:A:LYS:H	1:47:A:ILE:HD11	20	0.31	0.1	0.28
(1,5139)	1:80:A:LYS:H	1:47:A:ILE:HD12	20	0.31	0.1	0.28
(1,5139)	1:80:A:LYS:H	1:47:A:ILE:HD13	20	0.31	0.1	0.28
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	20	0.3	0.05	0.3
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	20	0.3	0.05	0.3
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	20	0.3	0.05	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	20	0.29	0.04	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	20	0.29	0.04	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	20	0.29	0.04	0.3
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	20	0.29	0.06	0.3
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	20	0.29	0.06	0.3
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	20	0.29	0.06	0.3
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	20	0.28	0.05	0.3
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	20	0.28	0.05	0.3
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	20	0.28	0.05	0.3
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG21	20	0.28	0.05	0.3
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG22	20	0.28	0.05	0.3

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG23	20	0.28	0.05	0.3
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	20	0.24	0.07	0.23
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	20	0.24	0.07	0.23
(1,2551)	1:98:A:ILE:HG21	1:98:A:ILE:HA	20	0.24	0.02	0.25
(1,2551)	1:98:A:ILE:HG22	1:98:A:ILE:HA	20	0.24	0.02	0.25
(1,2551)	1:98:A:ILE:HG23	1:98:A:ILE:HA	20	0.24	0.02	0.25
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	20	0.22	0.04	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	20	0.22	0.04	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	20	0.22	0.04	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG21	20	0.22	0.04	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG22	20	0.22	0.04	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG23	20	0.22	0.04	0.22
(1,2871)	1:175:A:ILE:HG13	1:175:A:ILE:HA	20	0.17	0.02	0.17
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	20	0.17	0.02	0.17
(1,2920)	1:54:A:ILE:HD11	1:52:A:TYR:HA	19	0.97	0.29	1.03
(1,2920)	1:54:A:ILE:HD13	1:52:A:TYR:HA	19	0.97	0.29	1.03
(1,2920)	1:54:A:ILE:HD12	1:52:A:TYR:HA	19	0.97	0.29	1.03
(1,2920)	1:54:A:ILE:HD11	1:58:A:ASP:HA	19	0.97	0.29	1.03
(1,2920)	1:54:A:ILE:HD12	1:58:A:ASP:HA	19	0.97	0.29	1.03
(1,2920)	1:54:A:ILE:HD13	1:58:A:ASP:HA	19	0.97	0.29	1.03
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD21	19	0.86	0.14	0.88
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD22	19	0.86	0.14	0.88
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD21	19	0.86	0.14	0.88
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD22	19	0.86	0.14	0.88
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD21	19	0.86	0.14	0.88
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD22	19	0.86	0.14	0.88
(1,2539)	1:54:A:ILE:HD13	1:14:A:ALA:HA	19	0.81	0.3	0.89
(1,2539)	1:54:A:ILE:HD12	1:14:A:ALA:HA	19	0.81	0.3	0.89
(1,2539)	1:54:A:ILE:HD11	1:14:A:ALA:HA	19	0.81	0.3	0.89
(1,2539)	1:54:A:ILE:HD12	1:11:A:VAL:HA	19	0.81	0.3	0.89
(1,2442)	1:101:A:ILE:HD11	1:100:A:GLU:H	19	0.66	0.17	0.69
(1,2442)	1:101:A:ILE:HD13	1:100:A:GLU:H	19	0.66	0.17	0.69
(1,2442)	1:101:A:ILE:HD12	1:100:A:GLU:H	19	0.66	0.17	0.69
(1,2373)	1:26:A:ILE:HD12	1:44:A:ARG:H	19	0.6	0.19	0.65
(1,2373)	1:26:A:ILE:HD11	1:43:A:VAL:H	19	0.6	0.19	0.65
(1,2373)	1:26:A:ILE:HD13	1:43:A:VAL:H	19	0.6	0.19	0.65
(1,2373)	1:26:A:ILE:HD11	1:44:A:ARG:H	19	0.6	0.19	0.65
(1,2373)	1:26:A:ILE:HD13	1:44:A:ARG:H	19	0.6	0.19	0.65
(1,2373)	1:26:A:ILE:HD12	1:43:A:VAL:H	19	0.6	0.19	0.65
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	19	0.55	0.26	0.5
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	19	0.55	0.26	0.5
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	19	0.55	0.26	0.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3063)	1:56:A:ARG:H	1:59:A:ILE:HG21	19	0.55	0.26	0.5
(1,3063)	1:56:A:ARG:H	1:59:A:ILE:HG22	19	0.55	0.26	0.5
(1,3063)	1:56:A:ARG:H	1:59:A:ILE:HG23	19	0.55	0.26	0.5
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD11	19	0.51	0.16	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD12	19	0.51	0.16	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD13	19	0.51	0.16	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD21	19	0.51	0.16	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD22	19	0.51	0.16	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD23	19	0.51	0.16	0.51
(1,5128)	1:197:A:ARG:H	1:200:A:LEU:HG	19	0.51	0.16	0.51
(1,5128)	1:197:A:ARG:H	1:198:A:LYS:HD2	19	0.51	0.16	0.51
(1,5128)	1:197:A:ARG:H	1:198:A:LYS:HD3	19	0.51	0.16	0.51
(1,2530)	1:36:A:VAL:HG13	1:37:A:LYS:HA	19	0.48	0.19	0.4
(1,2530)	1:36:A:VAL:HG12	1:37:A:LYS:HA	19	0.48	0.19	0.4
(1,2530)	1:36:A:VAL:HG11	1:37:A:LYS:HA	19	0.48	0.19	0.4
(1,2530)	1:36:A:VAL:HG21	1:37:A:LYS:HA	19	0.48	0.19	0.4
(1,2530)	1:36:A:VAL:HG23	1:37:A:LYS:HA	19	0.48	0.19	0.4
(1,2549)	1:36:A:VAL:HG13	1:37:A:LYS:HA	19	0.48	0.19	0.4
(1,2549)	1:36:A:VAL:HG12	1:37:A:LYS:HA	19	0.48	0.19	0.4
(1,2549)	1:36:A:VAL:HG11	1:37:A:LYS:HA	19	0.48	0.19	0.4
(1,2549)	1:36:A:VAL:HG21	1:37:A:LYS:HA	19	0.48	0.19	0.4
(1,2549)	1:36:A:VAL:HG23	1:37:A:LYS:HA	19	0.48	0.19	0.4
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG2	19	0.46	0.11	0.44
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG3	19	0.46	0.11	0.44
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	19	0.46	0.11	0.44
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	19	0.46	0.11	0.44
(1,3053)	1:55:A:ALA:HB3	1:40:A:GLN:HA	19	0.44	0.12	0.47
(1,3053)	1:55:A:ALA:HB1	1:40:A:GLN:HA	19	0.44	0.12	0.47
(1,3053)	1:55:A:ALA:HB2	1:40:A:GLN:HA	19	0.44	0.12	0.47
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	19	0.43	0.17	0.37
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	19	0.43	0.17	0.37
(1,4965)	1:84:A:PHE:H	1:88:A:ARG:HE	19	0.43	0.17	0.37
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD1	19	0.39	0.12	0.35
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD2	19	0.39	0.12	0.35
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD1	19	0.39	0.12	0.35
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD2	19	0.39	0.12	0.35
(1,2481)	1:187:A:ALA:HB1	1:190:A:TYR:HD1	19	0.39	0.12	0.35
(1,2481)	1:187:A:ALA:HB1	1:190:A:TYR:HD2	19	0.39	0.12	0.35
(1,2481)	1:187:A:ALA:HB3	1:191:A:ASN:HD21	19	0.39	0.12	0.35
(1,2481)	1:187:A:ALA:HB3	1:191:A:ASN:HD22	19	0.39	0.12	0.35
(1,2481)	1:187:A:ALA:HB2	1:191:A:ASN:HD21	19	0.39	0.12	0.35
(1,2481)	1:187:A:ALA:HB2	1:191:A:ASN:HD22	19	0.39	0.12	0.35

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	19	0.33	0.11	0.3
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	19	0.33	0.11	0.3
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	19	0.33	0.11	0.3
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	19	0.33	0.11	0.3
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	19	0.33	0.11	0.3
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	19	0.33	0.11	0.3
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD11	19	0.33	0.11	0.3
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD12	19	0.33	0.11	0.3
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD13	19	0.33	0.11	0.3
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD21	19	0.33	0.11	0.3
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD22	19	0.33	0.11	0.3
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD23	19	0.33	0.11	0.3
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	19	0.32	0.07	0.34
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	19	0.32	0.07	0.34
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	19	0.27	0.1	0.26
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	19	0.27	0.1	0.26
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	19	0.27	0.1	0.26
(1,3346)	1:177:A:MET:HE1	1:183:A:ILE:HD11	19	0.27	0.1	0.26
(1,3346)	1:177:A:MET:HE1	1:183:A:ILE:HD12	19	0.27	0.1	0.26
(1,3346)	1:177:A:MET:HE1	1:183:A:ILE:HD13	19	0.27	0.1	0.26
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	19	0.26	0.03	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	19	0.24	0.04	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	19	0.24	0.04	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	19	0.24	0.04	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	19	0.24	0.04	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	19	0.24	0.04	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	19	0.24	0.04	0.23
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	19	0.23	0.11	0.2
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	19	0.23	0.11	0.2
(1,5496)	1:20:A:TRP:HE1	1:62:A:VAL:HB	19	0.23	0.11	0.2
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	19	0.2	0.08	0.18
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	19	0.2	0.08	0.18
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	19	0.19	0.06	0.2
(1,2457)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	18	1.02	0.34	0.96
(1,2457)	1:90:A:VAL:HG21	1:94:A:TRP:HZ3	18	1.02	0.34	0.96
(1,2457)	1:90:A:VAL:HG13	1:94:A:TRP:HZ3	18	1.02	0.34	0.96
(1,2457)	1:90:A:VAL:HG12	1:94:A:TRP:HZ3	18	1.02	0.34	0.96
(1,2457)	1:90:A:VAL:HG22	1:94:A:TRP:HZ3	18	1.02	0.34	0.96
(1,2457)	1:90:A:VAL:HG11	1:94:A:TRP:HZ3	18	1.02	0.34	0.96
(1,2457)	1:90:A:VAL:HG23	1:66:A:ASN:H	18	1.02	0.34	0.96
(1,2459)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	18	1.02	0.34	0.96
(1,2459)	1:90:A:VAL:HG21	1:94:A:TRP:HZ3	18	1.02	0.34	0.96

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2459)	1:90:A:VAL:HG13	1:94:A:TRP:HZ3	18	1.02	0.34	0.96
(1,2459)	1:90:A:VAL:HG12	1:94:A:TRP:HZ3	18	1.02	0.34	0.96
(1,2459)	1:90:A:VAL:HG22	1:94:A:TRP:HZ3	18	1.02	0.34	0.96
(1,2459)	1:90:A:VAL:HG11	1:94:A:TRP:HZ3	18	1.02	0.34	0.96
(1,2459)	1:90:A:VAL:HG23	1:66:A:ASN:H	18	1.02	0.34	0.96
(1,2534)	1:101:A:ILE:HG22	1:105:A:SER:HA	18	0.77	0.24	0.8
(1,2534)	1:101:A:ILE:HG22	1:140:A:PRO:HA	18	0.77	0.24	0.8
(1,2534)	1:101:A:ILE:HG21	1:140:A:PRO:HA	18	0.77	0.24	0.8
(1,2534)	1:101:A:ILE:HG23	1:105:A:SER:HA	18	0.77	0.24	0.8
(1,2534)	1:101:A:ILE:HG23	1:140:A:PRO:HA	18	0.77	0.24	0.8
(1,2534)	1:101:A:ILE:HG21	1:105:A:SER:HA	18	0.77	0.24	0.8
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	18	0.72	0.11	0.75
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	18	0.72	0.11	0.75
(1,2696)	1:181:A:ILE:HB	1:183:A:ILE:HB	18	0.72	0.11	0.75
(1,2375)	1:60:A:LYS:HD3	1:61:A:GLU:H	18	0.57	0.24	0.48
(1,2375)	1:60:A:LYS:HD3	1:11:A:VAL:H	18	0.57	0.24	0.48
(1,2375)	1:60:A:LYS:HD2	1:61:A:GLU:H	18	0.57	0.24	0.48
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	18	0.46	0.12	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	18	0.46	0.12	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	18	0.46	0.12	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	18	0.46	0.12	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	18	0.46	0.12	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	18	0.46	0.12	0.47
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	18	0.46	0.19	0.38
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	18	0.46	0.19	0.38
(1,3144)	1:20:A:TRP:HD1	1:16:A:GLU:HG2	18	0.46	0.19	0.38
(1,3144)	1:20:A:TRP:HD1	1:16:A:GLU:HG3	18	0.46	0.19	0.38
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	18	0.36	0.15	0.3
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	18	0.36	0.15	0.3
(1,4907)	1:20:A:TRP:HE1	1:78:A:LEU:HB2	18	0.36	0.15	0.3
(1,4907)	1:20:A:TRP:HE1	1:78:A:LEU:HB3	18	0.36	0.15	0.3
(1,5578)	1:153:A:LEU:HA	1:157:A:VAL:H	18	0.32	0.08	0.3
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	18	0.32	0.08	0.3
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	18	0.23	0.05	0.24
(1,2988)	1:89:A:VAL:HB	1:86:A:LYS:HA	18	0.23	0.05	0.24
(1,2988)	1:86:A:LYS:HG2	1:86:A:LYS:HA	18	0.23	0.05	0.24
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	18	0.2	0.09	0.16
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	18	0.2	0.09	0.16
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	18	0.14	0.03	0.13
(1,2535)	1:101:A:ILE:HD11	1:97:A:ASP:HA	17	0.61	0.24	0.71
(1,2535)	1:101:A:ILE:HD13	1:97:A:ASP:HA	17	0.61	0.24	0.71
(1,2535)	1:101:A:ILE:HD12	1:97:A:ASP:HA	17	0.61	0.24	0.71

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2535)	1:101:A:ILE:HD12	1:96:A:MET:HA	17	0.61	0.24	0.71
(1,2535)	1:101:A:ILE:HD11	1:96:A:MET:HA	17	0.61	0.24	0.71
(1,5803)	1:18:A:THR:HG21	1:16:A:GLU:HB2	17	0.52	0.14	0.51
(1,5803)	1:18:A:THR:HG21	1:16:A:GLU:HB3	17	0.52	0.14	0.51
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB2	17	0.52	0.14	0.51
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB3	17	0.52	0.14	0.51
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB2	17	0.52	0.14	0.51
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB3	17	0.52	0.14	0.51
(1,5803)	1:152:A:LYS:HD2	1:113:A:GLU:HB2	17	0.52	0.14	0.51
(1,5803)	1:152:A:LYS:HD2	1:113:A:GLU:HB3	17	0.52	0.14	0.51
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	17	0.41	0.14	0.42
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	17	0.41	0.14	0.42
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE2	17	0.41	0.14	0.42
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE3	17	0.41	0.14	0.42
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	17	0.4	0.14	0.4
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	17	0.4	0.14	0.4
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	17	0.4	0.14	0.4
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG2	17	0.39	0.09	0.44
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG3	17	0.39	0.09	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG2	17	0.39	0.09	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG3	17	0.39	0.09	0.44
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	17	0.36	0.17	0.31
(1,2385)	1:34:A:ILE:HB	1:53:A:SER:H	17	0.36	0.17	0.31
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG21	17	0.36	0.23	0.3
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG22	17	0.36	0.23	0.3
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG23	17	0.36	0.23	0.3
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG21	17	0.36	0.23	0.3
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG22	17	0.36	0.23	0.3
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG23	17	0.36	0.23	0.3
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG21	17	0.36	0.23	0.3
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG22	17	0.36	0.23	0.3
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG23	17	0.36	0.23	0.3
(1,2479)	1:194:A:THR:HG23	1:190:A:TYR:HD1	17	0.35	0.1	0.36
(1,2479)	1:194:A:THR:HG23	1:190:A:TYR:HD2	17	0.35	0.1	0.36
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD1	17	0.35	0.1	0.36
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD2	17	0.35	0.1	0.36
(1,2479)	1:194:A:THR:HG22	1:190:A:TYR:HD1	17	0.35	0.1	0.36
(1,2479)	1:194:A:THR:HG22	1:190:A:TYR:HD2	17	0.35	0.1	0.36
(1,2479)	1:194:A:THR:HG23	1:199:A:TYR:HD1	17	0.35	0.1	0.36
(1,2479)	1:194:A:THR:HG23	1:199:A:TYR:HD2	17	0.35	0.1	0.36
(1,2479)	1:194:A:THR:HG21	1:199:A:TYR:HD1	17	0.35	0.1	0.36
(1,2479)	1:194:A:THR:HG21	1:199:A:TYR:HD2	17	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)
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	17	0.35	0.18	0.3
(1,2826)	1:59:A:ILE:HB	1:61:A:GLU:HG2	17	0.35	0.18	0.3
(1,2826)	1:59:A:ILE:HB	1:61:A:GLU:HG3	17	0.35	0.18	0.3
(1,113)	1:176:A:TYR:HD1	1:182:A:PRO:HA	17	0.3	0.11	0.31
(1,113)	1:176:A:TYR:HD2	1:182:A:PRO:HA	17	0.3	0.11	0.31
(1,2975)	1:179:A:LEU:HD12	1:176:A:TYR:HA	17	0.28	0.11	0.23
(1,2975)	1:179:A:LEU:HD21	1:176:A:TYR:HA	17	0.28	0.11	0.23
(1,2975)	1:65:A:LEU:HD22	1:82:A:SER:HA	17	0.28	0.11	0.23
(1,2975)	1:179:A:LEU:HD22	1:176:A:TYR:HA	17	0.28	0.11	0.23
(1,2975)	1:179:A:LEU:HD11	1:176:A:TYR:HA	17	0.28	0.11	0.23
(1,2975)	1:179:A:LEU:HD13	1:176:A:TYR:HA	17	0.28	0.11	0.23
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	16	0.48	0.16	0.48
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	16	0.48	0.16	0.48
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB2	16	0.48	0.16	0.48
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB3	16	0.48	0.16	0.48
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD2	16	0.37	0.11	0.4
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD3	16	0.37	0.11	0.4
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD2	16	0.37	0.11	0.4
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD3	16	0.37	0.11	0.4
(1,5053)	1:78:A:LEU:H	1:75:A:LYS:HD2	16	0.36	0.15	0.34
(1,5053)	1:78:A:LEU:H	1:75:A:LYS:HD3	16	0.36	0.15	0.34
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG2	16	0.36	0.15	0.34
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG3	16	0.36	0.15	0.34
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB2	16	0.36	0.15	0.34
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB3	16	0.36	0.15	0.34
(1,5053)	1:78:A:LEU:H	1:64:A:ILE:HG12	16	0.36	0.15	0.34
(1,5053)	1:78:A:LEU:H	1:64:A:ILE:HG13	16	0.36	0.15	0.34
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	16	0.36	0.09	0.32
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB2	16	0.34	0.22	0.27
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB3	16	0.34	0.22	0.27
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB2	16	0.34	0.22	0.27
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB3	16	0.34	0.22	0.27
(1,2685)	1:67:A:LEU:HD11	1:71:A:GLU:HB2	16	0.34	0.22	0.27
(1,2685)	1:67:A:LEU:HD11	1:71:A:GLU:HB3	16	0.34	0.22	0.27
(1,2685)	1:67:A:LEU:HD21	1:71:A:GLU:HB2	16	0.34	0.22	0.27
(1,2685)	1:67:A:LEU:HD21	1:71:A:GLU:HB3	16	0.34	0.22	0.27
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB2	16	0.3	0.1	0.29
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB3	16	0.3	0.1	0.29
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB2	16	0.3	0.1	0.29
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB3	16	0.3	0.1	0.29
(1,2643)	1:187:A:ALA:HB1	1:190:A:TYR:HB2	16	0.3	0.1	0.29
(1,2643)	1:187:A:ALA:HB1	1:190:A:TYR:HB3	16	0.3	0.1	0.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	16	0.26	0.05	0.26
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	16	0.26	0.05	0.26
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	16	0.26	0.05	0.26
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD11	16	0.26	0.05	0.26
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD12	16	0.26	0.05	0.26
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD13	16	0.26	0.05	0.26
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD21	16	0.26	0.05	0.26
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD22	16	0.26	0.05	0.26
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD23	16	0.26	0.05	0.26
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	16	0.25	0.09	0.25
(1,4970)	1:64:A:ILE:H	1:62:A:VAL:HA	16	0.25	0.09	0.25
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	16	0.23	0.06	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	16	0.23	0.06	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	16	0.23	0.06	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	16	0.23	0.06	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	16	0.23	0.06	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	16	0.23	0.06	0.21
(1,5788)	1:98:A:ILE:HD12	1:121:A:ASN:HA	15	0.64	0.29	0.57
(1,5788)	1:98:A:ILE:HD12	1:105:A:SER:HA	15	0.64	0.29	0.57
(1,5788)	1:98:A:ILE:HD13	1:105:A:SER:HA	15	0.64	0.29	0.57
(1,5788)	1:98:A:ILE:HD11	1:105:A:SER:HA	15	0.64	0.29	0.57
(1,5788)	1:98:A:ILE:HD13	1:97:A:ASP:HA	15	0.64	0.29	0.57
(1,5788)	1:98:A:ILE:HD13	1:121:A:ASN:HA	15	0.64	0.29	0.57
(1,5788)	1:98:A:ILE:HD11	1:97:A:ASP:HA	15	0.64	0.29	0.57
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG11	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG12	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG13	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG21	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG22	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG23	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG11	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG12	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG13	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG21	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG22	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG23	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG21	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG22	15	0.58	0.18	0.62
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG23	15	0.58	0.18	0.62
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	15	0.48	0.25	0.5
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	15	0.48	0.25	0.5
(1,2828)	1:137:A:ILE:HB	1:101:A:ILE:HA	15	0.48	0.25	0.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2571)	1:130:A:MET:HE2	1:136:A:PRO:HA	15	0.48	0.17	0.44
(1,2571)	1:130:A:MET:HE3	1:136:A:PRO:HA	15	0.48	0.17	0.44
(1,2571)	1:130:A:MET:HE1	1:198:A:LYS:HA	15	0.48	0.17	0.44
(1,2571)	1:130:A:MET:HE1	1:136:A:PRO:HA	15	0.48	0.17	0.44
(1,2571)	1:130:A:MET:HE3	1:198:A:LYS:HA	15	0.48	0.17	0.44
(1,2571)	1:130:A:MET:HE2	1:198:A:LYS:HA	15	0.48	0.17	0.44
(1,2578)	1:64:A:ILE:HD13	1:62:A:VAL:HA	15	0.45	0.19	0.4
(1,2578)	1:64:A:ILE:HD12	1:62:A:VAL:HA	15	0.45	0.19	0.4
(1,2578)	1:64:A:ILE:HD11	1:62:A:VAL:HA	15	0.45	0.19	0.4
(1,2577)	1:166:A:ILE:HD11	1:160:A:GLN:HA	15	0.42	0.26	0.33
(1,2577)	1:166:A:ILE:HD12	1:160:A:GLN:HA	15	0.42	0.26	0.33
(1,2577)	1:166:A:ILE:HD13	1:160:A:GLN:HA	15	0.42	0.26	0.33
(1,2577)	1:166:A:ILE:HD12	1:161:A:GLY:HA2	15	0.42	0.26	0.33
(1,2577)	1:166:A:ILE:HD12	1:161:A:GLY:HA3	15	0.42	0.26	0.33
(1,2699)	1:8:A:VAL:HG21	1:85:A:LEU:HG	15	0.4	0.13	0.44
(1,2699)	1:8:A:VAL:HG22	1:85:A:LEU:HG	15	0.4	0.13	0.44
(1,2699)	1:8:A:VAL:HG23	1:85:A:LEU:HG	15	0.4	0.13	0.44
(1,2699)	1:8:A:VAL:HG12	1:85:A:LEU:HB2	15	0.4	0.13	0.44
(1,2699)	1:8:A:VAL:HG12	1:85:A:LEU:HB3	15	0.4	0.13	0.44
(1,2699)	1:8:A:VAL:HG11	1:85:A:LEU:HB2	15	0.4	0.13	0.44
(1,2699)	1:8:A:VAL:HG11	1:85:A:LEU:HB3	15	0.4	0.13	0.44
(1,2699)	1:8:A:VAL:HG13	1:85:A:LEU:HB2	15	0.4	0.13	0.44
(1,2699)	1:8:A:VAL:HG13	1:85:A:LEU:HB3	15	0.4	0.13	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD11	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD12	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD13	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD21	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD22	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD23	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD11	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD12	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD13	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD21	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD22	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD23	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD11	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD12	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD13	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD21	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD22	15	0.39	0.14	0.44
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD23	15	0.39	0.14	0.44
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	15	0.35	0.07	0.37

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	15	0.35	0.07	0.37
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	15	0.35	0.07	0.37
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	15	0.35	0.07	0.37
(1,3177)	1:122:A:PHE:HD1	1:203:A:PHE:HB2	15	0.35	0.07	0.37
(1,3177)	1:122:A:PHE:HD1	1:203:A:PHE:HB3	15	0.35	0.07	0.37
(1,3177)	1:122:A:PHE:HD2	1:203:A:PHE:HB2	15	0.35	0.07	0.37
(1,3177)	1:122:A:PHE:HD2	1:203:A:PHE:HB3	15	0.35	0.07	0.37
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	15	0.34	0.09	0.34
(1,4975)	1:75:A:LYS:H	1:73:A:SER:HA	15	0.34	0.09	0.34
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	15	0.3	0.09	0.29
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	15	0.25	0.08	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	15	0.25	0.08	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	15	0.25	0.08	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	15	0.25	0.08	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	15	0.25	0.08	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	15	0.25	0.08	0.24
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	15	0.24	0.09	0.23
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	15	0.24	0.09	0.23
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	15	0.18	0.09	0.14
(1,5848)	1:113:A:GLU:HB3	1:114:A:LEU:HG	15	0.18	0.09	0.14
(1,5848)	1:113:A:GLU:HB2	1:114:A:LEU:HG	15	0.18	0.09	0.14
(1,2973)	1:166:A:ILE:HB	1:166:A:ILE:HA	15	0.18	0.04	0.18
(1,2973)	1:85:A:LEU:HB2	1:82:A:SER:HA	15	0.18	0.04	0.18
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	15	0.13	0.02	0.13
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	15	0.12	0.03	0.11
(1,2561)	1:65:A:LEU:HG	1:86:A:LYS:HA	15	0.12	0.03	0.11
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB2	14	0.66	0.23	0.6
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB3	14	0.66	0.23	0.6
(1,2708)	1:137:A:ILE:HD11	1:139:A:LYS:HB2	14	0.66	0.23	0.6
(1,2708)	1:137:A:ILE:HD11	1:139:A:LYS:HB3	14	0.66	0.23	0.6
(1,2708)	1:137:A:ILE:HD13	1:140:A:PRO:HB2	14	0.66	0.23	0.6
(1,2708)	1:137:A:ILE:HD13	1:140:A:PRO:HB3	14	0.66	0.23	0.6
(1,2708)	1:137:A:ILE:HD12	1:139:A:LYS:HB2	14	0.66	0.23	0.6
(1,2708)	1:137:A:ILE:HD12	1:139:A:LYS:HB3	14	0.66	0.23	0.6
(1,2708)	1:137:A:ILE:HD11	1:140:A:PRO:HB2	14	0.66	0.23	0.6
(1,2708)	1:137:A:ILE:HD11	1:140:A:PRO:HB3	14	0.66	0.23	0.6
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB2	14	0.48	0.25	0.44
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB3	14	0.48	0.25	0.44
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB2	14	0.48	0.25	0.44
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB3	14	0.48	0.25	0.44
(1,3516)	1:22:A:PRO:HG2	1:46:A:PHE:HB2	14	0.48	0.25	0.44
(1,3516)	1:22:A:PRO:HG2	1:46:A:PHE:HB3	14	0.48	0.25	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3516)	1:22:A:PRO:HG3	1:46:A:PHE:HB2	14	0.48	0.25	0.44
(1,3516)	1:22:A:PRO:HG3	1:46:A:PHE:HB3	14	0.48	0.25	0.44
(1,3516)	1:80:A:LYS:HD2	1:46:A:PHE:HB2	14	0.48	0.25	0.44
(1,3516)	1:80:A:LYS:HD2	1:46:A:PHE:HB3	14	0.48	0.25	0.44
(1,3516)	1:80:A:LYS:HD3	1:46:A:PHE:HB2	14	0.48	0.25	0.44
(1,3516)	1:80:A:LYS:HD3	1:46:A:PHE:HB3	14	0.48	0.25	0.44
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	14	0.39	0.15	0.34
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	14	0.39	0.15	0.34
(1,5386)	1:200:A:LEU:H	1:196:A:TYR:HE1	14	0.39	0.15	0.34
(1,5386)	1:200:A:LEU:H	1:196:A:TYR:HE2	14	0.39	0.15	0.34
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	14	0.36	0.2	0.3
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	14	0.36	0.2	0.3
(1,5322)	1:149:A:ASN:H	1:146:A:LYS:HG2	14	0.36	0.2	0.3
(1,5322)	1:149:A:ASN:H	1:146:A:LYS:HG3	14	0.36	0.2	0.3
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	14	0.34	0.1	0.35
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	14	0.34	0.1	0.35
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	14	0.34	0.1	0.35
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	14	0.34	0.1	0.35
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	14	0.34	0.1	0.35
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	14	0.34	0.1	0.35
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	14	0.34	0.1	0.35
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	14	0.34	0.1	0.35
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	14	0.34	0.1	0.35
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	14	0.34	0.1	0.35
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	14	0.34	0.1	0.35
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	14	0.34	0.1	0.35
(1,3442)	1:59:A:ILE:HG21	1:61:A:GLU:HG2	14	0.34	0.1	0.35
(1,3442)	1:59:A:ILE:HG21	1:61:A:GLU:HG3	14	0.34	0.1	0.35
(1,3442)	1:59:A:ILE:HG22	1:61:A:GLU:HG2	14	0.34	0.1	0.35
(1,3442)	1:59:A:ILE:HG22	1:61:A:GLU:HG3	14	0.34	0.1	0.35
(1,3442)	1:59:A:ILE:HG23	1:61:A:GLU:HG2	14	0.34	0.1	0.35
(1,3442)	1:59:A:ILE:HG23	1:61:A:GLU:HG3	14	0.34	0.1	0.35
(1,2389)	1:42:A:LEU:HG	1:52:A:TYR:H	14	0.3	0.13	0.25
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	14	0.3	0.13	0.25
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD21	14	0.2	0.05	0.2
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD22	14	0.2	0.05	0.2
(1,5690)	1:65:A:LEU:HA	1:66:A:ASN:HD21	14	0.2	0.05	0.2
(1,5690)	1:65:A:LEU:HA	1:66:A:ASN:HD22	14	0.2	0.05	0.2
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE2	14	0.18	0.08	0.16
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE3	14	0.18	0.08	0.16
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE2	14	0.18	0.08	0.16
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE3	14	0.18	0.08	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE2	14	0.18	0.08	0.16
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE3	14	0.18	0.08	0.16
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE2	14	0.18	0.08	0.16
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE3	14	0.18	0.08	0.16
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE2	14	0.18	0.08	0.16
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE3	14	0.18	0.08	0.16
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	14	0.15	0.05	0.13
(1,2692)	1:195:A:ALA:HB2	1:153:A:LEU:HG	13	0.89	0.3	1.04
(1,2692)	1:195:A:ALA:HB1	1:153:A:LEU:HG	13	0.89	0.3	1.04
(1,2692)	1:195:A:ALA:HB3	1:153:A:LEU:HG	13	0.89	0.3	1.04
(1,2692)	1:195:A:ALA:HB1	1:150:A:LEU:HB2	13	0.89	0.3	1.04
(1,2692)	1:195:A:ALA:HB1	1:150:A:LEU:HB3	13	0.89	0.3	1.04
(1,2692)	1:195:A:ALA:HB3	1:150:A:LEU:HB2	13	0.89	0.3	1.04
(1,2692)	1:195:A:ALA:HB3	1:150:A:LEU:HB3	13	0.89	0.3	1.04
(1,2692)	1:195:A:ALA:HB2	1:150:A:LEU:HB2	13	0.89	0.3	1.04
(1,2692)	1:195:A:ALA:HB2	1:150:A:LEU:HB3	13	0.89	0.3	1.04
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB2	13	0.65	0.24	0.72
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB3	13	0.65	0.24	0.72
(1,2649)	1:64:A:ILE:HD11	1:63:A:ASP:HB2	13	0.65	0.24	0.72
(1,2649)	1:64:A:ILE:HD11	1:63:A:ASP:HB3	13	0.65	0.24	0.72
(1,2649)	1:64:A:ILE:HD12	1:63:A:ASP:HB2	13	0.65	0.24	0.72
(1,2649)	1:64:A:ILE:HD12	1:63:A:ASP:HB3	13	0.65	0.24	0.72
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	13	0.37	0.05	0.37
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	13	0.37	0.05	0.37
(1,5366)	1:79:A:GLN:HE22	1:82:A:SER:HB2	13	0.37	0.05	0.37
(1,5366)	1:79:A:GLN:HE22	1:82:A:SER:HB3	13	0.37	0.05	0.37
(1,2841)	1:166:A:ILE:HD11	1:157:A:VAL:H	13	0.33	0.22	0.26
(1,2841)	1:166:A:ILE:HD12	1:157:A:VAL:H	13	0.33	0.22	0.26
(1,2841)	1:166:A:ILE:HD11	1:159:A:HIS:H	13	0.33	0.22	0.26
(1,2841)	1:166:A:ILE:HD13	1:157:A:VAL:H	13	0.33	0.22	0.26
(1,2841)	1:166:A:ILE:HD11	1:175:A:ILE:H	13	0.33	0.22	0.26
(1,2474)	1:101:A:ILE:HD13	1:127:A:TYR:HD1	13	0.32	0.15	0.32
(1,2474)	1:101:A:ILE:HD13	1:127:A:TYR:HD2	13	0.32	0.15	0.32
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD1	13	0.32	0.15	0.32
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD2	13	0.32	0.15	0.32
(1,2474)	1:101:A:ILE:HD13	1:101:A:ILE:H	13	0.32	0.15	0.32
(1,2474)	1:101:A:ILE:HD11	1:127:A:TYR:HD1	13	0.32	0.15	0.32
(1,2474)	1:101:A:ILE:HD11	1:127:A:TYR:HD2	13	0.32	0.15	0.32
(1,3051)	1:34:A:ILE:HG22	1:53:A:SER:HA	13	0.28	0.09	0.27
(1,3051)	1:43:A:VAL:HG23	1:53:A:SER:HA	13	0.28	0.09	0.27
(1,3051)	1:34:A:ILE:HG23	1:53:A:SER:HA	13	0.28	0.09	0.27
(1,3051)	1:34:A:ILE:HG21	1:53:A:SER:HA	13	0.28	0.09	0.27

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	13	0.27	0.08	0.26
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	13	0.27	0.08	0.26
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	13	0.22	0.08	0.23
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	13	0.22	0.08	0.23
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	13	0.21	0.04	0.21
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	13	0.21	0.04	0.21
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	13	0.21	0.04	0.21
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	13	0.21	0.04	0.21
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	13	0.21	0.04	0.21
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	13	0.21	0.04	0.21
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	13	0.21	0.04	0.21
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	13	0.21	0.04	0.21
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	13	0.21	0.04	0.21
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	13	0.21	0.04	0.21
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	13	0.21	0.04	0.21
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	13	0.21	0.04	0.21
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG2	13	0.17	0.08	0.13
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG3	13	0.17	0.08	0.13
(1,5292)	1:18:A:THR:H	1:19:A:GLU:HG2	13	0.17	0.08	0.13
(1,5292)	1:18:A:THR:H	1:19:A:GLU:HG3	13	0.17	0.08	0.13
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	13	0.15	0.04	0.14
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	13	0.15	0.04	0.14
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	13	0.12	0.01	0.13
(1,5812)	1:64:A:ILE:HD12	1:8:A:VAL:HB	12	0.76	0.19	0.8
(1,5812)	1:9:A:VAL:HG13	1:8:A:VAL:HB	12	0.76	0.19	0.8
(1,5812)	1:9:A:VAL:HG21	1:8:A:VAL:HB	12	0.76	0.19	0.8
(1,5812)	1:64:A:ILE:HD13	1:8:A:VAL:HB	12	0.76	0.19	0.8
(1,5812)	1:64:A:ILE:HD11	1:8:A:VAL:HB	12	0.76	0.19	0.8
(1,5812)	1:9:A:VAL:HG11	1:8:A:VAL:HB	12	0.76	0.19	0.8
(1,5812)	1:9:A:VAL:HG12	1:8:A:VAL:HB	12	0.76	0.19	0.8
(1,5812)	1:9:A:VAL:HG22	1:8:A:VAL:HB	12	0.76	0.19	0.8
(1,3435)	1:12:A:VAL:HG12	1:60:A:LYS:HE2	12	0.71	0.14	0.66
(1,3435)	1:12:A:VAL:HG12	1:60:A:LYS:HE3	12	0.71	0.14	0.66
(1,3435)	1:12:A:VAL:HG23	1:60:A:LYS:HE2	12	0.71	0.14	0.66
(1,3435)	1:12:A:VAL:HG23	1:60:A:LYS:HE3	12	0.71	0.14	0.66
(1,3435)	1:12:A:VAL:HG21	1:60:A:LYS:HE2	12	0.71	0.14	0.66
(1,3435)	1:12:A:VAL:HG21	1:60:A:LYS:HE3	12	0.71	0.14	0.66
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	12	0.71	0.14	0.66
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	12	0.71	0.14	0.66
(1,3435)	1:12:A:VAL:HG13	1:60:A:LYS:HE2	12	0.71	0.14	0.66
(1,3435)	1:12:A:VAL:HG13	1:60:A:LYS:HE3	12	0.71	0.14	0.66
(1,3436)	1:12:A:VAL:HG12	1:60:A:LYS:HE2	12	0.71	0.14	0.66

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3436)	1:12:A:VAL:HG12	1:60:A:LYS:HE3	12	0.71	0.14	0.66
(1,3436)	1:12:A:VAL:HG23	1:60:A:LYS:HE2	12	0.71	0.14	0.66
(1,3436)	1:12:A:VAL:HG23	1:60:A:LYS:HE3	12	0.71	0.14	0.66
(1,3436)	1:12:A:VAL:HG21	1:60:A:LYS:HE2	12	0.71	0.14	0.66
(1,3436)	1:12:A:VAL:HG21	1:60:A:LYS:HE3	12	0.71	0.14	0.66
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	12	0.71	0.14	0.66
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	12	0.71	0.14	0.66
(1,3436)	1:12:A:VAL:HG13	1:60:A:LYS:HE2	12	0.71	0.14	0.66
(1,3436)	1:12:A:VAL:HG13	1:60:A:LYS:HE3	12	0.71	0.14	0.66
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD21	12	0.35	0.14	0.4
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD22	12	0.35	0.14	0.4
(1,168)	1:190:A:TYR:HE1	1:191:A:ASN:HD21	12	0.35	0.14	0.4
(1,168)	1:190:A:TYR:HE1	1:191:A:ASN:HD22	12	0.35	0.14	0.4
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB2	12	0.34	0.2	0.38
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB3	12	0.34	0.2	0.38
(1,2636)	1:65:A:LEU:HD11	1:66:A:ASN:HB2	12	0.34	0.2	0.38
(1,2636)	1:65:A:LEU:HD11	1:66:A:ASN:HB3	12	0.34	0.2	0.38
(1,2636)	1:65:A:LEU:HD21	1:63:A:ASP:HB2	12	0.34	0.2	0.38
(1,2636)	1:65:A:LEU:HD21	1:63:A:ASP:HB3	12	0.34	0.2	0.38
(1,2636)	1:65:A:LEU:HD11	1:63:A:ASP:HB2	12	0.34	0.2	0.38
(1,2636)	1:65:A:LEU:HD11	1:63:A:ASP:HB3	12	0.34	0.2	0.38
(1,2636)	1:65:A:LEU:HD22	1:63:A:ASP:HB2	12	0.34	0.2	0.38
(1,2636)	1:65:A:LEU:HD22	1:63:A:ASP:HB3	12	0.34	0.2	0.38
(1,2636)	1:65:A:LEU:HD13	1:63:A:ASP:HB2	12	0.34	0.2	0.38
(1,2636)	1:65:A:LEU:HD13	1:63:A:ASP:HB3	12	0.34	0.2	0.38
(1,5642)	1:143:A:LEU:HG	1:191:A:ASN:HD21	12	0.33	0.12	0.39
(1,5642)	1:143:A:LEU:HG	1:191:A:ASN:HD22	12	0.33	0.12	0.39
(1,5642)	1:187:A:ALA:HB2	1:191:A:ASN:HD21	12	0.33	0.12	0.39
(1,5642)	1:187:A:ALA:HB2	1:191:A:ASN:HD22	12	0.33	0.12	0.39
(1,5642)	1:187:A:ALA:HB1	1:191:A:ASN:HD21	12	0.33	0.12	0.39
(1,5642)	1:187:A:ALA:HB1	1:191:A:ASN:HD22	12	0.33	0.12	0.39
(1,5642)	1:187:A:ALA:HB3	1:191:A:ASN:HD21	12	0.33	0.12	0.39
(1,5642)	1:187:A:ALA:HB3	1:191:A:ASN:HD22	12	0.33	0.12	0.39
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD2	12	0.28	0.16	0.21
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD3	12	0.28	0.16	0.21
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD2	12	0.28	0.16	0.21
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD3	12	0.28	0.16	0.21
(1,2917)	1:196:A:TYR:HA	1:201:A:TYR:H	12	0.26	0.08	0.26
(1,2917)	1:196:A:TYR:HA	1:195:A:ALA:H	12	0.26	0.08	0.26
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	12	0.22	0.1	0.2
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	12	0.22	0.1	0.2
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB2	12	0.21	0.06	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB3	12	0.21	0.06	0.2
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB1	12	0.21	0.06	0.2
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB2	12	0.21	0.06	0.2
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB3	12	0.21	0.06	0.2
(1,3381)	1:72:A:LEU:HB2	1:79:A:GLN:HG2	12	0.2	0.08	0.18
(1,3381)	1:72:A:LEU:HB2	1:79:A:GLN:HG3	12	0.2	0.08	0.18
(1,3381)	1:72:A:LEU:HB3	1:79:A:GLN:HG2	12	0.2	0.08	0.18
(1,3381)	1:72:A:LEU:HB3	1:79:A:GLN:HG3	12	0.2	0.08	0.18
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG2	12	0.2	0.08	0.18
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG3	12	0.2	0.08	0.18
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG2	12	0.2	0.08	0.18
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG3	12	0.2	0.08	0.18
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	12	0.2	0.05	0.19
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	12	0.19	0.08	0.15
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	12	0.19	0.08	0.15
(1,3274)	1:22:A:PRO:HD2	1:47:A:ILE:HG12	12	0.19	0.08	0.15
(1,3274)	1:22:A:PRO:HD2	1:47:A:ILE:HG13	12	0.19	0.08	0.15
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	12	0.15	0.02	0.16
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	12	0.15	0.02	0.16
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	12	0.14	0.02	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	12	0.13	0.02	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	12	0.13	0.02	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	12	0.13	0.02	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	12	0.13	0.02	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	12	0.13	0.02	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	12	0.13	0.02	0.12
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	12	0.12	0.02	0.12
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	12	0.12	0.02	0.12
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	12	0.12	0.02	0.12
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	11	0.46	0.14	0.42
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB2	11	0.38	0.14	0.33
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB3	11	0.38	0.14	0.33
(1,2260)	1:101:A:ILE:HA	1:100:A:GLU:HG2	11	0.38	0.14	0.33
(1,2260)	1:101:A:ILE:HA	1:100:A:GLU:HG3	11	0.38	0.14	0.33
(1,2575)	1:64:A:ILE:HG23	1:78:A:LEU:HA	11	0.34	0.13	0.31
(1,2575)	1:64:A:ILE:HG21	1:78:A:LEU:HA	11	0.34	0.13	0.31
(1,2575)	1:64:A:ILE:HG22	1:78:A:LEU:HA	11	0.34	0.13	0.31
(1,2575)	1:64:A:ILE:HG21	1:82:A:SER:HA	11	0.34	0.13	0.31
(1,2400)	1:34:A:ILE:HD13	1:52:A:TYR:H	11	0.32	0.2	0.21
(1,2400)	1:34:A:ILE:HD11	1:52:A:TYR:H	11	0.32	0.2	0.21
(1,2400)	1:34:A:ILE:HD13	1:32:A:ASP:H	11	0.32	0.2	0.21
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB1	11	0.29	0.14	0.31

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB2	11	0.29	0.14	0.31
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB3	11	0.29	0.14	0.31
(1,5356)	1:48:A:ASP:H	1:44:A:ARG:HG2	11	0.29	0.14	0.31
(1,5356)	1:48:A:ASP:H	1:44:A:ARG:HG3	11	0.29	0.14	0.31
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	11	0.24	0.07	0.22
(1,5522)	1:9:A:VAL:HG22	1:23:A:ALA:H	11	0.23	0.08	0.24
(1,5522)	1:9:A:VAL:HG23	1:23:A:ALA:H	11	0.23	0.08	0.24
(1,5522)	1:9:A:VAL:HG21	1:23:A:ALA:H	11	0.23	0.08	0.24
(1,5522)	1:64:A:ILE:HD12	1:23:A:ALA:H	11	0.23	0.08	0.24
(1,5522)	1:64:A:ILE:HD11	1:23:A:ALA:H	11	0.23	0.08	0.24
(1,120)	1:199:A:TYR:HE1	1:137:A:ILE:HG12	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE1	1:137:A:ILE:HG13	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD11	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD12	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD13	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD21	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD22	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD23	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD11	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD12	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD13	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD21	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD22	11	0.2	0.06	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD23	11	0.2	0.06	0.21
(1,2443)	1:83:A:ILE:HD13	1:83:A:ILE:H	11	0.19	0.07	0.15
(1,2443)	1:83:A:ILE:HD11	1:83:A:ILE:H	11	0.19	0.07	0.15
(1,2443)	1:83:A:ILE:HD12	1:83:A:ILE:H	11	0.19	0.07	0.15
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	11	0.14	0.03	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	11	0.12	0.02	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	11	0.12	0.02	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	11	0.12	0.02	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	11	0.12	0.02	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	11	0.12	0.02	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	11	0.12	0.02	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	11	0.12	0.02	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	11	0.12	0.02	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	11	0.12	0.02	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	11	0.12	0.02	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	11	0.12	0.02	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	11	0.12	0.02	0.12
(1,2903)	1:11:A:VAL:HG13	1:54:A:ILE:HB	10	0.52	0.21	0.55
(1,2903)	1:11:A:VAL:HG23	1:54:A:ILE:HB	10	0.52	0.21	0.55

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2903)	1:11:A:VAL:HG11	1:54:A:ILE:HB	10	0.52	0.21	0.55
(1,2903)	1:11:A:VAL:HG12	1:54:A:ILE:HB	10	0.52	0.21	0.55
(1,2903)	1:11:A:VAL:HG22	1:54:A:ILE:HB	10	0.52	0.21	0.55
(1,5020)	1:85:A:LEU:H	1:88:A:ARG:HE	10	0.46	0.19	0.45
(1,5020)	1:85:A:LEU:H	1:46:A:PHE:HD1	10	0.46	0.19	0.45
(1,5020)	1:85:A:LEU:H	1:46:A:PHE:HD2	10	0.46	0.19	0.45
(1,2866)	1:210:A:ALA:HA	1:5:A:LEU:HB2	10	0.42	0.17	0.45
(1,2866)	1:210:A:ALA:HA	1:5:A:LEU:HB3	10	0.42	0.17	0.45
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG12	10	0.42	0.17	0.45
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG13	10	0.42	0.17	0.45
(1,3544)	1:97:A:ASP:HB3	1:99:A:SER:HA	10	0.42	0.2	0.38
(1,3544)	1:198:A:LYS:HE2	1:137:A:ILE:HA	10	0.42	0.2	0.38
(1,2403)	1:3:A:GLU:HB2	1:4:A:LEU:H	10	0.37	0.13	0.34
(1,2403)	1:3:A:GLU:HB3	1:4:A:LEU:H	10	0.37	0.13	0.34
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD2	10	0.3	0.1	0.29
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD3	10	0.3	0.1	0.29
(1,5466)	1:47:A:ILE:H	1:77:A:GLY:HA2	10	0.3	0.1	0.29
(1,5466)	1:47:A:ILE:H	1:77:A:GLY:HA3	10	0.3	0.1	0.29
(1,5602)	1:34:A:ILE:HG22	1:53:A:SER:H	10	0.29	0.11	0.29
(1,5602)	1:34:A:ILE:HG23	1:53:A:SER:H	10	0.29	0.11	0.29
(1,5602)	1:34:A:ILE:HG21	1:53:A:SER:H	10	0.29	0.11	0.29
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD11	10	0.29	0.12	0.26
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD12	10	0.29	0.12	0.26
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD13	10	0.29	0.12	0.26
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD21	10	0.29	0.12	0.26
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD22	10	0.29	0.12	0.26
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD23	10	0.29	0.12	0.26
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD11	10	0.29	0.12	0.26
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD12	10	0.29	0.12	0.26
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD13	10	0.29	0.12	0.26
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD21	10	0.29	0.12	0.26
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD22	10	0.29	0.12	0.26
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD23	10	0.29	0.12	0.26
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB2	10	0.24	0.1	0.19
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB3	10	0.24	0.1	0.19
(1,3477)	1:83:A:ILE:H	1:65:A:LEU:HB2	10	0.24	0.1	0.19
(1,3477)	1:83:A:ILE:H	1:65:A:LEU:HB3	10	0.24	0.1	0.19
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE1	10	0.19	0.04	0.18
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE2	10	0.19	0.04	0.18
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG21	10	0.16	0.04	0.16
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG22	10	0.16	0.04	0.16
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG23	10	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2606)	1:64:A:ILE:HD11	1:78:A:LEU:HA	9	0.83	0.38	0.94
(1,2606)	1:64:A:ILE:HD12	1:78:A:LEU:HA	9	0.83	0.38	0.94
(1,2606)	1:64:A:ILE:HD13	1:78:A:LEU:HA	9	0.83	0.38	0.94
(1,2606)	1:64:A:ILE:HD13	1:82:A:SER:HA	9	0.83	0.38	0.94
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG11	9	0.79	0.29	0.9
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG12	9	0.79	0.29	0.9
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG13	9	0.79	0.29	0.9
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG21	9	0.79	0.29	0.9
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG22	9	0.79	0.29	0.9
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG23	9	0.79	0.29	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD11	9	0.79	0.29	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD12	9	0.79	0.29	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD13	9	0.79	0.29	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD21	9	0.79	0.29	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD22	9	0.79	0.29	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD23	9	0.79	0.29	0.9
(1,2657)	1:12:A:VAL:HG23	1:60:A:LYS:HE2	9	0.69	0.09	0.67
(1,2657)	1:12:A:VAL:HG23	1:60:A:LYS:HE3	9	0.69	0.09	0.67
(1,2657)	1:12:A:VAL:HG21	1:60:A:LYS:HE2	9	0.69	0.09	0.67
(1,2657)	1:12:A:VAL:HG21	1:60:A:LYS:HE3	9	0.69	0.09	0.67
(1,2657)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	9	0.69	0.09	0.67
(1,2657)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	9	0.69	0.09	0.67
(1,2657)	1:12:A:VAL:HG23	1:58:A:ASP:HB2	9	0.69	0.09	0.67
(1,2657)	1:12:A:VAL:HG23	1:58:A:ASP:HB3	9	0.69	0.09	0.67
(1,2657)	1:12:A:VAL:HG12	1:58:A:ASP:HB2	9	0.69	0.09	0.67
(1,2657)	1:12:A:VAL:HG12	1:58:A:ASP:HB3	9	0.69	0.09	0.67
(1,3339)	1:7:A:LYS:HB3	1:5:A:LEU:HG	9	0.67	0.33	0.57
(1,3339)	1:123:A:LEU:HB3	1:150:A:LEU:HG	9	0.67	0.33	0.57
(1,5557)	1:128:A:LYS:HG2	1:95:A:LYS:H	9	0.63	0.18	0.69
(1,5557)	1:124:A:GLN:HB3	1:95:A:LYS:H	9	0.63	0.18	0.69
(1,5557)	1:197:A:ARG:HG2	1:201:A:TYR:H	9	0.63	0.18	0.69
(1,5557)	1:128:A:LYS:HG3	1:95:A:LYS:H	9	0.63	0.18	0.69
(1,5697)	1:139:A:LYS:HD3	1:138:A:ASN:HD21	9	0.46	0.17	0.4
(1,5697)	1:139:A:LYS:HD3	1:138:A:ASN:HD22	9	0.46	0.17	0.4
(1,5697)	1:124:A:GLN:HB2	1:121:A:ASN:HD21	9	0.46	0.17	0.4
(1,5697)	1:124:A:GLN:HB2	1:121:A:ASN:HD22	9	0.46	0.17	0.4
(1,5697)	1:124:A:GLN:HB3	1:121:A:ASN:HD21	9	0.46	0.17	0.4
(1,5697)	1:124:A:GLN:HB3	1:121:A:ASN:HD22	9	0.46	0.17	0.4
(1,5697)	1:139:A:LYS:HD2	1:138:A:ASN:HD21	9	0.46	0.17	0.4
(1,5697)	1:139:A:LYS:HD2	1:138:A:ASN:HD22	9	0.46	0.17	0.4
(1,2531)	1:142:A:VAL:HG13	1:147:A:ASP:HA	9	0.42	0.09	0.38
(1,2531)	1:142:A:VAL:HG11	1:147:A:ASP:HA	9	0.42	0.09	0.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2531)	1:142:A:VAL:HG22	1:143:A:LEU:HA	9	0.42	0.09	0.38
(1,2531)	1:142:A:VAL:HG23	1:143:A:LEU:HA	9	0.42	0.09	0.38
(1,2531)	1:142:A:VAL:HG21	1:143:A:LEU:HA	9	0.42	0.09	0.38
(1,2422)	1:126:A:LEU:HD23	1:130:A:MET:H	9	0.41	0.2	0.38
(1,2422)	1:126:A:LEU:HD21	1:130:A:MET:H	9	0.41	0.2	0.38
(1,2422)	1:126:A:LEU:HD11	1:130:A:MET:H	9	0.41	0.2	0.38
(1,2422)	1:126:A:LEU:HD12	1:130:A:MET:H	9	0.41	0.2	0.38
(1,2422)	1:126:A:LEU:HD21	1:125:A:GLN:H	9	0.41	0.2	0.38
(1,2422)	1:126:A:LEU:HD22	1:130:A:MET:H	9	0.41	0.2	0.38
(1,2422)	1:126:A:LEU:HD13	1:125:A:GLN:H	9	0.41	0.2	0.38
(1,2835)	1:126:A:LEU:HD23	1:130:A:MET:H	9	0.41	0.2	0.38
(1,2835)	1:126:A:LEU:HD21	1:130:A:MET:H	9	0.41	0.2	0.38
(1,2835)	1:126:A:LEU:HD11	1:130:A:MET:H	9	0.41	0.2	0.38
(1,2835)	1:126:A:LEU:HD12	1:130:A:MET:H	9	0.41	0.2	0.38
(1,2835)	1:126:A:LEU:HD21	1:125:A:GLN:H	9	0.41	0.2	0.38
(1,2835)	1:126:A:LEU:HD22	1:130:A:MET:H	9	0.41	0.2	0.38
(1,2835)	1:126:A:LEU:HD13	1:125:A:GLN:H	9	0.41	0.2	0.38
(1,2489)	1:87:A:THR:HG22	1:84:A:PHE:HD1	9	0.39	0.19	0.31
(1,2489)	1:87:A:THR:HG22	1:84:A:PHE:HD2	9	0.39	0.19	0.31
(1,2489)	1:87:A:THR:HG23	1:84:A:PHE:HD1	9	0.39	0.19	0.31
(1,2489)	1:87:A:THR:HG23	1:84:A:PHE:HD2	9	0.39	0.19	0.31
(1,2489)	1:87:A:THR:HG21	1:84:A:PHE:HD1	9	0.39	0.19	0.31
(1,2489)	1:87:A:THR:HG21	1:84:A:PHE:HD2	9	0.39	0.19	0.31
(1,2489)	1:87:A:THR:HG22	1:89:A:VAL:H	9	0.39	0.19	0.31
(1,2489)	1:87:A:THR:HG23	1:89:A:VAL:H	9	0.39	0.19	0.31
(1,5681)	1:94:A:TRP:HZ3	1:94:A:TRP:H	9	0.37	0.13	0.43
(1,5681)	1:44:A:ARG:HE	1:50:A:LYS:H	9	0.37	0.13	0.43
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE1	9	0.32	0.1	0.31
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE2	9	0.32	0.1	0.31
(1,183)	1:50:A:LYS:H	1:52:A:TYR:HE1	9	0.32	0.1	0.31
(1,183)	1:50:A:LYS:H	1:52:A:TYR:HE2	9	0.32	0.1	0.31
(1,2717)	1:130:A:MET:HE2	1:137:A:ILE:HB	9	0.31	0.13	0.28
(1,2717)	1:130:A:MET:HE3	1:133:A:ARG:HG2	9	0.31	0.13	0.28
(1,2717)	1:130:A:MET:HE3	1:133:A:ARG:HG3	9	0.31	0.13	0.28
(1,2717)	1:130:A:MET:HE1	1:198:A:LYS:HB2	9	0.31	0.13	0.28
(1,2717)	1:130:A:MET:HE1	1:198:A:LYS:HB3	9	0.31	0.13	0.28
(1,2717)	1:130:A:MET:HE3	1:198:A:LYS:HB2	9	0.31	0.13	0.28
(1,2717)	1:130:A:MET:HE3	1:198:A:LYS:HB3	9	0.31	0.13	0.28
(1,2717)	1:130:A:MET:HE1	1:133:A:ARG:HG2	9	0.31	0.13	0.28
(1,2717)	1:130:A:MET:HE1	1:133:A:ARG:HG3	9	0.31	0.13	0.28
(1,2717)	1:130:A:MET:HE2	1:133:A:ARG:HG2	9	0.31	0.13	0.28
(1,2717)	1:130:A:MET:HE2	1:133:A:ARG:HG3	9	0.31	0.13	0.28

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG21	9	0.26	0.06	0.29
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG22	9	0.26	0.06	0.29
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG23	9	0.26	0.06	0.29
(1,3161)	1:133:A:ARG:HE	1:135:A:THR:HG21	9	0.26	0.06	0.29
(1,3161)	1:133:A:ARG:HE	1:135:A:THR:HG22	9	0.26	0.06	0.29
(1,3161)	1:133:A:ARG:HE	1:135:A:THR:HG23	9	0.26	0.06	0.29
(1,5428)	1:23:A:ALA:H	1:20:A:TRP:HZ3	9	0.21	0.1	0.18
(1,5428)	1:23:A:ALA:H	1:46:A:PHE:HD1	9	0.21	0.1	0.18
(1,5428)	1:23:A:ALA:H	1:46:A:PHE:HD2	9	0.21	0.1	0.18
(1,2562)	1:72:A:LEU:HG	1:69:A:GLU:HA	9	0.19	0.05	0.2
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD11	9	0.18	0.05	0.19
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD12	9	0.18	0.05	0.19
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD13	9	0.18	0.05	0.19
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG11	9	0.18	0.05	0.18
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG12	9	0.18	0.05	0.18
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG13	9	0.18	0.05	0.18
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG21	9	0.18	0.05	0.18
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG22	9	0.18	0.05	0.18
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG23	9	0.18	0.05	0.18
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD21	9	0.17	0.09	0.13
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD22	9	0.17	0.09	0.13
(1,5118)	1:7:A:LYS:H	1:5:A:LEU:HG	9	0.16	0.03	0.16
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD11	9	0.14	0.04	0.13
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD12	9	0.14	0.04	0.13
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD13	9	0.14	0.04	0.13
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB1	9	0.13	0.01	0.12
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB2	9	0.13	0.01	0.12
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB3	9	0.13	0.01	0.12
(1,5220)	1:185:A:ASN:H	1:183:A:ILE:HG21	9	0.13	0.01	0.12
(1,5220)	1:185:A:ASN:H	1:183:A:ILE:HG22	9	0.13	0.01	0.12
(1,5220)	1:185:A:ASN:H	1:183:A:ILE:HG23	9	0.13	0.01	0.12
(1,3379)	1:75:A:LYS:HG2	1:19:A:GLU:HG2	8	0.73	0.38	0.83
(1,3379)	1:75:A:LYS:HG2	1:19:A:GLU:HG3	8	0.73	0.38	0.83
(1,3379)	1:75:A:LYS:HG3	1:19:A:GLU:HG2	8	0.73	0.38	0.83
(1,3379)	1:75:A:LYS:HG3	1:19:A:GLU:HG3	8	0.73	0.38	0.83
(1,3379)	1:7:A:LYS:HG3	1:61:A:GLU:HG2	8	0.73	0.38	0.83
(1,3379)	1:7:A:LYS:HG3	1:61:A:GLU:HG3	8	0.73	0.38	0.83
(1,2905)	1:126:A:LEU:HD12	1:199:A:TYR:HD1	8	0.64	0.21	0.7
(1,2905)	1:126:A:LEU:HD12	1:199:A:TYR:HD2	8	0.64	0.21	0.7
(1,2905)	1:126:A:LEU:HD13	1:199:A:TYR:HD1	8	0.64	0.21	0.7
(1,2905)	1:126:A:LEU:HD13	1:199:A:TYR:HD2	8	0.64	0.21	0.7
(1,2905)	1:126:A:LEU:HD11	1:199:A:TYR:HD1	8	0.64	0.21	0.7

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2905)	1:126:A:LEU:HD11	1:199:A:TYR:HD2	8	0.64	0.21	0.7
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG21	8	0.48	0.2	0.42
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG22	8	0.48	0.2	0.42
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG23	8	0.48	0.2	0.42
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG21	8	0.48	0.2	0.42
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG22	8	0.48	0.2	0.42
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG23	8	0.48	0.2	0.42
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB2	8	0.42	0.17	0.43
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB3	8	0.42	0.17	0.43
(1,5416)	1:10:A:SER:H	1:22:A:PRO:HB2	8	0.42	0.17	0.43
(1,5416)	1:10:A:SER:H	1:22:A:PRO:HB3	8	0.42	0.17	0.43
(1,2872)	1:100:A:GLU:HB3	1:101:A:ILE:HD11	8	0.41	0.17	0.42
(1,2872)	1:100:A:GLU:HB3	1:101:A:ILE:HD12	8	0.41	0.17	0.42
(1,2872)	1:100:A:GLU:HB3	1:101:A:ILE:HD13	8	0.41	0.17	0.42
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD11	8	0.41	0.17	0.42
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD12	8	0.41	0.17	0.42
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD13	8	0.41	0.17	0.42
(1,2745)	1:137:A:ILE:HD13	1:126:A:LEU:HB2	8	0.39	0.09	0.4
(1,2745)	1:137:A:ILE:HD13	1:126:A:LEU:HB3	8	0.39	0.09	0.4
(1,2745)	1:137:A:ILE:HD11	1:126:A:LEU:HB2	8	0.39	0.09	0.4
(1,2745)	1:137:A:ILE:HD11	1:126:A:LEU:HB3	8	0.39	0.09	0.4
(1,2745)	1:137:A:ILE:HD12	1:126:A:LEU:HB2	8	0.39	0.09	0.4
(1,2745)	1:137:A:ILE:HD12	1:126:A:LEU:HB3	8	0.39	0.09	0.4
(1,2418)	1:200:A:LEU:HD23	1:199:A:TYR:H	8	0.38	0.19	0.37
(1,2418)	1:200:A:LEU:HD13	1:199:A:TYR:H	8	0.38	0.19	0.37
(1,2418)	1:200:A:LEU:HD21	1:150:A:LEU:H	8	0.38	0.19	0.37
(1,2418)	1:200:A:LEU:HD21	1:199:A:TYR:H	8	0.38	0.19	0.37
(1,2418)	1:200:A:LEU:HD12	1:153:A:LEU:H	8	0.38	0.19	0.37
(1,2418)	1:200:A:LEU:HD22	1:153:A:LEU:H	8	0.38	0.19	0.37
(1,2418)	1:200:A:LEU:HD22	1:199:A:TYR:H	8	0.38	0.19	0.37
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG21	8	0.36	0.11	0.36
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG22	8	0.36	0.11	0.36
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG23	8	0.36	0.11	0.36
(1,2255)	1:105:A:SER:HB2	1:101:A:ILE:HG21	8	0.36	0.11	0.36
(1,2255)	1:105:A:SER:HB2	1:101:A:ILE:HG22	8	0.36	0.11	0.36
(1,2255)	1:105:A:SER:HB2	1:101:A:ILE:HG23	8	0.36	0.11	0.36
(1,5679)	1:139:A:LYS:HB2	1:138:A:ASN:HD21	8	0.34	0.12	0.33
(1,5679)	1:139:A:LYS:HB2	1:138:A:ASN:HD22	8	0.34	0.12	0.33
(1,5679)	1:139:A:LYS:HB3	1:138:A:ASN:HD21	8	0.34	0.12	0.33
(1,5679)	1:139:A:LYS:HB3	1:138:A:ASN:HD22	8	0.34	0.12	0.33
(1,5679)	1:139:A:LYS:HD2	1:138:A:ASN:HD21	8	0.34	0.12	0.33
(1,5679)	1:139:A:LYS:HD2	1:138:A:ASN:HD22	8	0.34	0.12	0.33

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5679)	1:139:A:LYS:HD3	1:138:A:ASN:HD21	8	0.34	0.12	0.33
(1,5679)	1:139:A:LYS:HD3	1:138:A:ASN:HD22	8	0.34	0.12	0.33
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG2	8	0.34	0.11	0.38
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG3	8	0.34	0.11	0.38
(1,2415)	1:19:A:GLU:H	1:19:A:GLU:HG2	8	0.34	0.11	0.38
(1,2415)	1:19:A:GLU:H	1:19:A:GLU:HG3	8	0.34	0.11	0.38
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG2	8	0.34	0.11	0.38
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG3	8	0.34	0.11	0.38
(1,4985)	1:19:A:GLU:H	1:19:A:GLU:HG2	8	0.34	0.11	0.38
(1,4985)	1:19:A:GLU:H	1:19:A:GLU:HG3	8	0.34	0.11	0.38
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD11	8	0.31	0.09	0.34
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD12	8	0.31	0.09	0.34
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD13	8	0.31	0.09	0.34
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD21	8	0.31	0.09	0.34
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD22	8	0.31	0.09	0.34
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD23	8	0.31	0.09	0.34
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD11	8	0.31	0.09	0.34
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD12	8	0.31	0.09	0.34
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD13	8	0.31	0.09	0.34
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD21	8	0.31	0.09	0.34
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD22	8	0.31	0.09	0.34
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD23	8	0.31	0.09	0.34
(1,2682)	1:62:A:VAL:HB	1:9:A:VAL:HB	8	0.28	0.1	0.27
(1,3270)	1:144:A:GLY:HA3	1:146:A:LYS:HD2	8	0.26	0.08	0.28
(1,3270)	1:144:A:GLY:HA3	1:146:A:LYS:HD3	8	0.26	0.08	0.28
(1,3270)	1:80:A:LYS:HA	1:83:A:ILE:HG12	8	0.26	0.08	0.28
(1,3270)	1:80:A:LYS:HA	1:83:A:ILE:HG13	8	0.26	0.08	0.28
(1,3270)	1:182:A:PRO:HD2	1:146:A:LYS:HD2	8	0.26	0.08	0.28
(1,3270)	1:182:A:PRO:HD2	1:146:A:LYS:HD3	8	0.26	0.08	0.28
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG2	8	0.26	0.09	0.22
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG3	8	0.26	0.09	0.22
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB2	8	0.25	0.12	0.2
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB3	8	0.25	0.12	0.2
(1,5396)	1:124:A:GLN:H	1:98:A:ILE:HG12	8	0.25	0.12	0.2
(1,5396)	1:124:A:GLN:H	1:98:A:ILE:HG13	8	0.25	0.12	0.2
(1,5554)	1:128:A:LYS:HB2	1:129:A:PHE:H	8	0.25	0.11	0.2
(1,5554)	1:128:A:LYS:HB3	1:129:A:PHE:H	8	0.25	0.11	0.2
(1,2411)	1:88:A:ARG:HD2	1:88:A:ARG:H	8	0.25	0.07	0.25
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB2	8	0.25	0.11	0.2
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB3	8	0.25	0.11	0.2
(1,5534)	1:78:A:LEU:HB3	1:81:A:ALA:H	8	0.23	0.08	0.2
(1,5534)	1:78:A:LEU:HB2	1:81:A:ALA:H	8	0.23	0.08	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5534)	1:47:A:ILE:HB	1:81:A:ALA:H	8	0.23	0.08	0.2
(1,5430)	1:24:A:LEU:H	1:52:A:TYR:HE1	8	0.23	0.13	0.18
(1,5430)	1:24:A:LEU:H	1:52:A:TYR:HE2	8	0.23	0.13	0.18
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE1	8	0.23	0.13	0.18
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE2	8	0.23	0.13	0.18
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG2	8	0.22	0.06	0.22
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG3	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG11	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG12	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG13	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG21	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG22	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG23	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD11	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD12	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD13	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD21	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD22	8	0.22	0.06	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD23	8	0.22	0.06	0.22
(1,2639)	1:11:A:VAL:HG11	1:20:A:TRP:HB2	8	0.15	0.03	0.15
(1,2639)	1:11:A:VAL:HG11	1:20:A:TRP:HB3	8	0.15	0.03	0.15
(1,2639)	1:11:A:VAL:HG22	1:10:A:SER:HB2	8	0.15	0.03	0.15
(1,2639)	1:11:A:VAL:HG22	1:10:A:SER:HB3	8	0.15	0.03	0.15
(1,2639)	1:11:A:VAL:HG12	1:20:A:TRP:HB2	8	0.15	0.03	0.15
(1,2639)	1:11:A:VAL:HG12	1:20:A:TRP:HB3	8	0.15	0.03	0.15
(1,2639)	1:11:A:VAL:HG21	1:10:A:SER:HB2	8	0.15	0.03	0.15
(1,2639)	1:11:A:VAL:HG21	1:10:A:SER:HB3	8	0.15	0.03	0.15
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB2	8	0.13	0.02	0.14
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB3	8	0.13	0.02	0.14
(1,3869)	1:153:A:LEU:HG	1:179:A:LEU:H	8	0.13	0.02	0.12
(1,2461)	1:64:A:ILE:HD12	1:66:A:ASN:H	7	0.73	0.14	0.68
(1,2461)	1:64:A:ILE:HD11	1:66:A:ASN:H	7	0.73	0.14	0.68
(1,2461)	1:64:A:ILE:HD13	1:66:A:ASN:H	7	0.73	0.14	0.68
(1,3399)	1:64:A:ILE:HG12	1:62:A:VAL:HB	7	0.66	0.22	0.76
(1,3399)	1:198:A:LYS:HD2	1:139:A:LYS:HB2	7	0.66	0.22	0.76
(1,3399)	1:198:A:LYS:HD2	1:139:A:LYS:HB3	7	0.66	0.22	0.76
(1,3399)	1:198:A:LYS:HD3	1:139:A:LYS:HB2	7	0.66	0.22	0.76
(1,3399)	1:198:A:LYS:HD3	1:139:A:LYS:HB3	7	0.66	0.22	0.76
(1,3399)	1:64:A:ILE:HG13	1:62:A:VAL:HB	7	0.66	0.22	0.76
(1,5625)	1:146:A:LYS:HG2	1:145:A:TYR:H	7	0.57	0.15	0.58
(1,5625)	1:143:A:LEU:HG	1:145:A:TYR:H	7	0.57	0.15	0.58
(1,5625)	1:64:A:ILE:HG12	1:82:A:SER:H	7	0.57	0.15	0.58

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG2	7	0.55	0.17	0.62
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG3	7	0.55	0.17	0.62
(1,5054)	1:78:A:LEU:H	1:47:A:ILE:HG12	7	0.55	0.17	0.62
(1,5054)	1:78:A:LEU:H	1:47:A:ILE:HG13	7	0.55	0.17	0.62
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB2	7	0.51	0.22	0.6
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB3	7	0.51	0.22	0.6
(1,160)	1:145:A:TYR:HE1	1:146:A:LYS:HD2	7	0.51	0.22	0.6
(1,160)	1:145:A:TYR:HE1	1:146:A:LYS:HD3	7	0.51	0.22	0.6
(1,160)	1:145:A:TYR:HE2	1:184:A:LEU:HB2	7	0.51	0.22	0.6
(1,160)	1:145:A:TYR:HE2	1:184:A:LEU:HB3	7	0.51	0.22	0.6
(1,2596)	1:90:A:VAL:HG21	1:85:A:LEU:HA	7	0.5	0.28	0.48
(1,2596)	1:90:A:VAL:HG23	1:85:A:LEU:HA	7	0.5	0.28	0.48
(1,2596)	1:90:A:VAL:HG22	1:85:A:LEU:HA	7	0.5	0.28	0.48
(1,2596)	1:90:A:VAL:HG13	1:85:A:LEU:HA	7	0.5	0.28	0.48
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG2	7	0.42	0.16	0.36
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG3	7	0.42	0.16	0.36
(1,5237)	1:145:A:TYR:H	1:143:A:LEU:HG	7	0.42	0.16	0.36
(1,2529)	1:5:A:LEU:HD12	1:2:A:ASP:HA	7	0.4	0.28	0.37
(1,2529)	1:5:A:LEU:HD11	1:2:A:ASP:HA	7	0.4	0.28	0.37
(1,2529)	1:5:A:LEU:HD13	1:2:A:ASP:HA	7	0.4	0.28	0.37
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD2	7	0.4	0.13	0.39
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD3	7	0.4	0.13	0.39
(1,3091)	1:129:A:PHE:H	1:88:A:ARG:HD2	7	0.4	0.13	0.39
(1,3091)	1:129:A:PHE:H	1:88:A:ARG:HD3	7	0.4	0.13	0.39
(1,5233)	1:1:A:ASN:HD22	1:61:A:GLU:HG2	7	0.34	0.17	0.44
(1,5233)	1:1:A:ASN:HD22	1:61:A:GLU:HG3	7	0.34	0.17	0.44
(1,5233)	1:1:A:ASN:HD21	1:61:A:GLU:HG2	7	0.34	0.17	0.44
(1,5233)	1:1:A:ASN:HD21	1:61:A:GLU:HG3	7	0.34	0.17	0.44
(1,5233)	1:1:A:ASN:HD22	1:9:A:VAL:HB	7	0.34	0.17	0.44
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG2	7	0.34	0.13	0.28
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG3	7	0.34	0.13	0.28
(1,128)	1:51:A:PHE:HD1	1:133:A:ARG:HB2	7	0.34	0.13	0.28
(1,128)	1:51:A:PHE:HD1	1:133:A:ARG:HB3	7	0.34	0.13	0.28
(1,128)	1:51:A:PHE:HD2	1:133:A:ARG:HB2	7	0.34	0.13	0.28
(1,128)	1:51:A:PHE:HD2	1:133:A:ARG:HB3	7	0.34	0.13	0.28
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB2	7	0.33	0.15	0.43
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB3	7	0.33	0.15	0.43
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD2	7	0.33	0.1	0.32
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD3	7	0.33	0.1	0.32
(1,3259)	1:80:A:LYS:HA	1:80:A:LYS:HE2	7	0.33	0.1	0.32
(1,3259)	1:80:A:LYS:HA	1:80:A:LYS:HE3	7	0.33	0.1	0.32
(1,5786)	1:115:A:ASP:HA	1:117:A:GLU:H	7	0.32	0.17	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD11	7	0.32	0.08	0.28
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD12	7	0.32	0.08	0.28
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD13	7	0.32	0.08	0.28
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG11	7	0.32	0.08	0.28
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG12	7	0.32	0.08	0.28
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG13	7	0.32	0.08	0.28
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG21	7	0.32	0.08	0.28
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG22	7	0.32	0.08	0.28
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG23	7	0.32	0.08	0.28
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE2	7	0.29	0.14	0.27
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE3	7	0.29	0.14	0.27
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG2	7	0.26	0.08	0.23
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG3	7	0.26	0.08	0.23
(1,3096)	1:19:A:GLU:H	1:16:A:GLU:HG2	7	0.26	0.08	0.23
(1,3096)	1:19:A:GLU:H	1:16:A:GLU:HG3	7	0.26	0.08	0.23
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE2	7	0.25	0.12	0.21
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE3	7	0.25	0.12	0.21
(1,2552)	1:101:A:ILE:HG22	1:102:A:LEU:HA	7	0.19	0.04	0.18
(1,2552)	1:101:A:ILE:HG23	1:102:A:LEU:HA	7	0.19	0.04	0.18
(1,2552)	1:101:A:ILE:HG21	1:102:A:LEU:HA	7	0.19	0.04	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD11	7	0.19	0.05	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD12	7	0.19	0.05	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD13	7	0.19	0.05	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD21	7	0.19	0.05	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD22	7	0.19	0.05	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD23	7	0.19	0.05	0.18
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG11	7	0.19	0.05	0.18
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG12	7	0.19	0.05	0.18
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG13	7	0.19	0.05	0.18
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG21	7	0.19	0.05	0.18
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG22	7	0.19	0.05	0.18
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG23	7	0.19	0.05	0.18
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB2	7	0.18	0.05	0.2
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB3	7	0.18	0.05	0.2
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB2	7	0.15	0.07	0.11
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB3	7	0.15	0.07	0.11
(1,5451)	1:126:A:LEU:H	1:128:A:LYS:HB2	7	0.15	0.07	0.11
(1,5451)	1:126:A:LEU:H	1:128:A:LYS:HB3	7	0.15	0.07	0.11
(1,2660)	1:65:A:LEU:HD13	1:63:A:ASP:HB2	6	0.59	0.25	0.44
(1,2660)	1:65:A:LEU:HD13	1:63:A:ASP:HB3	6	0.59	0.25	0.44
(1,2660)	1:65:A:LEU:HD11	1:63:A:ASP:HB2	6	0.59	0.25	0.44
(1,2660)	1:65:A:LEU:HD11	1:63:A:ASP:HB3	6	0.59	0.25	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3439)	1:102:A:LEU:HD23	1:147:A:ASP:HB2	6	0.54	0.21	0.53
(1,3439)	1:102:A:LEU:HD23	1:147:A:ASP:HB3	6	0.54	0.21	0.53
(1,3439)	1:42:A:LEU:HG	1:31:A:ASN:HB2	6	0.54	0.21	0.53
(1,3439)	1:42:A:LEU:HG	1:31:A:ASN:HB3	6	0.54	0.21	0.53
(1,3439)	1:142:A:VAL:HG13	1:147:A:ASP:HB2	6	0.54	0.21	0.53
(1,3439)	1:142:A:VAL:HG13	1:147:A:ASP:HB3	6	0.54	0.21	0.53
(1,3439)	1:102:A:LEU:HD21	1:147:A:ASP:HB2	6	0.54	0.21	0.53
(1,3439)	1:102:A:LEU:HD21	1:147:A:ASP:HB3	6	0.54	0.21	0.53
(1,3439)	1:102:A:LEU:HD11	1:147:A:ASP:HB2	6	0.54	0.21	0.53
(1,3439)	1:102:A:LEU:HD11	1:147:A:ASP:HB3	6	0.54	0.21	0.53
(1,3439)	1:102:A:LEU:HD22	1:147:A:ASP:HB2	6	0.54	0.21	0.53
(1,3439)	1:102:A:LEU:HD22	1:147:A:ASP:HB3	6	0.54	0.21	0.53
(1,3312)	1:158:A:TYR:HB2	1:157:A:VAL:HB	6	0.53	0.15	0.49
(1,3312)	1:58:A:ASP:HB2	1:57:A:LYS:HB2	6	0.53	0.15	0.49
(1,3312)	1:58:A:ASP:HB2	1:57:A:LYS:HB3	6	0.53	0.15	0.49
(1,5850)	1:113:A:GLU:HG3	1:113:A:GLU:H	6	0.49	0.28	0.48
(1,5850)	1:113:A:GLU:HG2	1:114:A:LEU:H	6	0.49	0.28	0.48
(1,5861)	1:116:A:PRO:HG3	1:117:A:GLU:H	6	0.42	0.13	0.46
(1,5861)	1:116:A:PRO:HG2	1:117:A:GLU:H	6	0.42	0.13	0.46
(1,2238)	1:207:A:CYS:HA	1:211:A:ASN:HD21	6	0.42	0.13	0.42
(1,2238)	1:207:A:CYS:HA	1:211:A:ASN:HD22	6	0.42	0.13	0.42
(1,2238)	1:207:A:CYS:HA	1:213:A:GLN:HE21	6	0.42	0.13	0.42
(1,2238)	1:207:A:CYS:HA	1:213:A:GLN:HE22	6	0.42	0.13	0.42
(1,2426)	1:101:A:ILE:HG22	1:103:A:GLU:H	6	0.4	0.17	0.36
(1,2426)	1:101:A:ILE:HG23	1:103:A:GLU:H	6	0.4	0.17	0.36
(1,2426)	1:101:A:ILE:HG21	1:103:A:GLU:H	6	0.4	0.17	0.36
(1,5247)	1:40:A:GLN:HE21	1:55:A:ALA:HA	6	0.34	0.16	0.28
(1,5247)	1:40:A:GLN:HE21	1:37:A:LYS:HA	6	0.34	0.16	0.28
(1,2947)	1:30:A:CYS:HB2	1:29:A:SER:HB2	6	0.34	0.12	0.32
(1,2947)	1:30:A:CYS:HB2	1:29:A:SER:HB3	6	0.34	0.12	0.32
(1,2947)	1:133:A:ARG:HD3	1:136:A:PRO:HA	6	0.34	0.12	0.32
(1,2947)	1:133:A:ARG:HD2	1:136:A:PRO:HA	6	0.34	0.12	0.32
(1,2502)	1:42:A:LEU:HG	1:27:A:SER:HA	6	0.3	0.12	0.32
(1,2502)	1:42:A:LEU:HG	1:53:A:SER:HA	6	0.3	0.12	0.32
(1,3505)	1:197:A:ARG:HG3	1:197:A:ARG:HA	6	0.28	0.14	0.2
(1,3505)	1:197:A:ARG:HG2	1:197:A:ARG:HA	6	0.28	0.14	0.2
(1,5290)	1:73:A:SER:H	1:79:A:GLN:HG2	6	0.27	0.13	0.22
(1,5290)	1:73:A:SER:H	1:79:A:GLN:HG3	6	0.27	0.13	0.22
(1,5290)	1:73:A:SER:H	1:69:A:GLU:HG2	6	0.27	0.13	0.22
(1,5290)	1:73:A:SER:H	1:69:A:GLU:HG3	6	0.27	0.13	0.22
(1,2425)	1:54:A:ILE:HG23	1:12:A:VAL:H	6	0.26	0.1	0.23
(1,2425)	1:54:A:ILE:HG21	1:12:A:VAL:H	6	0.26	0.1	0.23

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2425)	1:54:A:ILE:HG21	1:57:A:LYS:H	6	0.26	0.1	0.23
(1,2425)	1:54:A:ILE:HG22	1:12:A:VAL:H	6	0.26	0.1	0.23
(1,1218)	1:62:A:VAL:HA	1:62:A:VAL:HB	6	0.16	0.01	0.16
(1,625)	1:143:A:LEU:H	1:142:A:VAL:HB	6	0.15	0.02	0.16
(1,5835)	1:110:A:LYS:HA	1:110:A:LYS:H	6	0.14	0.02	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD11	6	0.13	0.02	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD12	6	0.13	0.02	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD13	6	0.13	0.02	0.13
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD11	6	0.13	0.02	0.13
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD12	6	0.13	0.02	0.13
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD13	6	0.13	0.02	0.13
(1,2435)	1:153:A:LEU:HG	1:179:A:LEU:H	6	0.13	0.03	0.12
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE1	6	0.12	0.02	0.11
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE2	6	0.12	0.02	0.11
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE3	6	0.12	0.02	0.11
(1,263)	1:137:A:ILE:HG12	1:136:A:PRO:HA	6	0.11	0.03	0.1
(1,263)	1:137:A:ILE:HG13	1:136:A:PRO:HA	6	0.11	0.03	0.1
(1,2383)	1:43:A:VAL:HG22	1:52:A:TYR:H	5	0.7	0.24	0.56
(1,2383)	1:43:A:VAL:HG21	1:52:A:TYR:H	5	0.7	0.24	0.56
(1,2383)	1:43:A:VAL:HG23	1:52:A:TYR:H	5	0.7	0.24	0.56
(1,5801)	1:146:A:LYS:HE2	1:182:A:PRO:HG2	5	0.61	0.11	0.59
(1,5801)	1:146:A:LYS:HE2	1:182:A:PRO:HG3	5	0.61	0.11	0.59
(1,5801)	1:112:A:LYS:HE2	1:116:A:PRO:HG2	5	0.61	0.11	0.59
(1,5801)	1:112:A:LYS:HE2	1:116:A:PRO:HG3	5	0.61	0.11	0.59
(1,2379)	1:24:A:LEU:HD11	1:44:A:ARG:H	5	0.55	0.1	0.51
(1,2379)	1:24:A:LEU:HD12	1:46:A:PHE:H	5	0.55	0.1	0.51
(1,2379)	1:24:A:LEU:HD23	1:44:A:ARG:H	5	0.55	0.1	0.51
(1,2379)	1:24:A:LEU:HD21	1:44:A:ARG:H	5	0.55	0.1	0.51
(1,3448)	1:43:A:VAL:HG12	1:41:A:CYS:HB2	5	0.5	0.29	0.42
(1,3448)	1:43:A:VAL:HG12	1:41:A:CYS:HB3	5	0.5	0.29	0.42
(1,3448)	1:43:A:VAL:HG11	1:41:A:CYS:HB2	5	0.5	0.29	0.42
(1,3448)	1:43:A:VAL:HG11	1:41:A:CYS:HB3	5	0.5	0.29	0.42
(1,3448)	1:43:A:VAL:HG13	1:41:A:CYS:HB2	5	0.5	0.29	0.42
(1,3448)	1:43:A:VAL:HG13	1:41:A:CYS:HB3	5	0.5	0.29	0.42
(1,3448)	1:101:A:ILE:HG13	1:96:A:MET:HG2	5	0.5	0.29	0.42
(1,3448)	1:101:A:ILE:HG13	1:96:A:MET:HG3	5	0.5	0.29	0.42
(1,2573)	1:187:A:ALA:HB1	1:186:A:SER:HB2	5	0.47	0.14	0.47
(1,2573)	1:187:A:ALA:HB1	1:186:A:SER:HB3	5	0.47	0.14	0.47
(1,2573)	1:187:A:ALA:HB3	1:186:A:SER:HB2	5	0.47	0.14	0.47
(1,2573)	1:187:A:ALA:HB3	1:186:A:SER:HB3	5	0.47	0.14	0.47
(1,2573)	1:187:A:ALA:HB2	1:186:A:SER:HB2	5	0.47	0.14	0.47
(1,2573)	1:187:A:ALA:HB2	1:186:A:SER:HB3	5	0.47	0.14	0.47

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,172)	1:122:A:PHE:HE1	1:126:A:LEU:HG	5	0.44	0.11	0.39
(1,172)	1:122:A:PHE:HE1	1:200:A:LEU:HB2	5	0.44	0.11	0.39
(1,172)	1:122:A:PHE:HE1	1:200:A:LEU:HB3	5	0.44	0.11	0.39
(1,172)	1:122:A:PHE:HE2	1:126:A:LEU:HG	5	0.44	0.11	0.39
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG2	5	0.42	0.16	0.5
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG3	5	0.42	0.16	0.5
(1,2466)	1:60:A:LYS:HD3	1:20:A:TRP:HD1	5	0.4	0.23	0.37
(1,2466)	1:60:A:LYS:HD3	1:17:A:ARG:HE	5	0.4	0.23	0.37
(1,2466)	1:60:A:LYS:HD2	1:17:A:ARG:HE	5	0.4	0.23	0.37
(1,3330)	1:90:A:VAL:HB	1:91:A:PRO:HG2	5	0.4	0.2	0.33
(1,3330)	1:90:A:VAL:HB	1:91:A:PRO:HG3	5	0.4	0.2	0.33
(1,3330)	1:100:A:GLU:HG3	1:101:A:ILE:HG12	5	0.4	0.2	0.33
(1,3330)	1:100:A:GLU:HG3	1:101:A:ILE:HG13	5	0.4	0.2	0.33
(1,3330)	1:100:A:GLU:HG2	1:101:A:ILE:HG12	5	0.4	0.2	0.33
(1,3330)	1:100:A:GLU:HG2	1:101:A:ILE:HG13	5	0.4	0.2	0.33
(1,2471)	1:12:A:VAL:HG23	1:20:A:TRP:HD1	5	0.39	0.14	0.42
(1,2471)	1:12:A:VAL:HG22	1:20:A:TRP:HD1	5	0.39	0.14	0.42
(1,2471)	1:12:A:VAL:HG12	1:17:A:ARG:HE	5	0.39	0.14	0.42
(1,2471)	1:12:A:VAL:HG11	1:17:A:ARG:HE	5	0.39	0.14	0.42
(1,5318)	1:36:A:VAL:H	1:37:A:LYS:HG2	5	0.39	0.15	0.45
(1,5318)	1:36:A:VAL:H	1:37:A:LYS:HG3	5	0.39	0.15	0.45
(1,5318)	1:36:A:VAL:H	1:34:A:ILE:HB	5	0.39	0.15	0.45
(1,3287)	1:140:A:PRO:HD3	1:139:A:LYS:HD2	5	0.37	0.15	0.32
(1,3287)	1:140:A:PRO:HD3	1:139:A:LYS:HD3	5	0.37	0.15	0.32
(1,3287)	1:53:A:SER:HB3	1:37:A:LYS:HD2	5	0.37	0.15	0.32
(1,3287)	1:53:A:SER:HB3	1:37:A:LYS:HD3	5	0.37	0.15	0.32
(1,3287)	1:53:A:SER:HB2	1:37:A:LYS:HD2	5	0.37	0.15	0.32
(1,3287)	1:53:A:SER:HB2	1:37:A:LYS:HD3	5	0.37	0.15	0.32
(1,3287)	1:140:A:PRO:HD2	1:139:A:LYS:HD2	5	0.37	0.15	0.32
(1,3287)	1:140:A:PRO:HD2	1:139:A:LYS:HD3	5	0.37	0.15	0.32
(1,2548)	1:150:A:LEU:HD12	1:141:A:PRO:HA	5	0.34	0.15	0.44
(1,2548)	1:150:A:LEU:HD22	1:141:A:PRO:HA	5	0.34	0.15	0.44
(1,2548)	1:150:A:LEU:HD11	1:141:A:PRO:HA	5	0.34	0.15	0.44
(1,5785)	1:111:A:GLU:H	1:111:A:GLU:HG2	5	0.32	0.12	0.26
(1,5785)	1:111:A:GLU:H	1:111:A:GLU:HG3	5	0.32	0.12	0.26
(1,5785)	1:222:A:LEU:H	1:221:A:GLU:HG2	5	0.32	0.12	0.26
(1,5785)	1:222:A:LEU:H	1:221:A:GLU:HG3	5	0.32	0.12	0.26
(1,5842)	1:111:A:GLU:H	1:111:A:GLU:HG2	5	0.32	0.12	0.26
(1,5842)	1:111:A:GLU:H	1:111:A:GLU:HG3	5	0.32	0.12	0.26
(1,5842)	1:222:A:LEU:H	1:221:A:GLU:HG2	5	0.32	0.12	0.26
(1,5842)	1:222:A:LEU:H	1:221:A:GLU:HG3	5	0.32	0.12	0.26
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD11	5	0.31	0.11	0.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD12	5	0.31	0.11	0.29
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD13	5	0.31	0.11	0.29
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD21	5	0.31	0.11	0.29
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD22	5	0.31	0.11	0.29
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD23	5	0.31	0.11	0.29
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD11	5	0.31	0.11	0.29
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD12	5	0.31	0.11	0.29
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD13	5	0.31	0.11	0.29
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD21	5	0.31	0.11	0.29
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD22	5	0.31	0.11	0.29
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD23	5	0.31	0.11	0.29
(1,2804)	1:171:A:VAL:HG13	1:175:A:ILE:HD11	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG13	1:175:A:ILE:HD12	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG13	1:175:A:ILE:HD13	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG11	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG12	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG13	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG21	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG22	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG23	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG11	1:175:A:ILE:HD11	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG11	1:175:A:ILE:HD12	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG11	1:175:A:ILE:HD13	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG11	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG12	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG13	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG21	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG22	5	0.28	0.17	0.25
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG23	5	0.28	0.17	0.25
(1,3431)	1:83:A:ILE:HG21	1:87:A:THR:HG21	5	0.27	0.09	0.24
(1,3431)	1:83:A:ILE:HG21	1:87:A:THR:HG22	5	0.27	0.09	0.24
(1,3431)	1:83:A:ILE:HG21	1:87:A:THR:HG23	5	0.27	0.09	0.24
(1,3431)	1:83:A:ILE:HG23	1:87:A:THR:HG21	5	0.27	0.09	0.24
(1,3431)	1:83:A:ILE:HG23	1:87:A:THR:HG22	5	0.27	0.09	0.24
(1,3431)	1:83:A:ILE:HG23	1:87:A:THR:HG23	5	0.27	0.09	0.24
(1,3431)	1:83:A:ILE:HG22	1:87:A:THR:HG21	5	0.27	0.09	0.24
(1,3431)	1:83:A:ILE:HG22	1:87:A:THR:HG22	5	0.27	0.09	0.24
(1,3431)	1:83:A:ILE:HG22	1:87:A:THR:HG23	5	0.27	0.09	0.24
(1,3431)	1:36:A:VAL:HG11	1:35:A:THR:HG21	5	0.27	0.09	0.24
(1,3431)	1:36:A:VAL:HG11	1:35:A:THR:HG22	5	0.27	0.09	0.24
(1,3431)	1:36:A:VAL:HG11	1:35:A:THR:HG23	5	0.27	0.09	0.24
(1,750)	1:114:A:LEU:H	1:114:A:LEU:HG	5	0.25	0.04	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2554)	1:175:A:ILE:HD12	1:192:A:VAL:HA	5	0.24	0.19	0.12
(1,2554)	1:175:A:ILE:HD13	1:153:A:LEU:HA	5	0.24	0.19	0.12
(1,2554)	1:175:A:ILE:HD12	1:153:A:LEU:HA	5	0.24	0.19	0.12
(1,2998)	1:178:A:ASP:HB3	1:153:A:LEU:HA	5	0.24	0.09	0.25
(1,2998)	1:204:A:GLU:HB3	1:197:A:ARG:HA	5	0.24	0.09	0.25
(1,2998)	1:204:A:GLU:HB2	1:197:A:ARG:HA	5	0.24	0.09	0.25
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB2	5	0.24	0.1	0.21
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB3	5	0.24	0.1	0.21
(1,3221)	1:38:A:LYS:HA	1:38:A:LYS:HD2	5	0.23	0.06	0.22
(1,3221)	1:38:A:LYS:HA	1:38:A:LYS:HD3	5	0.23	0.06	0.22
(1,3221)	1:170:A:ALA:HA	1:173:A:LYS:HD2	5	0.23	0.06	0.22
(1,3221)	1:170:A:ALA:HA	1:173:A:LYS:HD3	5	0.23	0.06	0.22
(1,2645)	1:54:A:ILE:HG21	1:57:A:LYS:HE2	5	0.22	0.2	0.13
(1,2645)	1:54:A:ILE:HG21	1:57:A:LYS:HE3	5	0.22	0.2	0.13
(1,2645)	1:54:A:ILE:HG23	1:41:A:CYS:HB2	5	0.22	0.2	0.13
(1,2645)	1:54:A:ILE:HG23	1:41:A:CYS:HB3	5	0.22	0.2	0.13
(1,2645)	1:54:A:ILE:HG21	1:41:A:CYS:HB2	5	0.22	0.2	0.13
(1,2645)	1:54:A:ILE:HG21	1:41:A:CYS:HB3	5	0.22	0.2	0.13
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG11	5	0.22	0.06	0.2
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG12	5	0.22	0.06	0.2
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG13	5	0.22	0.06	0.2
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG21	5	0.22	0.06	0.2
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG22	5	0.22	0.06	0.2
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG23	5	0.22	0.06	0.2
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG11	5	0.22	0.06	0.2
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG12	5	0.22	0.06	0.2
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG13	5	0.22	0.06	0.2
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG21	5	0.22	0.06	0.2
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG22	5	0.22	0.06	0.2
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG23	5	0.22	0.06	0.2
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD21	5	0.22	0.03	0.23
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD22	5	0.22	0.03	0.23
(1,5070)	1:40:A:GLN:H	1:56:A:ARG:H	5	0.22	0.09	0.19
(1,2289)	1:119:A:ARG:HA	1:117:A:GLU:H	5	0.21	0.1	0.2
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG2	5	0.2	0.08	0.16
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG3	5	0.2	0.08	0.16
(1,3097)	1:177:A:MET:H	1:174:A:GLN:HG2	5	0.19	0.05	0.22
(1,3097)	1:177:A:MET:H	1:174:A:GLN:HG3	5	0.19	0.05	0.22
(1,3097)	1:82:A:SER:H	1:79:A:GLN:HG2	5	0.19	0.05	0.22
(1,3097)	1:82:A:SER:H	1:79:A:GLN:HG3	5	0.19	0.05	0.22
(1,5807)	1:99:A:SER:H	1:97:A:ASP:HB2	5	0.18	0.05	0.18
(1,5807)	1:99:A:SER:H	1:97:A:ASP:HB3	5	0.18	0.05	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5807)	1:2:A:ASP:H	1:2:A:ASP:HB2	5	0.18	0.05	0.18
(1,5807)	1:2:A:ASP:H	1:2:A:ASP:HB3	5	0.18	0.05	0.18
(1,2428)	1:64:A:ILE:HD13	1:65:A:LEU:H	5	0.17	0.05	0.17
(1,3604)	1:149:A:ASN:HB2	1:150:A:LEU:H	5	0.16	0.04	0.15
(1,3604)	1:149:A:ASN:HB3	1:150:A:LEU:H	5	0.16	0.04	0.15
(1,362)	1:150:A:LEU:HG	1:119:A:ARG:HA	5	0.15	0.03	0.14
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG11	5	0.12	0.01	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG12	5	0.12	0.01	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG13	5	0.12	0.01	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG21	5	0.12	0.01	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG22	5	0.12	0.01	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG23	5	0.12	0.01	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG11	5	0.12	0.01	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG12	5	0.12	0.01	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG13	5	0.12	0.01	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG21	5	0.12	0.01	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG22	5	0.12	0.01	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG23	5	0.12	0.01	0.13
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG11	5	0.12	0.01	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG12	5	0.12	0.01	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG13	5	0.12	0.01	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG21	5	0.12	0.01	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG22	5	0.12	0.01	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG23	5	0.12	0.01	0.12
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD2	5	0.12	0.02	0.11
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD3	5	0.12	0.02	0.11
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD2	5	0.12	0.02	0.11
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD3	5	0.12	0.02	0.11
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE1	5	0.11	0.01	0.11
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE2	5	0.11	0.01	0.11
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE1	5	0.11	0.01	0.11
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE2	5	0.11	0.01	0.11
(1,5556)	1:96:A:MET:HB2	1:95:A:LYS:H	4	0.58	0.3	0.65
(1,5556)	1:197:A:ARG:HB3	1:201:A:TYR:H	4	0.58	0.3	0.65
(1,2884)	1:61:A:GLU:HG2	1:3:A:GLU:HA	4	0.57	0.28	0.6
(1,2884)	1:61:A:GLU:HG3	1:3:A:GLU:HA	4	0.57	0.28	0.6
(1,2448)	1:130:A:MET:HE2	1:200:A:LEU:H	4	0.55	0.24	0.64
(1,2448)	1:130:A:MET:HE1	1:200:A:LEU:H	4	0.55	0.24	0.64
(1,5559)	1:24:A:LEU:HD22	1:8:A:VAL:H	4	0.54	0.09	0.5
(1,5559)	1:24:A:LEU:HD11	1:8:A:VAL:H	4	0.54	0.09	0.5
(1,5559)	1:24:A:LEU:HD21	1:8:A:VAL:H	4	0.54	0.09	0.5
(1,5559)	1:5:A:LEU:HD23	1:2:A:ASP:H	4	0.54	0.09	0.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5547)	1:100:A:GLU:HG3	1:100:A:GLU:H	4	0.48	0.29	0.42
(1,5547)	1:100:A:GLU:HG2	1:100:A:GLU:H	4	0.48	0.29	0.42
(1,2541)	1:142:A:VAL:HB	1:148:A:LEU:HA	4	0.48	0.19	0.56
(1,2541)	1:142:A:VAL:HB	1:141:A:PRO:HA	4	0.48	0.19	0.56
(1,3433)	1:4:A:LEU:HD23	1:56:A:ARG:HD2	4	0.42	0.09	0.44
(1,3433)	1:4:A:LEU:HD23	1:56:A:ARG:HD3	4	0.42	0.09	0.44
(1,3433)	1:12:A:VAL:HG12	1:17:A:ARG:HD2	4	0.42	0.09	0.44
(1,3433)	1:12:A:VAL:HG12	1:17:A:ARG:HD3	4	0.42	0.09	0.44
(1,3433)	1:12:A:VAL:HG23	1:17:A:ARG:HD2	4	0.42	0.09	0.44
(1,3433)	1:12:A:VAL:HG23	1:17:A:ARG:HD3	4	0.42	0.09	0.44
(1,3433)	1:4:A:LEU:HD21	1:56:A:ARG:HD2	4	0.42	0.09	0.44
(1,3433)	1:4:A:LEU:HD21	1:56:A:ARG:HD3	4	0.42	0.09	0.44
(1,5373)	1:134:A:GLY:H	1:133:A:ARG:HD2	4	0.34	0.16	0.3
(1,5373)	1:134:A:GLY:H	1:133:A:ARG:HD3	4	0.34	0.16	0.3
(1,5373)	1:134:A:GLY:H	1:44:A:ARG:HD2	4	0.34	0.16	0.3
(1,5373)	1:134:A:GLY:H	1:44:A:ARG:HD3	4	0.34	0.16	0.3
(1,3340)	1:19:A:GLU:HB2	1:75:A:LYS:HG2	4	0.34	0.08	0.35
(1,3340)	1:19:A:GLU:HB2	1:75:A:LYS:HG3	4	0.34	0.08	0.35
(1,3340)	1:19:A:GLU:HB3	1:75:A:LYS:HG2	4	0.34	0.08	0.35
(1,3340)	1:19:A:GLU:HB3	1:75:A:LYS:HG3	4	0.34	0.08	0.35
(1,3340)	1:76:A:PRO:HG2	1:75:A:LYS:HG2	4	0.34	0.08	0.35
(1,3340)	1:76:A:PRO:HG2	1:75:A:LYS:HG3	4	0.34	0.08	0.35
(1,3340)	1:76:A:PRO:HG3	1:75:A:LYS:HG2	4	0.34	0.08	0.35
(1,3340)	1:76:A:PRO:HG3	1:75:A:LYS:HG3	4	0.34	0.08	0.35
(1,5553)	1:148:A:LEU:HG	1:142:A:VAL:H	4	0.32	0.13	0.24
(1,3200)	1:184:A:LEU:HA	1:183:A:ILE:HG12	4	0.31	0.08	0.29
(1,3200)	1:184:A:LEU:HA	1:183:A:ILE:HG13	4	0.31	0.08	0.29
(1,5331)	1:75:A:LYS:H	1:71:A:GLU:HG2	4	0.3	0.09	0.29
(1,5331)	1:75:A:LYS:H	1:71:A:GLU:HG3	4	0.3	0.09	0.29
(1,5572)	1:94:A:TRP:HD1	1:94:A:TRP:H	4	0.28	0.08	0.3
(1,2842)	1:181:A:ILE:HD13	1:176:A:TYR:HB2	4	0.26	0.12	0.22
(1,2842)	1:181:A:ILE:HD13	1:176:A:TYR:HB3	4	0.26	0.12	0.22
(1,2842)	1:181:A:ILE:HD11	1:176:A:TYR:HB2	4	0.26	0.12	0.22
(1,2842)	1:181:A:ILE:HD11	1:176:A:TYR:HB3	4	0.26	0.12	0.22
(1,5313)	1:20:A:TRP:HE1	1:71:A:GLU:HG2	4	0.24	0.11	0.19
(1,5313)	1:20:A:TRP:HE1	1:71:A:GLU:HG3	4	0.24	0.11	0.19
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD11	4	0.24	0.02	0.24
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD12	4	0.24	0.02	0.24
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD13	4	0.24	0.02	0.24
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD11	4	0.24	0.02	0.24
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD12	4	0.24	0.02	0.24
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD13	4	0.24	0.02	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD11	4	0.24	0.02	0.24
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD12	4	0.24	0.02	0.24
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD13	4	0.24	0.02	0.24
(1,3351)	1:17:A:ARG:HB2	1:60:A:LYS:HB2	4	0.22	0.03	0.22
(1,3351)	1:17:A:ARG:HB2	1:60:A:LYS:HB3	4	0.22	0.03	0.22
(1,3351)	1:17:A:ARG:HB3	1:60:A:LYS:HB2	4	0.22	0.03	0.22
(1,3351)	1:17:A:ARG:HB3	1:60:A:LYS:HB3	4	0.22	0.03	0.22
(1,3351)	1:61:A:GLU:HB2	1:60:A:LYS:HB2	4	0.22	0.03	0.22
(1,3351)	1:61:A:GLU:HB2	1:60:A:LYS:HB3	4	0.22	0.03	0.22
(1,3351)	1:61:A:GLU:HB3	1:60:A:LYS:HB2	4	0.22	0.03	0.22
(1,3351)	1:61:A:GLU:HB3	1:60:A:LYS:HB3	4	0.22	0.03	0.22
(1,5828)	1:108:A:LYS:H	1:108:A:LYS:HB2	4	0.22	0.02	0.22
(1,5828)	1:108:A:LYS:H	1:108:A:LYS:HB3	4	0.22	0.02	0.22
(1,5226)	1:82:A:SER:H	1:79:A:GLN:HA	4	0.22	0.1	0.2
(1,5226)	1:82:A:SER:H	1:78:A:LEU:HA	4	0.22	0.1	0.2
(1,4994)	1:222:A:LEU:H	1:222:A:LEU:HG	4	0.21	0.05	0.21
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG21	4	0.2	0.03	0.2
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG22	4	0.2	0.03	0.2
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG23	4	0.2	0.03	0.2
(1,5314)	1:20:A:TRP:HE1	1:75:A:LYS:HG2	4	0.2	0.12	0.15
(1,5314)	1:20:A:TRP:HE1	1:75:A:LYS:HG3	4	0.2	0.12	0.15
(1,5314)	1:20:A:TRP:HE1	1:18:A:THR:HG21	4	0.2	0.12	0.15
(1,5314)	1:20:A:TRP:HE1	1:18:A:THR:HG22	4	0.2	0.12	0.15
(1,5314)	1:20:A:TRP:HE1	1:18:A:THR:HG23	4	0.2	0.12	0.15
(1,5052)	1:78:A:LEU:H	1:75:A:LYS:HB2	4	0.19	0.04	0.2
(1,5052)	1:78:A:LEU:H	1:75:A:LYS:HB3	4	0.19	0.04	0.2
(1,5052)	1:78:A:LEU:H	1:78:A:LEU:HB2	4	0.19	0.04	0.2
(1,5052)	1:78:A:LEU:H	1:78:A:LEU:HB3	4	0.19	0.04	0.2
(1,152)	1:176:A:TYR:HE1	1:181:A:ILE:HB	4	0.19	0.03	0.19
(1,152)	1:176:A:TYR:HE2	1:181:A:ILE:HB	4	0.19	0.03	0.19
(1,2948)	1:63:A:ASP:HB2	1:64:A:ILE:HA	4	0.18	0.01	0.18
(1,2948)	1:96:A:MET:HG2	1:101:A:ILE:HA	4	0.18	0.01	0.18
(1,2948)	1:63:A:ASP:HB3	1:64:A:ILE:HA	4	0.18	0.01	0.18
(1,2887)	1:101:A:ILE:HB	1:99:A:SER:H	4	0.18	0.04	0.19
(1,2212)	1:138:A:ASN:HD21	1:137:A:ILE:HA	4	0.17	0.03	0.17
(1,2212)	1:138:A:ASN:HD22	1:137:A:ILE:HA	4	0.17	0.03	0.17
(1,5689)	1:137:A:ILE:HA	1:138:A:ASN:HD21	4	0.17	0.03	0.17
(1,5689)	1:137:A:ILE:HA	1:138:A:ASN:HD22	4	0.17	0.03	0.17
(1,5813)	1:108:A:LYS:HG2	1:106:A:SER:HB2	4	0.16	0.04	0.16
(1,5813)	1:108:A:LYS:HG2	1:106:A:SER:HB3	4	0.16	0.04	0.16
(1,5813)	1:108:A:LYS:HG3	1:106:A:SER:HB2	4	0.16	0.04	0.16
(1,5813)	1:108:A:LYS:HG3	1:106:A:SER:HB3	4	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2978)	1:98:A:ILE:HG13	1:98:A:ILE:HA	4	0.15	0.02	0.15
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD11	4	0.14	0.03	0.14
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD12	4	0.14	0.03	0.14
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD13	4	0.14	0.03	0.14
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD21	4	0.14	0.03	0.14
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD22	4	0.14	0.03	0.14
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD23	4	0.14	0.03	0.14
(1,5397)	1:127:A:TYR:H	1:137:A:ILE:HG12	4	0.14	0.03	0.14
(1,5397)	1:127:A:TYR:H	1:137:A:ILE:HG13	4	0.14	0.03	0.14
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD11	4	0.13	0.03	0.12
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD12	4	0.13	0.03	0.12
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD13	4	0.13	0.03	0.12
(1,3868)	1:102:A:LEU:HB2	1:103:A:GLU:H	4	0.13	0.02	0.13
(1,3868)	1:102:A:LEU:HB3	1:103:A:GLU:H	4	0.13	0.02	0.13
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB1	4	0.13	0.02	0.14
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB2	4	0.13	0.02	0.14
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB3	4	0.13	0.02	0.14
(1,4502)	1:133:A:ARG:HE	1:202:A:GLY:H	4	0.13	0.02	0.12
(1,335)	1:120:A:ASP:HB2	1:117:A:GLU:HA	4	0.12	0.01	0.12
(1,335)	1:120:A:ASP:HB3	1:117:A:GLU:HA	4	0.12	0.01	0.12
(1,175)	1:190:A:TYR:HA	1:190:A:TYR:HD1	4	0.12	0.01	0.12
(1,175)	1:190:A:TYR:HA	1:190:A:TYR:HD2	4	0.12	0.01	0.12
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG11	4	0.11	0.01	0.11
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG12	4	0.11	0.01	0.11
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG13	4	0.11	0.01	0.11
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG21	4	0.11	0.01	0.11
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG22	4	0.11	0.01	0.11
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG23	4	0.11	0.01	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG11	4	0.11	0.01	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG12	4	0.11	0.01	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG13	4	0.11	0.01	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG21	4	0.11	0.01	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG22	4	0.11	0.01	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG23	4	0.11	0.01	0.11
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD11	4	0.11	0.01	0.11
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD12	4	0.11	0.01	0.11
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD13	4	0.11	0.01	0.11
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD11	4	0.11	0.01	0.11
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD12	4	0.11	0.01	0.11
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD13	4	0.11	0.01	0.11
(1,4583)	1:98:A:ILE:HD11	1:121:A:ASN:H	4	0.11	0.0	0.11
(1,4583)	1:98:A:ILE:HD12	1:121:A:ASN:H	4	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,4583)	1:98:A:ILE:HD13	1:121:A:ASN:H	4	0.11	0.0	0.11
(1,2665)	1:47:A:ILE:HD11	1:76:A:PRO:HB2	3	0.41	0.17	0.4
(1,2665)	1:47:A:ILE:HD11	1:76:A:PRO:HB3	3	0.41	0.17	0.4
(1,2665)	1:47:A:ILE:HD13	1:48:A:ASP:HB2	3	0.41	0.17	0.4
(1,2665)	1:47:A:ILE:HD13	1:48:A:ASP:HB3	3	0.41	0.17	0.4
(1,2462)	1:197:A:ARG:HD2	1:201:A:TYR:HD1	3	0.4	0.14	0.47
(1,2462)	1:197:A:ARG:HD2	1:201:A:TYR:HD2	3	0.4	0.14	0.47
(1,2462)	1:197:A:ARG:HD3	1:201:A:TYR:HD1	3	0.4	0.14	0.47
(1,2462)	1:197:A:ARG:HD3	1:201:A:TYR:HD2	3	0.4	0.14	0.47
(1,2462)	1:197:A:ARG:HD2	1:196:A:TYR:HE1	3	0.4	0.14	0.47
(1,2462)	1:197:A:ARG:HD2	1:196:A:TYR:HE2	3	0.4	0.14	0.47
(1,5333)	1:221:A:GLU:H	1:222:A:LEU:HB2	3	0.39	0.08	0.35
(1,5333)	1:221:A:GLU:H	1:222:A:LEU:HB3	3	0.39	0.08	0.35
(1,5333)	1:221:A:GLU:H	1:222:A:LEU:HG	3	0.39	0.08	0.35
(1,3289)	1:144:A:GLY:HA2	1:184:A:LEU:HG	3	0.36	0.25	0.2
(1,3289)	1:68:A:PRO:HD2	1:72:A:LEU:HG	3	0.36	0.25	0.2
(1,2632)	1:198:A:LYS:HD3	1:139:A:LYS:HE2	3	0.33	0.07	0.37
(1,2632)	1:198:A:LYS:HD3	1:139:A:LYS:HE3	3	0.33	0.07	0.37
(1,2632)	1:198:A:LYS:HD3	1:199:A:TYR:HB2	3	0.33	0.07	0.37
(1,2632)	1:198:A:LYS:HD3	1:199:A:TYR:HB3	3	0.33	0.07	0.37
(1,2632)	1:198:A:LYS:HD2	1:199:A:TYR:HB2	3	0.33	0.07	0.37
(1,2632)	1:198:A:LYS:HD2	1:199:A:TYR:HB3	3	0.33	0.07	0.37
(1,5821)	1:108:A:LYS:HB2	1:109:A:ASP:H	3	0.32	0.02	0.32
(1,5821)	1:108:A:LYS:HB2	1:108:A:LYS:H	3	0.32	0.02	0.32
(1,3398)	1:15:A:THR:HG21	1:16:A:GLU:HG2	3	0.31	0.08	0.31
(1,3398)	1:15:A:THR:HG21	1:16:A:GLU:HG3	3	0.31	0.08	0.31
(1,3398)	1:15:A:THR:HG22	1:16:A:GLU:HG2	3	0.31	0.08	0.31
(1,3398)	1:15:A:THR:HG22	1:16:A:GLU:HG3	3	0.31	0.08	0.31
(1,3398)	1:15:A:THR:HG23	1:16:A:GLU:HG2	3	0.31	0.08	0.31
(1,3398)	1:15:A:THR:HG23	1:16:A:GLU:HG3	3	0.31	0.08	0.31
(1,5549)	1:204:A:GLU:HB2	1:201:A:TYR:H	3	0.3	0.15	0.25
(1,5549)	1:204:A:GLU:HB3	1:201:A:TYR:H	3	0.3	0.15	0.25
(1,5417)	1:10:A:SER:H	1:22:A:PRO:HB2	3	0.29	0.09	0.24
(1,5417)	1:10:A:SER:H	1:22:A:PRO:HB3	3	0.29	0.09	0.24
(1,5417)	1:10:A:SER:H	1:3:A:GLU:HB2	3	0.29	0.09	0.24
(1,5417)	1:10:A:SER:H	1:3:A:GLU:HB3	3	0.29	0.09	0.24
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD11	3	0.28	0.08	0.31
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD12	3	0.28	0.08	0.31
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD13	3	0.28	0.08	0.31
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD21	3	0.28	0.08	0.31
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD22	3	0.28	0.08	0.31
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD23	3	0.28	0.08	0.31

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3217)	1:98:A:ILE:HA	1:96:A:MET:HG2	3	0.28	0.07	0.23
(1,3217)	1:98:A:ILE:HA	1:96:A:MET:HG3	3	0.28	0.07	0.23
(1,3217)	1:128:A:LYS:HA	1:96:A:MET:HG2	3	0.28	0.07	0.23
(1,3217)	1:128:A:LYS:HA	1:96:A:MET:HG3	3	0.28	0.07	0.23
(1,5267)	1:160:A:GLN:HE21	1:175:A:ILE:HD11	3	0.27	0.05	0.27
(1,5267)	1:160:A:GLN:HE21	1:175:A:ILE:HD12	3	0.27	0.05	0.27
(1,5267)	1:160:A:GLN:HE21	1:175:A:ILE:HD13	3	0.27	0.05	0.27
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG11	3	0.27	0.05	0.27
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG12	3	0.27	0.05	0.27
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG13	3	0.27	0.05	0.27
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG21	3	0.27	0.05	0.27
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG22	3	0.27	0.05	0.27
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG23	3	0.27	0.05	0.27
(1,2306)	1:81:A:ALA:HA	1:78:A:LEU:HA	3	0.27	0.09	0.26
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG11	3	0.27	0.11	0.32
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG12	3	0.27	0.11	0.32
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG13	3	0.27	0.11	0.32
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG21	3	0.27	0.11	0.32
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG22	3	0.27	0.11	0.32
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG23	3	0.27	0.11	0.32
(1,2726)	1:61:A:GLU:HG3	1:60:A:LYS:HB2	3	0.23	0.09	0.23
(1,2726)	1:61:A:GLU:HG3	1:60:A:LYS:HB3	3	0.23	0.09	0.23
(1,5471)	1:79:A:GLN:HE21	1:72:A:LEU:HB2	3	0.22	0.06	0.25
(1,5471)	1:79:A:GLN:HE21	1:72:A:LEU:HB3	3	0.22	0.06	0.25
(1,5471)	1:79:A:GLN:HE22	1:72:A:LEU:HB2	3	0.22	0.06	0.25
(1,5471)	1:79:A:GLN:HE22	1:72:A:LEU:HB3	3	0.22	0.06	0.25
(1,150)	1:127:A:TYR:HE2	1:141:A:PRO:HG2	3	0.22	0.02	0.21
(1,150)	1:127:A:TYR:HE2	1:141:A:PRO:HG3	3	0.22	0.02	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD11	3	0.22	0.02	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD12	3	0.22	0.02	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD13	3	0.22	0.02	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD21	3	0.22	0.02	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD22	3	0.22	0.02	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD23	3	0.22	0.02	0.21
(1,3502)	1:22:A:PRO:HB2	1:21:A:TYR:HA	3	0.21	0.06	0.17
(1,5832)	1:109:A:ASP:H	1:108:A:LYS:HB2	3	0.21	0.02	0.2
(1,5832)	1:109:A:ASP:H	1:108:A:LYS:HB3	3	0.21	0.02	0.2
(1,5832)	1:108:A:LYS:H	1:108:A:LYS:HB2	3	0.21	0.02	0.2
(1,5832)	1:108:A:LYS:H	1:108:A:LYS:HB3	3	0.21	0.02	0.2
(1,2372)	1:96:A:MET:HE2	1:127:A:TYR:H	3	0.2	0.07	0.16
(1,2372)	1:96:A:MET:HE3	1:127:A:TYR:H	3	0.2	0.07	0.16
(1,2372)	1:96:A:MET:HE1	1:127:A:TYR:H	3	0.2	0.07	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2496)	1:46:A:PHE:HD1	1:44:A:ARG:HG2	3	0.19	0.02	0.18
(1,2496)	1:46:A:PHE:HD1	1:44:A:ARG:HG3	3	0.19	0.02	0.18
(1,2496)	1:46:A:PHE:HD2	1:23:A:ALA:HB1	3	0.19	0.02	0.18
(1,2496)	1:46:A:PHE:HD2	1:23:A:ALA:HB2	3	0.19	0.02	0.18
(1,2496)	1:46:A:PHE:HD2	1:23:A:ALA:HB3	3	0.19	0.02	0.18
(1,5623)	1:61:A:GLU:HG2	1:1:A:ASN:HD21	3	0.19	0.03	0.2
(1,5623)	1:61:A:GLU:HG2	1:1:A:ASN:HD22	3	0.19	0.03	0.2
(1,5623)	1:61:A:GLU:HG3	1:1:A:ASN:HD21	3	0.19	0.03	0.2
(1,5623)	1:61:A:GLU:HG3	1:1:A:ASN:HD22	3	0.19	0.03	0.2
(1,5103)	1:123:A:LEU:H	1:119:A:ARG:HB2	3	0.19	0.05	0.2
(1,5103)	1:123:A:LEU:H	1:119:A:ARG:HB3	3	0.19	0.05	0.2
(1,3721)	1:18:A:THR:HB	1:19:A:GLU:H	3	0.18	0.02	0.19
(1,732)	1:142:A:VAL:H	1:142:A:VAL:HB	3	0.18	0.02	0.19
(1,5792)	1:76:A:PRO:HD2	1:75:A:LYS:HB2	3	0.18	0.03	0.19
(1,5792)	1:76:A:PRO:HD2	1:75:A:LYS:HB3	3	0.18	0.03	0.19
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD11	3	0.17	0.05	0.19
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD12	3	0.17	0.05	0.19
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD13	3	0.17	0.05	0.19
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD21	3	0.17	0.05	0.19
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD22	3	0.17	0.05	0.19
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD23	3	0.17	0.05	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD11	3	0.17	0.05	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD12	3	0.17	0.05	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD13	3	0.17	0.05	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD21	3	0.17	0.05	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD22	3	0.17	0.05	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD23	3	0.17	0.05	0.19
(1,3507)	1:67:A:LEU:H	1:65:A:LEU:HB2	3	0.17	0.07	0.14
(1,3507)	1:67:A:LEU:H	1:65:A:LEU:HB3	3	0.17	0.07	0.14
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD11	3	0.17	0.01	0.18
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD12	3	0.17	0.01	0.18
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD13	3	0.17	0.01	0.18
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD11	3	0.17	0.01	0.18
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD12	3	0.17	0.01	0.18
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD13	3	0.17	0.01	0.18
(1,2869)	1:194:A:THR:HB	1:190:A:TYR:HD1	3	0.17	0.01	0.18
(1,2869)	1:194:A:THR:HB	1:190:A:TYR:HD2	3	0.17	0.01	0.18
(1,5235)	1:70:A:SER:H	1:69:A:GLU:HB2	3	0.17	0.05	0.15
(1,5235)	1:70:A:SER:H	1:69:A:GLU:HB3	3	0.17	0.05	0.15
(1,5359)	1:6:A:GLY:H	1:25:A:VAL:H	3	0.16	0.02	0.15
(1,2922)	1:64:A:ILE:HD12	1:62:A:VAL:HB	3	0.16	0.03	0.15
(1,2922)	1:64:A:ILE:HD13	1:85:A:LEU:HB2	3	0.16	0.03	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2922)	1:64:A:ILE:HD13	1:85:A:LEU:HB3	3	0.16	0.03	0.15
(1,2922)	1:64:A:ILE:HD11	1:62:A:VAL:HB	3	0.16	0.03	0.15
(1,3848)	1:223:A:GLU:HG2	1:223:A:GLU:H	3	0.15	0.02	0.15
(1,3848)	1:223:A:GLU:HG3	1:223:A:GLU:H	3	0.15	0.02	0.15
(1,5789)	1:108:A:LYS:H	1:107:A:SER:HB2	3	0.15	0.06	0.11
(1,5789)	1:108:A:LYS:H	1:107:A:SER:HB3	3	0.15	0.06	0.11
(1,3236)	1:17:A:ARG:HA	1:17:A:ARG:HD2	3	0.15	0.03	0.16
(1,3236)	1:17:A:ARG:HA	1:17:A:ARG:HD3	3	0.15	0.03	0.16
(1,5382)	1:74:A:THR:H	1:79:A:GLN:HB2	3	0.15	0.05	0.13
(1,5382)	1:74:A:THR:H	1:79:A:GLN:HB3	3	0.15	0.05	0.13
(1,5382)	1:74:A:THR:H	1:71:A:GLU:HG2	3	0.15	0.05	0.13
(1,5382)	1:74:A:THR:H	1:71:A:GLU:HG3	3	0.15	0.05	0.13
(1,4267)	1:198:A:LYS:HB2	1:199:A:TYR:H	3	0.14	0.01	0.14
(1,4267)	1:198:A:LYS:HB3	1:199:A:TYR:H	3	0.14	0.01	0.14
(1,5453)	1:172:A:TRP:H	1:174:A:GLN:HB2	3	0.14	0.03	0.13
(1,5453)	1:172:A:TRP:H	1:174:A:GLN:HB3	3	0.14	0.03	0.13
(1,249)	1:133:A:ARG:H	1:136:A:PRO:HA	3	0.13	0.04	0.11
(1,627)	1:10:A:SER:H	1:62:A:VAL:HB	3	0.13	0.02	0.14
(1,2398)	1:9:A:VAL:HG22	1:10:A:SER:H	3	0.13	0.02	0.15
(1,2398)	1:9:A:VAL:HG22	1:25:A:VAL:H	3	0.13	0.02	0.15
(1,2398)	1:9:A:VAL:HG23	1:10:A:SER:H	3	0.13	0.02	0.15
(1,3871)	1:198:A:LYS:HB2	1:201:A:TYR:H	3	0.13	0.03	0.12
(1,3871)	1:198:A:LYS:HB3	1:201:A:TYR:H	3	0.13	0.03	0.12
(1,5361)	1:199:A:TYR:H	1:197:A:ARG:HB2	3	0.13	0.03	0.12
(1,5361)	1:199:A:TYR:H	1:197:A:ARG:HB3	3	0.13	0.03	0.12
(1,5361)	1:199:A:TYR:H	1:150:A:LEU:HB2	3	0.13	0.03	0.12
(1,5361)	1:199:A:TYR:H	1:150:A:LEU:HB3	3	0.13	0.03	0.12
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD11	3	0.13	0.03	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD12	3	0.13	0.03	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD13	3	0.13	0.03	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD21	3	0.13	0.03	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD22	3	0.13	0.03	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD23	3	0.13	0.03	0.11
(1,3201)	1:2:A:ASP:HA	1:5:A:LEU:HG	3	0.13	0.03	0.11
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG21	3	0.12	0.03	0.11
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG22	3	0.12	0.03	0.11
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG23	3	0.12	0.03	0.11
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD11	3	0.12	0.01	0.12
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD12	3	0.12	0.01	0.12
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD13	3	0.12	0.01	0.12
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD21	3	0.12	0.01	0.12
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD22	3	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)
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD23	3	0.12	0.01	0.12
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD11	3	0.12	0.01	0.13
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD12	3	0.12	0.01	0.13
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD13	3	0.12	0.01	0.13
(1,725)	1:210:A:ALA:H	1:212:A:ILE:HB	3	0.12	0.01	0.11
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD11	3	0.12	0.01	0.12
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD12	3	0.12	0.01	0.12
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD13	3	0.12	0.01	0.12
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD21	3	0.12	0.01	0.12
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD22	3	0.12	0.01	0.12
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD23	3	0.12	0.01	0.12
(1,5851)	1:113:A:GLU:H	1:113:A:GLU:HA	3	0.12	0.0	0.12
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD11	3	0.11	0.01	0.11
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD12	3	0.11	0.01	0.11
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD13	3	0.11	0.01	0.11
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD21	3	0.11	0.01	0.11
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD22	3	0.11	0.01	0.11
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD23	3	0.11	0.01	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD11	3	0.11	0.01	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD12	3	0.11	0.01	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD13	3	0.11	0.01	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD21	3	0.11	0.01	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD22	3	0.11	0.01	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD23	3	0.11	0.01	0.11
(1,5497)	1:3:A:GLU:H	1:3:A:GLU:HB2	3	0.11	0.0	0.11
(1,5497)	1:3:A:GLU:H	1:3:A:GLU:HB3	3	0.11	0.0	0.11
(1,248)	1:130:A:MET:H	1:136:A:PRO:HA	3	0.11	0.01	0.1
(1,5808)	1:4:A:LEU:HA	1:4:A:LEU:HG	3	0.11	0.0	0.11
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG11	2	0.76	0.07	0.76
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG12	2	0.76	0.07	0.76
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG13	2	0.76	0.07	0.76
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG21	2	0.76	0.07	0.76
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG22	2	0.76	0.07	0.76
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG23	2	0.76	0.07	0.76
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG11	2	0.76	0.07	0.76
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG12	2	0.76	0.07	0.76
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG13	2	0.76	0.07	0.76
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG21	2	0.76	0.07	0.76
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG22	2	0.76	0.07	0.76
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG23	2	0.76	0.07	0.76
(1,5375)	1:202:A:GLY:H	1:204:A:GLU:HB2	2	0.62	0.07	0.62
(1,5375)	1:202:A:GLY:H	1:204:A:GLU:HB3	2	0.62	0.07	0.62

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2468)	1:84:A:PHE:HE1	1:88:A:ARG:HG2	2	0.52	0.04	0.52
(1,2468)	1:84:A:PHE:HE1	1:88:A:ARG:HG3	2	0.52	0.04	0.52
(1,2468)	1:84:A:PHE:HE2	1:88:A:ARG:HB2	2	0.52	0.04	0.52
(1,2468)	1:84:A:PHE:HE2	1:88:A:ARG:HB3	2	0.52	0.04	0.52
(1,5797)	1:71:A:GLU:HA	1:68:A:PRO:HD2	2	0.5	0.0	0.5
(1,5797)	1:71:A:GLU:HA	1:68:A:PRO:HD3	2	0.5	0.0	0.5
(1,5795)	1:167:A:ASP:HB2	1:168:A:SER:HB2	2	0.49	0.06	0.49
(1,5795)	1:167:A:ASP:HB2	1:168:A:SER:HB3	2	0.49	0.06	0.49
(1,5804)	1:167:A:ASP:HB2	1:168:A:SER:HB2	2	0.49	0.06	0.49
(1,5804)	1:167:A:ASP:HB2	1:168:A:SER:HB3	2	0.49	0.06	0.49
(1,2669)	1:85:A:LEU:HD12	1:8:A:VAL:HB	2	0.46	0.13	0.46
(1,5490)	1:63:A:ASP:H	1:61:A:GLU:HB2	2	0.46	0.12	0.46
(1,5490)	1:63:A:ASP:H	1:61:A:GLU:HB3	2	0.46	0.12	0.46
(1,5490)	1:63:A:ASP:H	1:67:A:LEU:HG	2	0.46	0.12	0.46
(1,5252)	1:88:A:ARG:HE	1:46:A:PHE:HB2	2	0.44	0.09	0.44
(1,5252)	1:88:A:ARG:HE	1:46:A:PHE:HB3	2	0.44	0.09	0.44
(1,5252)	1:88:A:ARG:HE	1:88:A:ARG:HA	2	0.44	0.09	0.44
(1,3338)	1:100:A:GLU:HB2	1:101:A:ILE:HG12	2	0.43	0.15	0.43
(1,3338)	1:100:A:GLU:HB2	1:101:A:ILE:HG13	2	0.43	0.15	0.43
(1,5266)	1:211:A:ASN:HD21	1:210:A:ALA:HB1	2	0.41	0.03	0.41
(1,5266)	1:211:A:ASN:HD21	1:210:A:ALA:HB2	2	0.41	0.03	0.41
(1,5266)	1:211:A:ASN:HD21	1:210:A:ALA:HB3	2	0.41	0.03	0.41
(1,132)	1:154:A:PHE:HD1	1:158:A:TYR:HB2	2	0.34	0.16	0.34
(1,132)	1:154:A:PHE:HD1	1:158:A:TYR:HB3	2	0.34	0.16	0.34
(1,3317)	1:39:A:ASP:HB3	1:38:A:LYS:HG2	2	0.32	0.09	0.32
(1,3317)	1:39:A:ASP:HB3	1:38:A:LYS:HG3	2	0.32	0.09	0.32
(1,3317)	1:39:A:ASP:HB2	1:38:A:LYS:HG2	2	0.32	0.09	0.32
(1,3317)	1:39:A:ASP:HB2	1:38:A:LYS:HG3	2	0.32	0.09	0.32
(1,5663)	1:160:A:GLN:HB2	1:157:A:VAL:H	2	0.32	0.02	0.32
(1,5663)	1:38:A:LYS:HG3	1:40:A:GLN:H	2	0.32	0.02	0.32
(1,5849)	1:113:A:GLU:HG3	1:113:A:GLU:HA	2	0.32	0.01	0.32
(1,5404)	1:89:A:VAL:H	1:89:A:VAL:HB	2	0.29	0.02	0.29
(1,5791)	1:102:A:LEU:HB2	1:105:A:SER:HB2	2	0.28	0.12	0.28
(1,5791)	1:102:A:LEU:HB2	1:105:A:SER:HB3	2	0.28	0.12	0.28
(1,5791)	1:102:A:LEU:HB3	1:105:A:SER:HB2	2	0.28	0.12	0.28
(1,5791)	1:102:A:LEU:HB3	1:105:A:SER:HB3	2	0.28	0.12	0.28
(1,2485)	1:34:A:ILE:HG12	1:51:A:PHE:HD1	2	0.26	0.08	0.26
(1,2485)	1:34:A:ILE:HG12	1:51:A:PHE:HD2	2	0.26	0.08	0.26
(1,3429)	1:181:A:ILE:HG21	1:182:A:PRO:HG2	2	0.26	0.08	0.26
(1,3429)	1:181:A:ILE:HG21	1:182:A:PRO:HG3	2	0.26	0.08	0.26
(1,3429)	1:181:A:ILE:HG22	1:182:A:PRO:HG2	2	0.26	0.08	0.26
(1,3429)	1:181:A:ILE:HG22	1:182:A:PRO:HG3	2	0.26	0.08	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3429)	1:181:A:ILE:HG23	1:182:A:PRO:HG2	2	0.26	0.08	0.26
(1,3429)	1:181:A:ILE:HG23	1:182:A:PRO:HG3	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD11	1:182:A:PRO:HG2	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD11	1:182:A:PRO:HG3	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD12	1:182:A:PRO:HG2	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD12	1:182:A:PRO:HG3	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD13	1:182:A:PRO:HG2	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD13	1:182:A:PRO:HG3	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD21	1:182:A:PRO:HG2	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD21	1:182:A:PRO:HG3	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD22	1:182:A:PRO:HG2	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD22	1:182:A:PRO:HG3	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD23	1:182:A:PRO:HG2	2	0.26	0.08	0.26
(1,3429)	1:184:A:LEU:HD23	1:182:A:PRO:HG3	2	0.26	0.08	0.26
(1,2564)	1:157:A:VAL:HG12	1:153:A:LEU:HA	2	0.25	0.15	0.25
(1,2607)	1:137:A:ILE:HD13	1:127:A:TYR:HA	2	0.24	0.03	0.24
(1,2607)	1:137:A:ILE:HD13	1:141:A:PRO:HD2	2	0.24	0.03	0.24
(1,2607)	1:137:A:ILE:HD13	1:141:A:PRO:HD3	2	0.24	0.03	0.24
(1,2837)	1:34:A:ILE:HG12	1:51:A:PHE:HA	2	0.24	0.12	0.24
(1,2840)	1:22:A:PRO:HA	1:81:A:ALA:HB1	2	0.24	0.02	0.24
(1,2840)	1:22:A:PRO:HA	1:81:A:ALA:HB2	2	0.24	0.02	0.24
(1,2840)	1:22:A:PRO:HA	1:81:A:ALA:HB3	2	0.24	0.02	0.24
(1,2314)	1:88:A:ARG:HA	1:88:A:ARG:HE	2	0.23	0.12	0.23
(1,2314)	1:88:A:ARG:HA	1:94:A:TRP:HD1	2	0.23	0.12	0.23
(1,2958)	1:72:A:LEU:H	1:70:A:SER:HB2	2	0.22	0.02	0.22
(1,2958)	1:72:A:LEU:H	1:70:A:SER:HB3	2	0.22	0.02	0.22
(1,2533)	1:9:A:VAL:HG22	1:25:A:VAL:HA	2	0.22	0.02	0.22
(1,2533)	1:9:A:VAL:HG21	1:25:A:VAL:HA	2	0.22	0.02	0.22
(1,5626)	1:142:A:VAL:HG11	1:145:A:TYR:H	2	0.21	0.06	0.21
(1,5626)	1:64:A:ILE:HG21	1:82:A:SER:H	2	0.21	0.06	0.21
(1,2946)	1:190:A:TYR:HB2	1:189:A:SER:HB2	2	0.2	0.02	0.2
(1,2946)	1:190:A:TYR:HB2	1:189:A:SER:HB3	2	0.2	0.02	0.2
(1,3524)	1:58:A:ASP:H	1:57:A:LYS:HE2	2	0.2	0.09	0.2
(1,3524)	1:58:A:ASP:H	1:57:A:LYS:HE3	2	0.2	0.09	0.2
(1,3524)	1:198:A:LYS:H	1:197:A:ARG:HD2	2	0.2	0.09	0.2
(1,3524)	1:198:A:LYS:H	1:197:A:ARG:HD3	2	0.2	0.09	0.2
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD11	2	0.2	0.07	0.2
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD12	2	0.2	0.07	0.2
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD13	2	0.2	0.07	0.2
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD21	2	0.2	0.07	0.2
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD22	2	0.2	0.07	0.2
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD23	2	0.2	0.07	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD11	2	0.2	0.07	0.2
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD12	2	0.2	0.07	0.2
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD13	2	0.2	0.07	0.2
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD21	2	0.2	0.07	0.2
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD22	2	0.2	0.07	0.2
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD23	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD11	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD12	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD13	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD21	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD22	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD23	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD11	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD12	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD13	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD21	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD22	2	0.2	0.07	0.2
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD23	2	0.2	0.07	0.2
(1,111)	1:20:A:TRP:HZ2	1:67:A:LEU:HB2	2	0.2	0.08	0.2
(1,111)	1:20:A:TRP:HZ2	1:67:A:LEU:HB3	2	0.2	0.08	0.2
(1,5536)	1:183:A:ILE:HG13	1:188:A:ALA:H	2	0.2	0.05	0.2
(1,5592)	1:43:A:VAL:HG11	1:44:A:ARG:H	2	0.18	0.08	0.18
(1,5592)	1:43:A:VAL:HG12	1:44:A:ARG:H	2	0.18	0.08	0.18
(1,2587)	1:137:A:ILE:HG13	1:127:A:TYR:HA	2	0.18	0.01	0.18
(1,3402)	1:35:A:THR:HG23	1:36:A:VAL:HB	2	0.18	0.06	0.18
(1,3402)	1:35:A:THR:HG22	1:36:A:VAL:HB	2	0.18	0.06	0.18
(1,5151)	1:105:A:SER:H	1:105:A:SER:HB2	2	0.18	0.08	0.18
(1,5151)	1:105:A:SER:H	1:105:A:SER:HB3	2	0.18	0.08	0.18
(1,117)	1:52:A:TYR:HD2	1:52:A:TYR:H	2	0.17	0.07	0.17
(1,5145)	1:52:A:TYR:HD2	1:52:A:TYR:H	2	0.17	0.07	0.17
(1,2977)	1:62:A:VAL:HB	1:62:A:VAL:HA	2	0.16	0.01	0.16
(1,2458)	1:171:A:VAL:HG12	1:174:A:GLN:H	2	0.16	0.01	0.16
(1,2458)	1:171:A:VAL:HG13	1:174:A:GLN:H	2	0.16	0.01	0.16
(1,5691)	1:22:A:PRO:HG3	1:23:A:ALA:H	2	0.16	0.0	0.16
(1,2257)	1:101:A:ILE:HA	1:100:A:GLU:H	2	0.16	0.04	0.16
(1,3846)	1:111:A:GLU:HG2	1:111:A:GLU:H	2	0.16	0.01	0.16
(1,3846)	1:111:A:GLU:HG3	1:111:A:GLU:H	2	0.16	0.01	0.16
(1,5041)	1:20:A:TRP:H	1:19:A:GLU:HG2	2	0.16	0.02	0.16
(1,5041)	1:20:A:TRP:H	1:19:A:GLU:HG3	2	0.16	0.02	0.16
(2,320)	1:118:A:GLU:CB	1:114:A:LEU:N	2	0.15	0.0	0.15
(1,34)	1:146:A:LYS:HB2	1:145:A:TYR:HD1	2	0.15	0.0	0.15
(1,34)	1:146:A:LYS:HB2	1:145:A:TYR:HD2	2	0.15	0.0	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,34)	1:146:A:LYS:HB3	1:145:A:TYR:HD1	2	0.15	0.0	0.15
(1,34)	1:146:A:LYS:HB3	1:145:A:TYR:HD2	2	0.15	0.0	0.15
(1,3849)	1:109:A:ASP:HB2	1:109:A:ASP:H	2	0.15	0.02	0.15
(1,3849)	1:109:A:ASP:HB3	1:109:A:ASP:H	2	0.15	0.02	0.15
(1,5845)	1:111:A:GLU:H	1:111:A:GLU:HA	2	0.15	0.0	0.15
(1,58)	1:96:A:MET:HB2	1:127:A:TYR:HD1	2	0.14	0.02	0.14
(1,58)	1:96:A:MET:HB2	1:127:A:TYR:HD2	2	0.14	0.02	0.14
(1,58)	1:96:A:MET:HB3	1:127:A:TYR:HD1	2	0.14	0.02	0.14
(1,58)	1:96:A:MET:HB3	1:127:A:TYR:HD2	2	0.14	0.02	0.14
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG11	2	0.14	0.04	0.14
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG12	2	0.14	0.04	0.14
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG13	2	0.14	0.04	0.14
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG21	2	0.14	0.04	0.14
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG22	2	0.14	0.04	0.14
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG23	2	0.14	0.04	0.14
(1,3669)	1:112:A:LYS:HB2	1:113:A:GLU:H	2	0.14	0.02	0.14
(1,3669)	1:112:A:LYS:HB3	1:113:A:GLU:H	2	0.14	0.02	0.14
(1,5546)	1:8:A:VAL:HB	1:8:A:VAL:H	2	0.14	0.02	0.14
(1,4775)	1:60:A:LYS:HG2	1:59:A:ILE:H	2	0.13	0.02	0.13
(1,4775)	1:60:A:LYS:HG3	1:59:A:ILE:H	2	0.13	0.02	0.13
(1,2630)	1:47:A:ILE:HD11	1:21:A:TYR:HB2	2	0.12	0.02	0.12
(1,2630)	1:47:A:ILE:HD11	1:21:A:TYR:HB3	2	0.12	0.02	0.12
(1,2839)	1:11:A:VAL:HG21	1:23:A:ALA:HA	2	0.12	0.02	0.12
(1,2839)	1:11:A:VAL:HG22	1:23:A:ALA:HA	2	0.12	0.02	0.12
(1,3774)	1:43:A:VAL:HG11	1:24:A:LEU:H	2	0.12	0.02	0.12
(1,3774)	1:43:A:VAL:HG12	1:24:A:LEU:H	2	0.12	0.02	0.12
(1,3774)	1:43:A:VAL:HG13	1:24:A:LEU:H	2	0.12	0.02	0.12
(1,3774)	1:43:A:VAL:HG21	1:24:A:LEU:H	2	0.12	0.02	0.12
(1,3774)	1:43:A:VAL:HG22	1:24:A:LEU:H	2	0.12	0.02	0.12
(1,3774)	1:43:A:VAL:HG23	1:24:A:LEU:H	2	0.12	0.02	0.12
(1,3982)	1:50:A:LYS:HD2	1:50:A:LYS:H	2	0.12	0.01	0.12
(1,3982)	1:50:A:LYS:HD3	1:50:A:LYS:H	2	0.12	0.01	0.12
(1,4745)	1:177:A:MET:HA	1:174:A:GLN:HE21	2	0.12	0.02	0.12
(1,4745)	1:177:A:MET:HA	1:174:A:GLN:HE22	2	0.12	0.02	0.12
(1,4922)	1:11:A:VAL:H	1:20:A:TRP:HD1	2	0.12	0.01	0.12
(2,36)	1:4:A:LEU:CB	1:210:A:ALA:N	2	0.12	0.02	0.12
(1,687)	1:2:A:ASP:H	1:61:A:GLU:HB2	2	0.12	0.01	0.12
(1,687)	1:2:A:ASP:H	1:61:A:GLU:HB3	2	0.12	0.01	0.12
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD11	2	0.12	0.01	0.12
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD12	2	0.12	0.01	0.12
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD13	2	0.12	0.01	0.12
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD21	2	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD22	2	0.12	0.01	0.12
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD23	2	0.12	0.01	0.12
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD11	2	0.12	0.01	0.12
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD12	2	0.12	0.01	0.12
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD13	2	0.12	0.01	0.12
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD21	2	0.12	0.01	0.12
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD22	2	0.12	0.01	0.12
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD23	2	0.12	0.01	0.12
(1,3927)	1:46:A:PHE:HE1	1:80:A:LYS:H	2	0.12	0.02	0.12
(1,3927)	1:46:A:PHE:HE2	1:80:A:LYS:H	2	0.12	0.02	0.12
(1,4956)	1:178:A:ASP:H	1:175:A:ILE:HG12	2	0.12	0.02	0.12
(1,4956)	1:178:A:ASP:H	1:175:A:ILE:HG13	2	0.12	0.02	0.12
(1,3486)	1:2:A:ASP:H	1:1:A:ASN:HB2	2	0.12	0.0	0.12
(1,3486)	1:2:A:ASP:H	1:1:A:ASN:HB3	2	0.12	0.0	0.12
(1,731)	1:148:A:LEU:H	1:142:A:VAL:HB	2	0.11	0.01	0.11
(1,955)	1:196:A:TYR:HE1	1:175:A:ILE:HG21	2	0.11	0.01	0.11
(1,955)	1:196:A:TYR:HE1	1:175:A:ILE:HG22	2	0.11	0.01	0.11
(1,955)	1:196:A:TYR:HE1	1:175:A:ILE:HG23	2	0.11	0.01	0.11
(1,955)	1:196:A:TYR:HE2	1:175:A:ILE:HG21	2	0.11	0.01	0.11
(1,955)	1:196:A:TYR:HE2	1:175:A:ILE:HG22	2	0.11	0.01	0.11
(1,955)	1:196:A:TYR:HE2	1:175:A:ILE:HG23	2	0.11	0.01	0.11
(1,4528)	1:205:A:GLU:HB2	1:29:A:SER:H	2	0.11	0.01	0.11
(1,4528)	1:205:A:GLU:HB3	1:29:A:SER:H	2	0.11	0.01	0.11
(1,5413)	1:170:A:ALA:H	1:168:A:SER:H	2	0.11	0.01	0.11
(4,59)	1:206:A:TYR:H	1:202:A:GLY:O	2	0.11	0.0	0.11
(1,3619)	1:15:A:THR:HG21	1:14:A:ALA:H	2	0.1	0.0	0.1
(1,3619)	1:15:A:THR:HG22	1:14:A:ALA:H	2	0.1	0.0	0.1
(1,3619)	1:15:A:THR:HG23	1:14:A:ALA:H	2	0.1	0.0	0.1

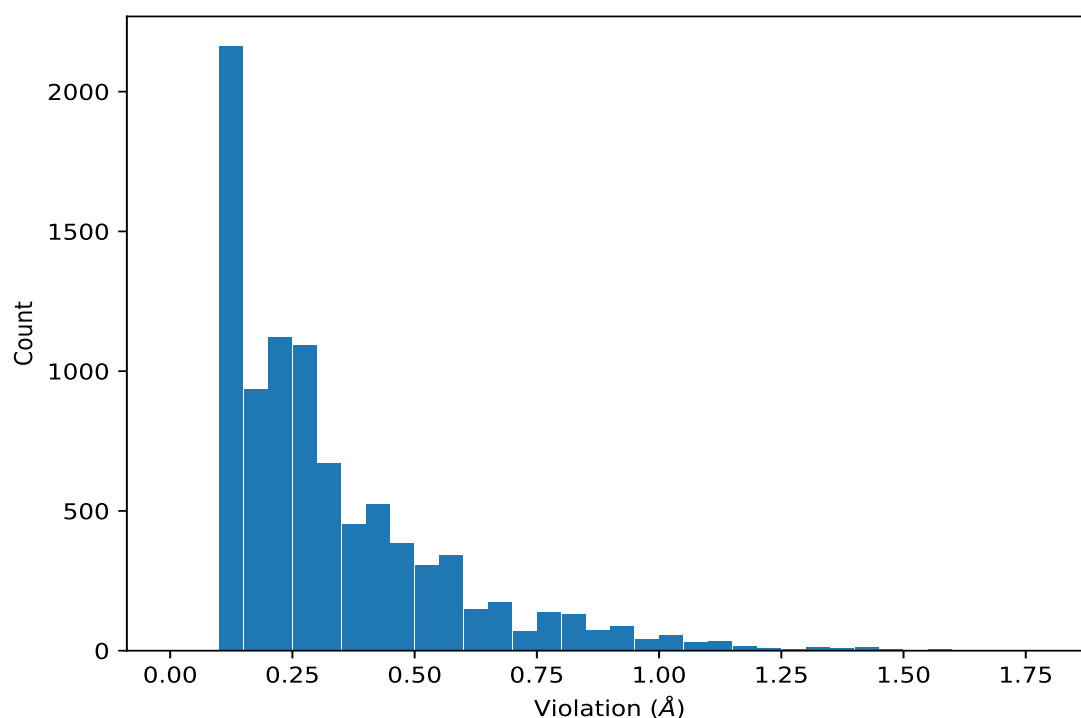
<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

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

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

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





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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5734)	1:54:A:ILE:HG21	1:11:A:VAL:H	19	1.78
(1,5734)	1:54:A:ILE:HG22	1:11:A:VAL:H	8	1.66
(1,5734)	1:54:A:ILE:HG21	1:60:A:LYS:H	20	1.64
(1,5734)	1:54:A:ILE:HG21	1:11:A:VAL:H	3	1.59
(1,2459)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	2	1.59
(1,2457)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	2	1.59
(1,2459)	1:90:A:VAL:HG13	1:94:A:TRP:HZ3	14	1.57
(1,2457)	1:90:A:VAL:HG13	1:94:A:TRP:HZ3	14	1.57
(1,5734)	1:54:A:ILE:HG22	1:11:A:VAL:H	14	1.56
(1,5734)	1:54:A:ILE:HG22	1:11:A:VAL:H	15	1.56
(1,2538)	1:183:A:ILE:HD11	1:172:A:TRP:HA	8	1.51
(1,5787)	1:98:A:ILE:HD13	1:100:A:GLU:H	7	1.5
(1,2538)	1:183:A:ILE:HD13	1:182:A:PRO:HA	20	1.49
(1,5734)	1:54:A:ILE:HG22	1:11:A:VAL:H	11	1.47
(1,2538)	1:183:A:ILE:HD12	1:182:A:PRO:HA	1	1.47
(1,2538)	1:183:A:ILE:HD13	1:184:A:LEU:HA	5	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2459)	1:90:A:VAL:HG13	1:94:A:TRP:HZ3	4	1.46
(1,2457)	1:90:A:VAL:HG13	1:94:A:TRP:HZ3	4	1.46
(1,5787)	1:98:A:ILE:HD11	1:100:A:GLU:H	4	1.45
(1,2538)	1:183:A:ILE:HD12	1:182:A:PRO:HA	6	1.45
(1,5787)	1:98:A:ILE:HD13	1:100:A:GLU:H	2	1.44
(1,5734)	1:54:A:ILE:HG23	1:60:A:LYS:H	2	1.43
(1,2459)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	1	1.43
(1,2457)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	1	1.43
(1,5734)	1:54:A:ILE:HG21	1:11:A:VAL:H	17	1.42
(1,2538)	1:183:A:ILE:HD12	1:182:A:PRO:HA	11	1.42
(1,2538)	1:183:A:ILE:HD12	1:172:A:TRP:HA	12	1.42
(1,2843)	1:181:A:ILE:HD11	1:153:A:LEU:HB2	8	1.41
(1,2843)	1:181:A:ILE:HD11	1:153:A:LEU:HB3	8	1.41
(1,2843)	1:181:A:ILE:HD13	1:182:A:PRO:HG2	16	1.39
(1,2843)	1:181:A:ILE:HD13	1:182:A:PRO:HG3	16	1.39
(1,5734)	1:54:A:ILE:HG22	1:53:A:SER:H	12	1.38
(1,2538)	1:183:A:ILE:HD13	1:182:A:PRO:HA	18	1.38
(1,5734)	1:54:A:ILE:HG21	1:11:A:VAL:H	13	1.37
(1,2459)	1:90:A:VAL:HG12	1:94:A:TRP:HZ3	5	1.37
(1,2457)	1:90:A:VAL:HG12	1:94:A:TRP:HZ3	5	1.37
(1,2538)	1:183:A:ILE:HD12	1:172:A:TRP:HA	15	1.36
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB2	3	1.34
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB3	3	1.34
(1,2538)	1:183:A:ILE:HD11	1:182:A:PRO:HA	3	1.34
(1,2538)	1:183:A:ILE:HD13	1:182:A:PRO:HA	10	1.34
(1,5787)	1:98:A:ILE:HD11	1:100:A:GLU:H	6	1.33
(1,2538)	1:183:A:ILE:HD11	1:182:A:PRO:HA	13	1.33
(1,5788)	1:98:A:ILE:HD13	1:97:A:ASP:HA	9	1.32
(1,5734)	1:54:A:ILE:HG21	1:11:A:VAL:H	1	1.32
(1,2848)	1:11:A:VAL:HG23	1:43:A:VAL:H	18	1.32
(1,5734)	1:54:A:ILE:HG22	1:11:A:VAL:H	16	1.31
(1,2920)	1:54:A:ILE:HD11	1:58:A:ASP:HA	20	1.31
(1,3339)	1:7:A:LYS:HB3	1:5:A:LEU:HG	19	1.3
(1,2920)	1:54:A:ILE:HD13	1:52:A:TYR:HA	16	1.3
(1,2539)	1:54:A:ILE:HD12	1:11:A:VAL:HA	12	1.3
(1,2606)	1:64:A:ILE:HD13	1:82:A:SER:HA	6	1.29
(1,5787)	1:98:A:ILE:HD13	1:100:A:GLU:H	11	1.28
(1,2538)	1:183:A:ILE:HD12	1:182:A:PRO:HA	19	1.28
(1,2606)	1:64:A:ILE:HD11	1:78:A:LEU:HA	2	1.27
(1,5787)	1:98:A:ILE:HD11	1:103:A:GLU:H	8	1.26
(1,5787)	1:98:A:ILE:HD11	1:103:A:GLU:H	15	1.24
(1,2692)	1:195:A:ALA:HB2	1:153:A:LEU:HG	1	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5734)	1:54:A:ILE:HG23	1:11:A:VAL:H	7	1.23
(1,2920)	1:54:A:ILE:HD12	1:52:A:TYR:HA	3	1.23
(1,2539)	1:54:A:ILE:HD11	1:14:A:ALA:HA	20	1.23
(1,167)	1:176:A:TYR:HE1	1:177:A:MET:H	1	1.23
(1,5734)	1:54:A:ILE:HG23	1:60:A:LYS:H	10	1.22
(1,2539)	1:54:A:ILE:HD13	1:14:A:ALA:HA	15	1.22
(1,167)	1:176:A:TYR:HE1	1:177:A:MET:H	13	1.22
(1,167)	1:176:A:TYR:HE1	1:177:A:MET:H	16	1.21
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG11	9	1.2
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG12	9	1.2
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG13	9	1.2
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG21	9	1.2
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG22	9	1.2
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG23	9	1.2
(1,3379)	1:7:A:LYS:HG3	1:61:A:GLU:HG2	18	1.2
(1,3379)	1:7:A:LYS:HG3	1:61:A:GLU:HG3	18	1.2
(1,167)	1:176:A:TYR:HE2	1:177:A:MET:H	10	1.19
(1,167)	1:176:A:TYR:HE1	1:177:A:MET:H	20	1.19
(1,5678)	1:137:A:ILE:HD11	1:130:A:MET:H	2	1.17
(1,2920)	1:54:A:ILE:HD11	1:52:A:TYR:HA	13	1.17
(1,2920)	1:54:A:ILE:HD12	1:58:A:ASP:HA	17	1.17
(1,2459)	1:90:A:VAL:HG23	1:66:A:ASN:H	17	1.17
(1,2457)	1:90:A:VAL:HG23	1:66:A:ASN:H	17	1.17
(1,167)	1:176:A:TYR:HE1	1:177:A:MET:H	15	1.16
(1,5787)	1:98:A:ILE:HD13	1:100:A:GLU:H	14	1.15
(1,5734)	1:54:A:ILE:HG22	1:11:A:VAL:H	9	1.15
(1,2534)	1:101:A:ILE:HG23	1:140:A:PRO:HA	5	1.15
(1,167)	1:176:A:TYR:HE1	1:177:A:MET:H	18	1.15
(1,5734)	1:54:A:ILE:HG22	1:11:A:VAL:H	6	1.14
(1,2843)	1:181:A:ILE:HD13	1:182:A:PRO:HG2	20	1.14
(1,2843)	1:181:A:ILE:HD13	1:182:A:PRO:HG3	20	1.14
(1,167)	1:176:A:TYR:HE1	1:145:A:TYR:H	5	1.14
(1,5787)	1:98:A:ILE:HD12	1:100:A:GLU:H	18	1.13
(1,2606)	1:64:A:ILE:HD13	1:82:A:SER:HA	13	1.13
(1,2459)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	19	1.13
(1,2457)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	19	1.13
(1,5787)	1:98:A:ILE:HD13	1:100:A:GLU:H	1	1.12
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD21	2	1.12
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD22	2	1.12
(1,2920)	1:54:A:ILE:HD11	1:52:A:TYR:HA	1	1.12
(1,2543)	1:64:A:ILE:HG12	1:62:A:VAL:HA	18	1.12
(1,2539)	1:54:A:ILE:HD11	1:14:A:ALA:HA	4	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2491)	1:43:A:VAL:HG13	1:52:A:TYR:HD1	18	1.12
(1,2491)	1:43:A:VAL:HG13	1:52:A:TYR:HD2	18	1.12
(1,167)	1:176:A:TYR:HE2	1:177:A:MET:H	2	1.12
(1,5734)	1:54:A:ILE:HG22	1:53:A:SER:H	4	1.11
(1,2843)	1:181:A:ILE:HD11	1:153:A:LEU:HB2	12	1.11
(1,2843)	1:181:A:ILE:HD11	1:153:A:LEU:HB3	12	1.11
(1,2543)	1:64:A:ILE:HG12	1:65:A:LEU:HA	8	1.11
(1,2543)	1:64:A:ILE:HG12	1:62:A:VAL:HA	14	1.11
(1,2534)	1:101:A:ILE:HG23	1:105:A:SER:HA	17	1.11
(1,5678)	1:137:A:ILE:HD12	1:130:A:MET:H	10	1.1
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG11	14	1.1
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG12	14	1.1
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG13	14	1.1
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG21	14	1.1
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG22	14	1.1
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG23	14	1.1
(1,2543)	1:64:A:ILE:HG12	1:62:A:VAL:HA	7	1.1
(1,3379)	1:7:A:LYS:HG3	1:61:A:GLU:HG2	15	1.09
(1,3379)	1:7:A:LYS:HG3	1:61:A:GLU:HG3	15	1.09
(1,3339)	1:7:A:LYS:HB3	1:5:A:LEU:HG	20	1.09
(1,2920)	1:54:A:ILE:HD13	1:52:A:TYR:HA	8	1.09
(1,2920)	1:54:A:ILE:HD11	1:58:A:ASP:HA	11	1.09
(1,2843)	1:181:A:ILE:HD12	1:182:A:PRO:HG2	1	1.09
(1,2843)	1:181:A:ILE:HD12	1:182:A:PRO:HG3	1	1.09
(1,5678)	1:137:A:ILE:HD13	1:130:A:MET:H	18	1.08
(1,5558)	1:9:A:VAL:HG11	1:8:A:VAL:H	14	1.08
(1,2908)	1:137:A:ILE:HD13	1:130:A:MET:H	18	1.08
(1,2543)	1:64:A:ILE:HG13	1:62:A:VAL:HA	5	1.08
(1,167)	1:176:A:TYR:HE2	1:177:A:MET:H	6	1.08
(1,5787)	1:98:A:ILE:HD13	1:103:A:GLU:H	19	1.07
(1,5678)	1:137:A:ILE:HD13	1:130:A:MET:H	9	1.07
(1,2848)	1:11:A:VAL:HG22	1:43:A:VAL:H	7	1.07
(1,2708)	1:137:A:ILE:HD12	1:139:A:LYS:HB2	13	1.07
(1,2708)	1:137:A:ILE:HD12	1:139:A:LYS:HB3	13	1.07
(1,2692)	1:195:A:ALA:HB3	1:153:A:LEU:HG	4	1.07
(1,167)	1:176:A:TYR:HE1	1:177:A:MET:H	11	1.07
(1,5787)	1:98:A:ILE:HD12	1:100:A:GLU:H	12	1.06
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	2	1.06
(1,3379)	1:75:A:LYS:HG2	1:19:A:GLU:HG2	8	1.06
(1,3379)	1:75:A:LYS:HG2	1:19:A:GLU:HG3	8	1.06
(1,2692)	1:195:A:ALA:HB3	1:150:A:LEU:HB2	20	1.06
(1,2692)	1:195:A:ALA:HB3	1:150:A:LEU:HB3	20	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2543)	1:64:A:ILE:HG12	1:65:A:LEU:HA	19	1.06
(1,2848)	1:11:A:VAL:HG21	1:43:A:VAL:H	6	1.05
(1,2692)	1:195:A:ALA:HB1	1:153:A:LEU:HG	6	1.05
(1,2692)	1:195:A:ALA:HB1	1:150:A:LEU:HB2	14	1.05
(1,2692)	1:195:A:ALA:HB1	1:150:A:LEU:HB3	14	1.05
(1,2534)	1:101:A:ILE:HG21	1:140:A:PRO:HA	6	1.05
(1,5678)	1:137:A:ILE:HD13	1:130:A:MET:H	1	1.04
(1,5678)	1:137:A:ILE:HD13	1:130:A:MET:H	13	1.04
(1,2920)	1:54:A:ILE:HD11	1:58:A:ASP:HA	12	1.04
(1,2908)	1:137:A:ILE:HD13	1:130:A:MET:H	1	1.04
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD1	19	1.04
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD2	19	1.04
(1,2843)	1:181:A:ILE:HD11	1:153:A:LEU:HB2	7	1.04
(1,2843)	1:181:A:ILE:HD11	1:153:A:LEU:HB3	7	1.04
(1,2692)	1:195:A:ALA:HB3	1:150:A:LEU:HB2	13	1.04
(1,2692)	1:195:A:ALA:HB3	1:150:A:LEU:HB3	13	1.04
(1,2692)	1:195:A:ALA:HB2	1:150:A:LEU:HB2	19	1.04
(1,2692)	1:195:A:ALA:HB2	1:150:A:LEU:HB3	19	1.04
(1,2543)	1:64:A:ILE:HG12	1:65:A:LEU:HA	1	1.04
(1,2536)	1:181:A:ILE:HD11	1:179:A:LEU:HA	13	1.04
(1,2482)	1:175:A:ILE:HD13	1:174:A:GLN:H	20	1.04
(1,167)	1:176:A:TYR:HE2	1:177:A:MET:H	19	1.04
(1,5788)	1:98:A:ILE:HD11	1:97:A:ASP:HA	17	1.03
(1,5678)	1:137:A:ILE:HD12	1:130:A:MET:H	8	1.03
(1,2920)	1:54:A:ILE:HD12	1:58:A:ASP:HA	7	1.03
(1,2920)	1:54:A:ILE:HD11	1:52:A:TYR:HA	19	1.03
(1,2908)	1:137:A:ILE:HD12	1:130:A:MET:H	8	1.03
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB2	6	1.03
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB3	6	1.03
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB2	17	1.03
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB3	17	1.03
(1,2606)	1:64:A:ILE:HD12	1:78:A:LEU:HA	16	1.03
(1,2543)	1:64:A:ILE:HG13	1:62:A:VAL:HA	15	1.03
(1,2383)	1:43:A:VAL:HG21	1:52:A:TYR:H	15	1.03
(1,167)	1:176:A:TYR:HE1	1:177:A:MET:H	8	1.03
(1,5787)	1:98:A:ILE:HD13	1:100:A:GLU:H	10	1.02
(1,5558)	1:9:A:VAL:HG11	1:8:A:VAL:H	9	1.02
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG11	6	1.02
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG12	6	1.02
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG13	6	1.02
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG21	6	1.02
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG22	6	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG23	6	1.02
(1,2692)	1:195:A:ALA:HB1	1:153:A:LEU:HG	16	1.02
(1,2543)	1:64:A:ILE:HG12	1:65:A:LEU:HA	3	1.02
(1,2538)	1:183:A:ILE:HD11	1:182:A:PRO:HA	2	1.02
(1,2529)	1:5:A:LEU:HD12	1:2:A:ASP:HA	3	1.02
(1,167)	1:176:A:TYR:HE2	1:145:A:TYR:H	14	1.02
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD21	20	1.01
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD22	20	1.01
(1,2828)	1:137:A:ILE:HB	1:101:A:ILE:HA	3	1.01
(1,2539)	1:54:A:ILE:HD13	1:14:A:ALA:HA	13	1.01
(1,2459)	1:90:A:VAL:HG11	1:94:A:TRP:HZ3	9	1.01
(1,2457)	1:90:A:VAL:HG11	1:94:A:TRP:HZ3	9	1.01
(1,2848)	1:11:A:VAL:HG21	1:44:A:ARG:H	5	1.0
(1,2843)	1:181:A:ILE:HD12	1:182:A:PRO:HG2	14	1.0
(1,2843)	1:181:A:ILE:HD12	1:182:A:PRO:HG3	14	1.0
(1,2660)	1:65:A:LEU:HD11	1:63:A:ASP:HB2	8	1.0
(1,2660)	1:65:A:LEU:HD11	1:63:A:ASP:HB3	8	1.0
(1,2482)	1:175:A:ILE:HD13	1:174:A:GLN:H	6	1.0
(1,2375)	1:60:A:LYS:HD3	1:11:A:VAL:H	19	1.0
(1,5787)	1:98:A:ILE:HD13	1:100:A:GLU:H	9	0.99
(1,5665)	1:200:A:LEU:HB3	1:205:A:GLU:H	15	0.99
(1,3436)	1:12:A:VAL:HG12	1:60:A:LYS:HE2	2	0.99
(1,3436)	1:12:A:VAL:HG12	1:60:A:LYS:HE3	2	0.99
(1,3435)	1:12:A:VAL:HG12	1:60:A:LYS:HE2	2	0.99
(1,3435)	1:12:A:VAL:HG12	1:60:A:LYS:HE3	2	0.99
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	20	0.99
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	20	0.99
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	20	0.99
(1,2920)	1:54:A:ILE:HD13	1:52:A:TYR:HA	2	0.99
(1,2543)	1:64:A:ILE:HG12	1:65:A:LEU:HA	12	0.99
(1,2539)	1:54:A:ILE:HD12	1:14:A:ALA:HA	7	0.99
(1,2539)	1:54:A:ILE:HD12	1:11:A:VAL:HA	16	0.99
(1,2534)	1:101:A:ILE:HG21	1:105:A:SER:HA	15	0.99
(1,5558)	1:12:A:VAL:HG12	1:17:A:ARG:H	3	0.98
(1,2848)	1:11:A:VAL:HG23	1:43:A:VAL:H	13	0.98
(1,2539)	1:54:A:ILE:HD13	1:14:A:ALA:HA	1	0.98
(1,2482)	1:175:A:ILE:HD11	1:174:A:GLN:H	17	0.98
(1,5787)	1:98:A:ILE:HD12	1:100:A:GLU:H	3	0.97
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD21	12	0.97
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD22	12	0.97
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD21	16	0.97
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD22	16	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD21	19	0.97
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD22	19	0.97
(1,2692)	1:195:A:ALA:HB1	1:153:A:LEU:HG	2	0.97
(1,2535)	1:101:A:ILE:HD12	1:97:A:ASP:HA	6	0.97
(1,2482)	1:175:A:ILE:HD13	1:174:A:GLN:H	1	0.97
(1,2461)	1:64:A:ILE:HD11	1:66:A:ASN:H	6	0.97
(1,2459)	1:90:A:VAL:HG11	1:94:A:TRP:HZ3	7	0.97
(1,2457)	1:90:A:VAL:HG11	1:94:A:TRP:HZ3	7	0.97
(1,167)	1:176:A:TYR:HE1	1:145:A:TYR:H	12	0.97
(1,5678)	1:137:A:ILE:HD11	1:130:A:MET:H	20	0.96
(1,5558)	1:9:A:VAL:HG13	1:8:A:VAL:H	5	0.96
(1,5558)	1:9:A:VAL:HG12	1:8:A:VAL:H	13	0.96
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	13	0.96
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	13	0.96
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	13	0.96
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	13	0.96
(1,2908)	1:137:A:ILE:HD11	1:130:A:MET:H	20	0.96
(1,2577)	1:166:A:ILE:HD11	1:160:A:GLN:HA	1	0.96
(1,2482)	1:175:A:ILE:HD13	1:172:A:TRP:HZ2	10	0.96
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD21	6	0.95
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD22	6	0.95
(1,5558)	1:12:A:VAL:HG12	1:17:A:ARG:H	10	0.95
(1,2920)	1:54:A:ILE:HD11	1:58:A:ASP:HA	4	0.95
(1,2596)	1:90:A:VAL:HG21	1:85:A:LEU:HA	14	0.95
(1,2543)	1:64:A:ILE:HG12	1:65:A:LEU:HA	4	0.95
(1,2442)	1:101:A:ILE:HD13	1:100:A:GLU:H	2	0.95
(1,5788)	1:98:A:ILE:HD12	1:105:A:SER:HA	4	0.94
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	9	0.94
(1,5558)	1:9:A:VAL:HG13	1:8:A:VAL:H	7	0.94
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG11	16	0.94
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG12	16	0.94
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG13	16	0.94
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG21	16	0.94
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG22	16	0.94
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG23	16	0.94
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD1	3	0.94
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD2	3	0.94
(1,2708)	1:137:A:ILE:HD13	1:140:A:PRO:HB2	20	0.94
(1,2708)	1:137:A:ILE:HD13	1:140:A:PRO:HB3	20	0.94
(1,2606)	1:64:A:ILE:HD13	1:78:A:LEU:HA	5	0.94
(1,2543)	1:64:A:ILE:HG12	1:62:A:VAL:HA	10	0.94
(1,2482)	1:175:A:ILE:HD13	1:174:A:GLN:H	3	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2459)	1:90:A:VAL:HG13	1:94:A:TRP:HZ3	11	0.94
(1,2457)	1:90:A:VAL:HG13	1:94:A:TRP:HZ3	11	0.94
(1,2375)	1:60:A:LYS:HD3	1:61:A:GLU:H	13	0.94
(1,167)	1:176:A:TYR:HE1	1:177:A:MET:H	4	0.94
(1,167)	1:176:A:TYR:HE2	1:177:A:MET:H	7	0.94
(1,5812)	1:64:A:ILE:HD12	1:8:A:VAL:HB	11	0.93
(1,5812)	1:9:A:VAL:HG11	1:8:A:VAL:HB	14	0.93
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	1	0.93
(1,5558)	1:9:A:VAL:HG12	1:8:A:VAL:H	8	0.93
(1,2884)	1:61:A:GLU:HG2	1:3:A:GLU:HA	16	0.93
(1,2708)	1:137:A:ILE:HD13	1:140:A:PRO:HB2	12	0.93
(1,2708)	1:137:A:ILE:HD13	1:140:A:PRO:HB3	12	0.93
(1,2539)	1:54:A:ILE:HD11	1:14:A:ALA:HA	11	0.93
(1,2534)	1:101:A:ILE:HG21	1:140:A:PRO:HA	7	0.93
(1,2534)	1:101:A:ILE:HG21	1:105:A:SER:HA	14	0.93
(1,2534)	1:101:A:ILE:HG21	1:140:A:PRO:HA	18	0.93
(1,2482)	1:175:A:ILE:HD13	1:174:A:GLN:H	5	0.93
(1,2482)	1:175:A:ILE:HD11	1:174:A:GLN:H	9	0.93
(1,2482)	1:175:A:ILE:HD12	1:174:A:GLN:H	19	0.93
(1,2383)	1:43:A:VAL:HG23	1:52:A:TYR:H	19	0.93
(1,5812)	1:64:A:ILE:HD12	1:8:A:VAL:HB	19	0.92
(1,5547)	1:100:A:GLU:HG2	1:100:A:GLU:H	2	0.92
(1,3448)	1:101:A:ILE:HG13	1:96:A:MET:HG2	14	0.92
(1,3448)	1:101:A:ILE:HG13	1:96:A:MET:HG3	14	0.92
(1,2577)	1:166:A:ILE:HD12	1:160:A:GLN:HA	18	0.92
(1,2535)	1:101:A:ILE:HD13	1:97:A:ASP:HA	14	0.92
(1,2482)	1:175:A:ILE:HD12	1:174:A:GLN:H	15	0.92
(1,2459)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	15	0.92
(1,2457)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	15	0.92
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD21	17	0.91
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD22	17	0.91
(1,5558)	1:9:A:VAL:HG12	1:8:A:VAL:H	1	0.91
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG12	11	0.91
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG13	11	0.91
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG12	13	0.91
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG13	13	0.91
(1,3063)	1:56:A:ARG:H	1:59:A:ILE:HG21	2	0.91
(1,3063)	1:56:A:ARG:H	1:59:A:ILE:HG22	2	0.91
(1,3063)	1:56:A:ARG:H	1:59:A:ILE:HG23	2	0.91
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	7	0.91
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	7	0.91
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	7	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2920)	1:54:A:ILE:HD12	1:52:A:TYR:HA	14	0.91
(1,2920)	1:54:A:ILE:HD13	1:58:A:ASP:HA	15	0.91
(1,2848)	1:11:A:VAL:HG21	1:44:A:ARG:H	11	0.91
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB2	13	0.91
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB3	13	0.91
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB2	18	0.91
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB3	18	0.91
(1,2543)	1:64:A:ILE:HG12	1:62:A:VAL:HA	20	0.91
(1,2534)	1:101:A:ILE:HG22	1:105:A:SER:HA	1	0.91
(1,5850)	1:113:A:GLU:HG2	1:114:A:LEU:H	10	0.9
(1,5678)	1:137:A:ILE:HD12	1:130:A:MET:H	15	0.9
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	4	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD11	8	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD12	8	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD13	8	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD21	8	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD22	8	0.9
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD23	8	0.9
(1,3544)	1:198:A:LYS:HE2	1:137:A:ILE:HA	13	0.9
(1,2908)	1:137:A:ILE:HD12	1:130:A:MET:H	15	0.9
(1,2848)	1:11:A:VAL:HG22	1:43:A:VAL:H	2	0.9
(1,2482)	1:175:A:ILE:HD11	1:174:A:GLN:H	8	0.9
(1,2482)	1:175:A:ILE:HD13	1:174:A:GLN:H	16	0.9
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD21	11	0.89
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD22	11	0.89
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD21	18	0.89
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD22	18	0.89
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD1	14	0.89
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD2	14	0.89
(1,2848)	1:11:A:VAL:HG22	1:44:A:ARG:H	10	0.89
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB2	18	0.89
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB3	18	0.89
(1,2841)	1:166:A:ILE:HD11	1:159:A:HIS:H	5	0.89
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG11	5	0.89
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG12	5	0.89
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG13	5	0.89
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG21	5	0.89
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG22	5	0.89
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG23	5	0.89
(1,2571)	1:130:A:MET:HE3	1:136:A:PRO:HA	7	0.89
(1,2539)	1:54:A:ILE:HD11	1:14:A:ALA:HA	3	0.89
(1,2482)	1:175:A:ILE:HD13	1:174:A:GLN:H	14	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2459)	1:90:A:VAL:HG22	1:94:A:TRP:HZ3	20	0.89
(1,2457)	1:90:A:VAL:HG22	1:94:A:TRP:HZ3	20	0.89
(1,2442)	1:101:A:ILE:HD11	1:100:A:GLU:H	8	0.89
(1,2375)	1:60:A:LYS:HD3	1:61:A:GLU:H	16	0.89
(1,5678)	1:137:A:ILE:HD13	1:130:A:MET:H	3	0.88
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD21	14	0.88
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD22	14	0.88
(1,5556)	1:197:A:ARG:HB3	1:201:A:TYR:H	3	0.88
(1,3379)	1:7:A:LYS:HG3	1:61:A:GLU:HG2	11	0.88
(1,3379)	1:7:A:LYS:HG3	1:61:A:GLU:HG3	11	0.88
(1,2908)	1:137:A:ILE:HD13	1:130:A:MET:H	3	0.88
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG21	10	0.88
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG22	10	0.88
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG23	10	0.88
(1,2657)	1:12:A:VAL:HG23	1:58:A:ASP:HB2	13	0.88
(1,2657)	1:12:A:VAL:HG23	1:58:A:ASP:HB3	13	0.88
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB2	14	0.88
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB3	14	0.88
(1,2482)	1:175:A:ILE:HD11	1:174:A:GLN:H	4	0.88
(1,2482)	1:175:A:ILE:HD12	1:174:A:GLN:H	7	0.88
(1,2482)	1:175:A:ILE:HD12	1:174:A:GLN:H	18	0.88
(1,5678)	1:137:A:ILE:HD13	1:130:A:MET:H	11	0.87
(1,5625)	1:64:A:ILE:HG12	1:82:A:SER:H	16	0.87
(1,2908)	1:137:A:ILE:HD13	1:130:A:MET:H	11	0.87
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD1	11	0.87
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD2	11	0.87
(1,2543)	1:64:A:ILE:HG13	1:62:A:VAL:HA	16	0.87
(1,2539)	1:54:A:ILE:HD12	1:11:A:VAL:HA	6	0.87
(1,2442)	1:101:A:ILE:HD12	1:100:A:GLU:H	6	0.87
(1,2375)	1:60:A:LYS:HD3	1:11:A:VAL:H	12	0.87
(1,5734)	1:54:A:ILE:HG23	1:53:A:SER:H	5	0.86
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD21	3	0.86
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD22	3	0.86
(1,5557)	1:128:A:LYS:HG2	1:95:A:LYS:H	17	0.86
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD1	5	0.86
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD2	5	0.86
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD1	8	0.86
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD2	8	0.86
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD1	9	0.86
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD2	9	0.86
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB2	4	0.86
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB3	4	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	11	0.86
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	11	0.86
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	20	0.86
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	20	0.86
(1,2649)	1:64:A:ILE:HD11	1:63:A:ASP:HB2	8	0.86
(1,2649)	1:64:A:ILE:HD11	1:63:A:ASP:HB3	8	0.86
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB2	12	0.86
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB3	12	0.86
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB2	19	0.86
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB3	19	0.86
(1,2543)	1:64:A:ILE:HG13	1:62:A:VAL:HA	2	0.86
(1,2442)	1:101:A:ILE:HD12	1:100:A:GLU:H	14	0.86
(1,5812)	1:9:A:VAL:HG11	1:8:A:VAL:HB	10	0.85
(1,3399)	1:64:A:ILE:HG12	1:62:A:VAL:HB	12	0.85
(1,2920)	1:54:A:ILE:HD11	1:58:A:ASP:HA	5	0.85
(1,2903)	1:11:A:VAL:HG11	1:54:A:ILE:HB	9	0.85
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD1	12	0.85
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD2	12	0.85
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD1	17	0.85
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD2	17	0.85
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG21	4	0.85
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG22	4	0.85
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG23	4	0.85
(1,2660)	1:65:A:LEU:HD11	1:63:A:ASP:HB2	10	0.85
(1,2660)	1:65:A:LEU:HD11	1:63:A:ASP:HB3	10	0.85
(1,2538)	1:183:A:ILE:HD13	1:182:A:PRO:HA	14	0.85
(1,2536)	1:181:A:ILE:HD12	1:179:A:LEU:HA	4	0.85
(1,2461)	1:64:A:ILE:HD13	1:66:A:ASN:H	17	0.85
(1,2373)	1:26:A:ILE:HD13	1:43:A:VAL:H	20	0.85
(1,167)	1:176:A:TYR:HE2	1:145:A:TYR:H	17	0.85
(1,5788)	1:98:A:ILE:HD12	1:121:A:ASN:HA	1	0.84
(1,5678)	1:137:A:ILE:HD11	1:130:A:MET:H	5	0.84
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD21	4	0.84
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD22	4	0.84
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD21	5	0.84
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD22	5	0.84
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD21	7	0.84
(1,5654)	1:53:A:SER:HA	1:31:A:ASN:HD22	7	0.84
(1,5556)	1:96:A:MET:HB2	1:95:A:LYS:H	12	0.84
(1,2908)	1:137:A:ILE:HD11	1:130:A:MET:H	5	0.84
(1,2905)	1:126:A:LEU:HD13	1:199:A:TYR:HD1	6	0.84
(1,2905)	1:126:A:LEU:HD13	1:199:A:TYR:HD2	6	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2905)	1:126:A:LEU:HD11	1:199:A:TYR:HD1	9	0.84
(1,2905)	1:126:A:LEU:HD11	1:199:A:TYR:HD2	9	0.84
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD1	16	0.84
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD2	16	0.84
(1,2848)	1:11:A:VAL:HG21	1:43:A:VAL:H	1	0.84
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB2	4	0.84
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB3	4	0.84
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	1	0.84
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	1	0.84
(1,2692)	1:195:A:ALA:HB1	1:153:A:LEU:HG	8	0.84
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB2	1	0.84
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB3	1	0.84
(1,2578)	1:64:A:ILE:HD13	1:62:A:VAL:HA	12	0.84
(1,2535)	1:101:A:ILE:HD13	1:97:A:ASP:HA	7	0.84
(1,2534)	1:101:A:ILE:HG22	1:140:A:PRO:HA	16	0.84
(1,2482)	1:175:A:ILE:HD13	1:174:A:GLN:H	13	0.84
(1,2375)	1:60:A:LYS:HD3	1:11:A:VAL:H	3	0.84
(1,5665)	1:50:A:LYS:HB2	1:133:A:ARG:H	5	0.83
(1,5665)	1:50:A:LYS:HB2	1:133:A:ARG:H	6	0.83
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB2	11	0.83
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB3	11	0.83
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB2	11	0.83
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB3	11	0.83
(1,3439)	1:42:A:LEU:HG	1:31:A:ASN:HB2	3	0.83
(1,3439)	1:42:A:LEU:HG	1:31:A:ASN:HB3	3	0.83
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	19	0.83
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	19	0.83
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	19	0.83
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	19	0.83
(1,3339)	1:123:A:LEU:HB3	1:150:A:LEU:HG	3	0.83
(1,3144)	1:20:A:TRP:HD1	1:16:A:GLU:HG2	20	0.83
(1,3144)	1:20:A:TRP:HD1	1:16:A:GLU:HG3	20	0.83
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD1	13	0.83
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD2	13	0.83
(1,2696)	1:181:A:ILE:HB	1:183:A:ILE:HB	19	0.83
(1,2577)	1:166:A:ILE:HD11	1:160:A:GLN:HA	7	0.83
(1,2549)	1:36:A:VAL:HG21	1:37:A:LYS:HA	8	0.83
(1,2543)	1:64:A:ILE:HG13	1:62:A:VAL:HA	6	0.83
(1,2543)	1:64:A:ILE:HG12	1:65:A:LEU:HA	11	0.83
(1,2530)	1:36:A:VAL:HG21	1:37:A:LYS:HA	8	0.83
(1,2466)	1:60:A:LYS:HD3	1:17:A:ARG:HE	14	0.83
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG11	18	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG12	18	0.83
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG13	18	0.83
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG21	18	0.83
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG22	18	0.83
(1,161)	1:52:A:TYR:HE1	1:11:A:VAL:HG23	18	0.83
(1,2908)	1:137:A:ILE:HD12	1:199:A:TYR:H	10	0.82
(1,2905)	1:126:A:LEU:HD12	1:199:A:TYR:HD1	18	0.82
(1,2905)	1:126:A:LEU:HD12	1:199:A:TYR:HD2	18	0.82
(1,2835)	1:126:A:LEU:HD13	1:125:A:GLN:H	17	0.82
(1,2543)	1:64:A:ILE:HG12	1:65:A:LEU:HA	9	0.82
(1,2459)	1:90:A:VAL:HG21	1:94:A:TRP:HZ3	18	0.82
(1,2457)	1:90:A:VAL:HG21	1:94:A:TRP:HZ3	18	0.82
(1,2422)	1:126:A:LEU:HD13	1:125:A:GLN:H	17	0.82
(1,2373)	1:26:A:ILE:HD12	1:43:A:VAL:H	7	0.82
(1,5787)	1:98:A:ILE:HD11	1:100:A:GLU:H	16	0.81
(1,5787)	1:98:A:ILE:HD11	1:100:A:GLU:H	17	0.81
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	12	0.81
(1,3016)	1:157:A:VAL:HG12	1:156:A:LEU:HA	19	0.81
(1,2908)	1:137:A:ILE:HD13	1:199:A:TYR:H	9	0.81
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD1	6	0.81
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD2	6	0.81
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD1	20	0.81
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD2	20	0.81
(1,2848)	1:11:A:VAL:HG23	1:44:A:ARG:H	8	0.81
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB2	11	0.81
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB3	11	0.81
(1,2596)	1:90:A:VAL:HG23	1:85:A:LEU:HA	9	0.81
(1,2536)	1:181:A:ILE:HD11	1:179:A:LEU:HA	17	0.81
(1,2489)	1:87:A:THR:HG22	1:89:A:VAL:H	19	0.81
(1,2375)	1:60:A:LYS:HD3	1:61:A:GLU:H	17	0.81
(1,5812)	1:9:A:VAL:HG12	1:8:A:VAL:HB	12	0.8
(1,5812)	1:9:A:VAL:HG21	1:8:A:VAL:HB	18	0.8
(1,5734)	1:54:A:ILE:HG22	1:11:A:VAL:H	18	0.8
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	7	0.8
(1,5558)	1:12:A:VAL:HG12	1:17:A:ARG:H	2	0.8
(1,5558)	1:9:A:VAL:HG13	1:8:A:VAL:H	16	0.8
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD11	1	0.8
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD12	1	0.8
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD13	1	0.8
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD21	1	0.8
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD22	1	0.8
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD23	1	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	12	0.8
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	12	0.8
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	12	0.8
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	12	0.8
(1,3399)	1:64:A:ILE:HG12	1:62:A:VAL:HB	8	0.8
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	2	0.8
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	2	0.8
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD1	18	0.8
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD2	18	0.8
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB2	10	0.8
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB3	10	0.8
(1,2657)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	12	0.8
(1,2657)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	12	0.8
(1,2538)	1:183:A:ILE:HD11	1:182:A:PRO:HA	4	0.8
(1,2536)	1:181:A:ILE:HD13	1:179:A:LEU:HA	6	0.8
(1,2535)	1:101:A:ILE:HD12	1:97:A:ASP:HA	13	0.8
(1,2461)	1:64:A:ILE:HD11	1:66:A:ASN:H	15	0.8
(1,2373)	1:26:A:ILE:HD13	1:44:A:ARG:H	8	0.8
(1,5812)	1:9:A:VAL:HG22	1:8:A:VAL:HB	20	0.79
(1,5697)	1:124:A:GLN:HB2	1:121:A:ASN:HD21	8	0.79
(1,5697)	1:124:A:GLN:HB2	1:121:A:ASN:HD22	8	0.79
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	12	0.79
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	12	0.79
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	12	0.79
(1,2920)	1:54:A:ILE:HD12	1:58:A:ASP:HA	10	0.79
(1,2905)	1:126:A:LEU:HD12	1:199:A:TYR:HD1	1	0.79
(1,2905)	1:126:A:LEU:HD12	1:199:A:TYR:HD2	1	0.79
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD1	10	0.79
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD2	10	0.79
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD1	15	0.79
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD2	15	0.79
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG21	5	0.79
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG22	5	0.79
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG23	5	0.79
(1,2685)	1:67:A:LEU:HD11	1:71:A:GLU:HB2	9	0.79
(1,2685)	1:67:A:LEU:HD11	1:71:A:GLU:HB3	9	0.79
(1,2535)	1:101:A:ILE:HD11	1:97:A:ASP:HA	1	0.79
(1,5788)	1:98:A:ILE:HD11	1:105:A:SER:HA	7	0.78
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	8	0.78
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD21	1	0.78
(1,5654)	1:51:A:PHE:HA	1:31:A:ASN:HD22	1	0.78
(1,3516)	1:22:A:PRO:HG2	1:46:A:PHE:HB2	14	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3516)	1:22:A:PRO:HG2	1:46:A:PHE:HB3	14	0.78
(1,3516)	1:22:A:PRO:HG3	1:46:A:PHE:HB2	14	0.78
(1,3516)	1:22:A:PRO:HG3	1:46:A:PHE:HB3	14	0.78
(1,3516)	1:80:A:LYS:HD2	1:46:A:PHE:HB2	16	0.78
(1,3516)	1:80:A:LYS:HD2	1:46:A:PHE:HB3	16	0.78
(1,3516)	1:80:A:LYS:HD3	1:46:A:PHE:HB2	16	0.78
(1,3516)	1:80:A:LYS:HD3	1:46:A:PHE:HB3	16	0.78
(1,3399)	1:198:A:LYS:HD3	1:139:A:LYS:HB2	11	0.78
(1,3399)	1:198:A:LYS:HD3	1:139:A:LYS:HB3	11	0.78
(1,3379)	1:75:A:LYS:HG3	1:19:A:GLU:HG2	9	0.78
(1,3379)	1:75:A:LYS:HG3	1:19:A:GLU:HG3	9	0.78
(1,3312)	1:58:A:ASP:HB2	1:57:A:LYS:HB2	12	0.78
(1,3312)	1:58:A:ASP:HB2	1:57:A:LYS:HB3	12	0.78
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	1	0.78
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	1	0.78
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	1	0.78
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	16	0.78
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	16	0.78
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG11	2	0.78
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG12	2	0.78
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG13	2	0.78
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG21	2	0.78
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG22	2	0.78
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG23	2	0.78
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	6	0.78
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	6	0.78
(1,2692)	1:195:A:ALA:HB1	1:150:A:LEU:HB2	9	0.78
(1,2692)	1:195:A:ALA:HB1	1:150:A:LEU:HB3	9	0.78
(1,2636)	1:65:A:LEU:HD21	1:63:A:ASP:HB2	11	0.78
(1,2636)	1:65:A:LEU:HD21	1:63:A:ASP:HB3	11	0.78
(1,2549)	1:36:A:VAL:HG13	1:37:A:LYS:HA	16	0.78
(1,2530)	1:36:A:VAL:HG13	1:37:A:LYS:HA	16	0.78
(1,2459)	1:90:A:VAL:HG22	1:94:A:TRP:HZ3	6	0.78
(1,2457)	1:90:A:VAL:HG22	1:94:A:TRP:HZ3	6	0.78
(1,2385)	1:34:A:ILE:HB	1:53:A:SER:H	9	0.78
(1,5812)	1:9:A:VAL:HG13	1:8:A:VAL:HB	3	0.77
(1,5665)	1:200:A:LEU:HB3	1:205:A:GLU:H	20	0.77
(1,5557)	1:197:A:ARG:HG2	1:201:A:TYR:H	15	0.77
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	4	0.77
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	4	0.77
(1,3439)	1:142:A:VAL:HG13	1:147:A:ASP:HB2	10	0.77
(1,3439)	1:142:A:VAL:HG13	1:147:A:ASP:HB3	10	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2549)	1:36:A:VAL:HG23	1:37:A:LYS:HA	20	0.77
(1,2543)	1:64:A:ILE:HG13	1:62:A:VAL:HA	13	0.77
(1,2535)	1:101:A:ILE:HD11	1:97:A:ASP:HA	4	0.77
(1,2530)	1:36:A:VAL:HG23	1:37:A:LYS:HA	20	0.77
(1,2482)	1:175:A:ILE:HD12	1:174:A:GLN:H	11	0.77
(1,2482)	1:175:A:ILE:HD11	1:174:A:GLN:H	12	0.77
(1,2448)	1:130:A:MET:HE1	1:200:A:LEU:H	18	0.77
(1,2400)	1:34:A:ILE:HD11	1:52:A:TYR:H	9	0.77
(1,2373)	1:26:A:ILE:HD11	1:44:A:ARG:H	18	0.77
(1,5850)	1:113:A:GLU:HG3	1:113:A:GLU:H	3	0.76
(1,5812)	1:9:A:VAL:HG21	1:8:A:VAL:HB	7	0.76
(1,5812)	1:64:A:ILE:HD13	1:8:A:VAL:HB	8	0.76
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB2	15	0.76
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB3	15	0.76
(1,5801)	1:112:A:LYS:HE2	1:116:A:PRO:HG2	11	0.76
(1,5801)	1:112:A:LYS:HE2	1:116:A:PRO:HG3	11	0.76
(1,5678)	1:137:A:ILE:HD13	1:130:A:MET:H	4	0.76
(1,5678)	1:137:A:ILE:HD13	1:130:A:MET:H	6	0.76
(1,5678)	1:137:A:ILE:HD12	1:130:A:MET:H	7	0.76
(1,3516)	1:22:A:PRO:HG2	1:46:A:PHE:HB2	13	0.76
(1,3516)	1:22:A:PRO:HG2	1:46:A:PHE:HB3	13	0.76
(1,3516)	1:22:A:PRO:HG3	1:46:A:PHE:HB2	13	0.76
(1,3516)	1:22:A:PRO:HG3	1:46:A:PHE:HB3	13	0.76
(1,3448)	1:43:A:VAL:HG13	1:41:A:CYS:HB2	12	0.76
(1,3448)	1:43:A:VAL:HG13	1:41:A:CYS:HB3	12	0.76
(1,3399)	1:64:A:ILE:HG12	1:62:A:VAL:HB	1	0.76
(1,2908)	1:137:A:ILE:HD13	1:130:A:MET:H	4	0.76
(1,2908)	1:137:A:ILE:HD13	1:130:A:MET:H	6	0.76
(1,2908)	1:137:A:ILE:HD12	1:130:A:MET:H	7	0.76
(1,2903)	1:11:A:VAL:HG22	1:54:A:ILE:HB	18	0.76
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD1	7	0.76
(1,2892)	1:175:A:ILE:HD11	1:176:A:TYR:HD2	7	0.76
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	14	0.76
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	14	0.76
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	10	0.76
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	10	0.76
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	13	0.76
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	13	0.76
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	18	0.76
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	18	0.76
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB2	1	0.76
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB3	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2534)	1:101:A:ILE:HG21	1:140:A:PRO:HA	3	0.76
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG21	13	0.75
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG22	13	0.75
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG23	13	0.75
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG21	17	0.75
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG22	17	0.75
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG23	17	0.75
(1,5558)	1:9:A:VAL:HG13	1:8:A:VAL:H	17	0.75
(1,5557)	1:128:A:LYS:HG2	1:95:A:LYS:H	11	0.75
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG2	6	0.75
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG3	6	0.75
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	16	0.75
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	16	0.75
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	16	0.75
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD1	4	0.75
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD2	4	0.75
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB2	11	0.75
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB3	11	0.75
(1,2708)	1:137:A:ILE:HD11	1:139:A:LYS:HB2	15	0.75
(1,2708)	1:137:A:ILE:HD11	1:139:A:LYS:HB3	15	0.75
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	12	0.75
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	12	0.75
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	15	0.75
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	15	0.75
(1,2578)	1:64:A:ILE:HD13	1:62:A:VAL:HA	18	0.75
(1,2459)	1:90:A:VAL:HG21	1:94:A:TRP:HZ3	12	0.75
(1,2457)	1:90:A:VAL:HG21	1:94:A:TRP:HZ3	12	0.75
(1,2442)	1:101:A:ILE:HD11	1:100:A:GLU:H	19	0.75
(1,2373)	1:26:A:ILE:HD11	1:43:A:VAL:H	2	0.75
(1,2373)	1:26:A:ILE:HD11	1:44:A:ARG:H	4	0.75
(1,167)	1:176:A:TYR:HE1	1:145:A:TYR:H	3	0.75
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB2	14	0.74
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB3	14	0.74
(1,5803)	1:18:A:THR:HG21	1:16:A:GLU:HB2	18	0.74
(1,5803)	1:18:A:THR:HG21	1:16:A:GLU:HB3	18	0.74
(1,5788)	1:98:A:ILE:HD12	1:121:A:ASN:HA	2	0.74
(1,5678)	1:137:A:ILE:HD11	1:130:A:MET:H	17	0.74
(1,5558)	1:12:A:VAL:HG11	1:17:A:ARG:H	19	0.74
(1,5558)	1:12:A:VAL:HG11	1:17:A:ARG:H	20	0.74
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG2	16	0.74
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG3	16	0.74
(1,5128)	1:197:A:ARG:H	1:200:A:LEU:HG	4	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2908)	1:137:A:ILE:HD11	1:130:A:MET:H	17	0.74
(1,2848)	1:11:A:VAL:HG23	1:43:A:VAL:H	4	0.74
(1,2657)	1:12:A:VAL:HG12	1:58:A:ASP:HB2	19	0.74
(1,2657)	1:12:A:VAL:HG12	1:58:A:ASP:HB3	19	0.74
(1,2442)	1:101:A:ILE:HD13	1:100:A:GLU:H	7	0.74
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB2	12	0.74
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB3	12	0.74
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG12	1	0.73
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG13	1	0.73
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	18	0.73
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	18	0.73
(1,2549)	1:36:A:VAL:HG11	1:37:A:LYS:HA	19	0.73
(1,2543)	1:64:A:ILE:HG13	1:62:A:VAL:HA	17	0.73
(1,2535)	1:101:A:ILE:HD11	1:97:A:ASP:HA	2	0.73
(1,2530)	1:36:A:VAL:HG11	1:37:A:LYS:HA	19	0.73
(1,2442)	1:101:A:ILE:HD13	1:100:A:GLU:H	3	0.73
(1,2403)	1:3:A:GLU:HB2	1:4:A:LEU:H	13	0.73
(1,5665)	1:50:A:LYS:HB3	1:133:A:ARG:H	13	0.72
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	16	0.72
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	13	0.72
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	13	0.72
(1,3330)	1:90:A:VAL:HB	1:91:A:PRO:HG2	12	0.72
(1,3330)	1:90:A:VAL:HB	1:91:A:PRO:HG3	12	0.72
(1,3016)	1:157:A:VAL:HG12	1:156:A:LEU:HA	5	0.72
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB2	3	0.72
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB3	3	0.72
(1,2649)	1:64:A:ILE:HD11	1:63:A:ASP:HB2	10	0.72
(1,2649)	1:64:A:ILE:HD11	1:63:A:ASP:HB3	10	0.72
(1,2535)	1:101:A:ILE:HD11	1:97:A:ASP:HA	20	0.72
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	18	0.71
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	18	0.71
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	18	0.71
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	18	0.71
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	18	0.71
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	18	0.71
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB2	17	0.71
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB3	17	0.71
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	6	0.71
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	6	0.71
(1,3399)	1:64:A:ILE:HG12	1:62:A:VAL:HB	18	0.71
(1,3289)	1:144:A:GLY:HA2	1:184:A:LEU:HG	17	0.71
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	4	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	4	0.71
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	4	0.71
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	15	0.71
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	15	0.71
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	15	0.71
(1,3016)	1:157:A:VAL:HG22	1:156:A:LEU:HA	20	0.71
(1,2903)	1:11:A:VAL:HG12	1:54:A:ILE:HB	16	0.71
(1,2573)	1:187:A:ALA:HB1	1:186:A:SER:HB2	4	0.71
(1,2573)	1:187:A:ALA:HB1	1:186:A:SER:HB3	4	0.71
(1,2535)	1:101:A:ILE:HD11	1:97:A:ASP:HA	12	0.71
(1,2534)	1:101:A:ILE:HG23	1:140:A:PRO:HA	13	0.71
(1,2442)	1:101:A:ILE:HD13	1:100:A:GLU:H	4	0.71
(1,2442)	1:101:A:ILE:HD13	1:100:A:GLU:H	11	0.71
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	12	0.71
(1,2379)	1:24:A:LEU:HD21	1:44:A:ARG:H	17	0.71
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB2	5	0.71
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB3	5	0.71
(1,5801)	1:146:A:LYS:HE2	1:182:A:PRO:HG2	13	0.7
(1,5801)	1:146:A:LYS:HE2	1:182:A:PRO:HG3	13	0.7
(1,5787)	1:98:A:ILE:HD11	1:100:A:GLU:H	13	0.7
(1,5678)	1:137:A:ILE:HD12	1:130:A:MET:H	14	0.7
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD21	10	0.7
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD22	10	0.7
(1,5558)	1:9:A:VAL:HG12	1:8:A:VAL:H	12	0.7
(1,5557)	1:128:A:LYS:HG3	1:95:A:LYS:H	19	0.7
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	9	0.7
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	9	0.7
(1,5020)	1:85:A:LEU:H	1:46:A:PHE:HD1	13	0.7
(1,5020)	1:85:A:LEU:H	1:46:A:PHE:HD2	13	0.7
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	5	0.7
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	5	0.7
(1,3016)	1:157:A:VAL:HG23	1:156:A:LEU:HA	7	0.7
(1,3016)	1:157:A:VAL:HG21	1:156:A:LEU:HA	13	0.7
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	15	0.7
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	15	0.7
(1,2908)	1:137:A:ILE:HD12	1:130:A:MET:H	14	0.7
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	13	0.7
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	3	0.7
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	3	0.7
(1,2696)	1:181:A:ILE:HB	1:183:A:ILE:HB	9	0.7
(1,2606)	1:64:A:ILE:HD12	1:78:A:LEU:HA	17	0.7
(1,2373)	1:26:A:ILE:HD13	1:43:A:VAL:H	15	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD21	9	0.69
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD22	9	0.69
(1,5557)	1:128:A:LYS:HG2	1:95:A:LYS:H	2	0.69
(1,5375)	1:202:A:GLY:H	1:204:A:GLU:HB2	19	0.69
(1,5375)	1:202:A:GLY:H	1:204:A:GLU:HB3	19	0.69
(1,5128)	1:197:A:ARG:H	1:200:A:LEU:HG	5	0.69
(1,3312)	1:158:A:TYR:HB2	1:157:A:VAL:HB	19	0.69
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	16	0.69
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	16	0.69
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD11	12	0.69
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD12	12	0.69
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD13	12	0.69
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG11	12	0.69
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG12	12	0.69
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG13	12	0.69
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG21	12	0.69
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG22	12	0.69
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG23	12	0.69
(1,2571)	1:130:A:MET:HE2	1:136:A:PRO:HA	1	0.69
(1,2536)	1:181:A:ILE:HD12	1:179:A:LEU:HA	16	0.69
(1,2448)	1:130:A:MET:HE2	1:200:A:LEU:H	8	0.69
(1,2442)	1:101:A:ILE:HD13	1:100:A:GLU:H	5	0.69
(1,2442)	1:101:A:ILE:HD13	1:100:A:GLU:H	12	0.69
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG11	6	0.69
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG12	6	0.69
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG13	6	0.69
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG21	6	0.69
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG22	6	0.69
(1,161)	1:52:A:TYR:HE2	1:11:A:VAL:HG23	6	0.69
(1,160)	1:145:A:TYR:HE1	1:146:A:LYS:HD2	7	0.69
(1,160)	1:145:A:TYR:HE1	1:146:A:LYS:HD3	7	0.69
(1,5812)	1:64:A:ILE:HD12	1:8:A:VAL:HB	1	0.68
(1,5788)	1:98:A:ILE:HD13	1:105:A:SER:HA	5	0.68
(1,5787)	1:98:A:ILE:HD12	1:103:A:GLU:H	5	0.68
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD21	13	0.68
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD22	13	0.68
(1,5559)	1:5:A:LEU:HD23	1:2:A:ASP:H	7	0.68
(1,5128)	1:197:A:ARG:H	1:198:A:LYS:HD2	7	0.68
(1,5128)	1:197:A:ARG:H	1:198:A:LYS:HD3	7	0.68
(1,5020)	1:85:A:LEU:H	1:88:A:ARG:HE	18	0.68
(1,3516)	1:22:A:PRO:HG2	1:46:A:PHE:HB2	2	0.68
(1,3516)	1:22:A:PRO:HG2	1:46:A:PHE:HB3	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3516)	1:22:A:PRO:HG3	1:46:A:PHE:HB2	2	0.68
(1,3516)	1:22:A:PRO:HG3	1:46:A:PHE:HB3	2	0.68
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	12	0.68
(1,3016)	1:157:A:VAL:HG21	1:156:A:LEU:HA	11	0.68
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	12	0.68
(1,2835)	1:126:A:LEU:HD21	1:125:A:GLN:H	13	0.68
(1,2699)	1:8:A:VAL:HG21	1:85:A:LEU:HG	10	0.68
(1,2696)	1:181:A:ILE:HB	1:183:A:ILE:HB	17	0.68
(1,2535)	1:101:A:ILE:HD11	1:97:A:ASP:HA	19	0.68
(1,2461)	1:64:A:ILE:HD11	1:66:A:ASN:H	13	0.68
(1,2422)	1:126:A:LEU:HD21	1:125:A:GLN:H	13	0.68
(1,167)	1:176:A:TYR:HE1	1:177:A:MET:H	9	0.68
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB2	10	0.67
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB3	10	0.67
(1,5558)	1:12:A:VAL:HG12	1:17:A:ARG:H	4	0.67
(1,5020)	1:85:A:LEU:H	1:88:A:ARG:HE	3	0.67
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	19	0.67
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	19	0.67
(1,3436)	1:12:A:VAL:HG21	1:60:A:LYS:HE2	4	0.67
(1,3436)	1:12:A:VAL:HG21	1:60:A:LYS:HE3	4	0.67
(1,3436)	1:12:A:VAL:HG21	1:60:A:LYS:HE2	16	0.67
(1,3436)	1:12:A:VAL:HG21	1:60:A:LYS:HE3	16	0.67
(1,3435)	1:12:A:VAL:HG21	1:60:A:LYS:HE2	4	0.67
(1,3435)	1:12:A:VAL:HG21	1:60:A:LYS:HE3	4	0.67
(1,3435)	1:12:A:VAL:HG21	1:60:A:LYS:HE2	16	0.67
(1,3435)	1:12:A:VAL:HG21	1:60:A:LYS:HE3	16	0.67
(1,3339)	1:123:A:LEU:HB3	1:150:A:LEU:HG	5	0.67
(1,3053)	1:55:A:ALA:HB3	1:40:A:GLN:HA	19	0.67
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG11	15	0.67
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG12	15	0.67
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG13	15	0.67
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG21	15	0.67
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG22	15	0.67
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG23	15	0.67
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG21	7	0.67
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG22	7	0.67
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG23	7	0.67
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	10	0.67
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	10	0.67
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	10	0.67
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	10	0.67
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	10	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	10	0.67
(1,2657)	1:12:A:VAL:HG21	1:60:A:LYS:HE2	4	0.67
(1,2657)	1:12:A:VAL:HG21	1:60:A:LYS:HE3	4	0.67
(1,2657)	1:12:A:VAL:HG21	1:60:A:LYS:HE2	16	0.67
(1,2657)	1:12:A:VAL:HG21	1:60:A:LYS:HE3	16	0.67
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD1	4	0.67
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD2	4	0.67
(1,5787)	1:98:A:ILE:HD11	1:100:A:GLU:H	20	0.66
(1,5557)	1:197:A:ARG:HG2	1:201:A:TYR:H	12	0.66
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	18	0.66
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	18	0.66
(1,5322)	1:149:A:ASN:H	1:146:A:LYS:HG2	20	0.66
(1,5322)	1:149:A:ASN:H	1:146:A:LYS:HG3	20	0.66
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG2	12	0.66
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG3	12	0.66
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG2	14	0.66
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG3	14	0.66
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	7	0.66
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	7	0.66
(1,3516)	1:22:A:PRO:HG2	1:46:A:PHE:HB2	17	0.66
(1,3516)	1:22:A:PRO:HG2	1:46:A:PHE:HB3	17	0.66
(1,3516)	1:22:A:PRO:HG3	1:46:A:PHE:HB2	17	0.66
(1,3516)	1:22:A:PRO:HG3	1:46:A:PHE:HB3	17	0.66
(1,3091)	1:129:A:PHE:H	1:88:A:ARG:HD2	15	0.66
(1,3091)	1:129:A:PHE:H	1:88:A:ARG:HD3	15	0.66
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	9	0.66
(1,3016)	1:157:A:VAL:HG23	1:156:A:LEU:HA	6	0.66
(1,3016)	1:157:A:VAL:HG22	1:156:A:LEU:HA	12	0.66
(1,3016)	1:157:A:VAL:HG22	1:156:A:LEU:HA	17	0.66
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	9	0.66
(1,2848)	1:11:A:VAL:HG23	1:44:A:ARG:H	19	0.66
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB2	9	0.66
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB3	9	0.66
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB2	15	0.66
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB3	15	0.66
(1,2841)	1:166:A:ILE:HD11	1:175:A:ILE:H	19	0.66
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	17	0.66
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	17	0.66
(1,2549)	1:36:A:VAL:HG13	1:37:A:LYS:HA	12	0.66
(1,2536)	1:181:A:ILE:HD12	1:179:A:LEU:HA	18	0.66
(1,2532)	1:183:A:ILE:HG22	1:182:A:PRO:HA	3	0.66
(1,2530)	1:36:A:VAL:HG13	1:37:A:LYS:HA	12	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2461)	1:64:A:ILE:HD12	1:66:A:ASN:H	2	0.66
(1,2418)	1:200:A:LEU:HD22	1:153:A:LEU:H	19	0.66
(1,2373)	1:26:A:ILE:HD12	1:43:A:VAL:H	10	0.66
(1,5665)	1:50:A:LYS:HB2	1:133:A:ARG:H	18	0.65
(1,5558)	1:9:A:VAL:HG12	1:8:A:VAL:H	18	0.65
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	17	0.65
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	17	0.65
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	17	0.65
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	17	0.65
(1,3016)	1:157:A:VAL:HG23	1:156:A:LEU:HA	3	0.65
(1,3016)	1:157:A:VAL:HG21	1:156:A:LEU:HA	10	0.65
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	13	0.65
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	13	0.65
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	17	0.65
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	19	0.65
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	19	0.65
(1,2536)	1:181:A:ILE:HD13	1:179:A:LEU:HA	19	0.65
(1,2429)	1:181:A:ILE:HD11	1:180:A:GLY:H	4	0.65
(1,2429)	1:181:A:ILE:HD12	1:180:A:GLY:H	9	0.65
(1,2426)	1:101:A:ILE:HG23	1:103:A:GLU:H	17	0.65
(1,2373)	1:26:A:ILE:HD12	1:44:A:ARG:H	1	0.65
(1,2373)	1:26:A:ILE:HD13	1:44:A:ARG:H	6	0.65
(1,172)	1:122:A:PHE:HE2	1:126:A:LEU:HG	9	0.65
(1,5678)	1:137:A:ILE:HD13	1:130:A:MET:H	16	0.64
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE2	16	0.64
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE3	16	0.64
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	11	0.64
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	11	0.64
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	15	0.64
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	15	0.64
(1,3436)	1:12:A:VAL:HG13	1:60:A:LYS:HE2	17	0.64
(1,3436)	1:12:A:VAL:HG13	1:60:A:LYS:HE3	17	0.64
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	11	0.64
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	11	0.64
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	15	0.64
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	15	0.64
(1,3435)	1:12:A:VAL:HG13	1:60:A:LYS:HE2	17	0.64
(1,3435)	1:12:A:VAL:HG13	1:60:A:LYS:HE3	17	0.64
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	13	0.64
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	13	0.64
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	13	0.64
(1,2908)	1:137:A:ILE:HD13	1:130:A:MET:H	16	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD1	1	0.64
(1,2892)	1:175:A:ILE:HD12	1:176:A:TYR:HD2	1	0.64
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG11	12	0.64
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG12	12	0.64
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG13	12	0.64
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG21	12	0.64
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG22	12	0.64
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG23	12	0.64
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG11	13	0.64
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG12	13	0.64
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG13	13	0.64
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG21	13	0.64
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG22	13	0.64
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG23	13	0.64
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG21	12	0.64
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG22	12	0.64
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG23	12	0.64
(1,2657)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	11	0.64
(1,2657)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	11	0.64
(1,2657)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	15	0.64
(1,2657)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	15	0.64
(1,2536)	1:181:A:ILE:HD12	1:179:A:LEU:HA	2	0.64
(1,2442)	1:101:A:ILE:HD11	1:100:A:GLU:H	20	0.64
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	3	0.63
(1,5625)	1:146:A:LYS:HG2	1:145:A:TYR:H	7	0.63
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	20	0.63
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	20	0.63
(1,5128)	1:197:A:ARG:H	1:200:A:LEU:HG	3	0.63
(1,4965)	1:84:A:PHE:H	1:88:A:ARG:HE	11	0.63
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	8	0.63
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	8	0.63
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD11	11	0.63
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD12	11	0.63
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD13	11	0.63
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD21	11	0.63
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD22	11	0.63
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD23	11	0.63
(1,3016)	1:157:A:VAL:HG11	1:156:A:LEU:HA	4	0.63
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG12	12	0.63
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG13	12	0.63
(1,2848)	1:11:A:VAL:HG21	1:44:A:ARG:H	20	0.63
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	8	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2699)	1:8:A:VAL:HG23	1:85:A:LEU:HG	3	0.63
(1,2665)	1:47:A:ILE:HD13	1:48:A:ASP:HB2	15	0.63
(1,2665)	1:47:A:ILE:HD13	1:48:A:ASP:HB3	15	0.63
(1,2645)	1:54:A:ILE:HG21	1:57:A:LYS:HE2	2	0.63
(1,2645)	1:54:A:ILE:HG21	1:57:A:LYS:HE3	2	0.63
(1,2536)	1:181:A:ILE:HD11	1:179:A:LEU:HA	3	0.63
(1,2536)	1:181:A:ILE:HD13	1:179:A:LEU:HA	11	0.63
(1,2481)	1:187:A:ALA:HB1	1:190:A:TYR:HD1	12	0.63
(1,2481)	1:187:A:ALA:HB1	1:190:A:TYR:HD2	12	0.63
(1,2429)	1:181:A:ILE:HD13	1:180:A:GLY:H	17	0.63
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG21	11	0.62
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG22	11	0.62
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG23	11	0.62
(1,5625)	1:146:A:LYS:HG2	1:145:A:TYR:H	14	0.62
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	2	0.62
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	2	0.62
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	2	0.62
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG2	3	0.62
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG3	3	0.62
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG2	13	0.62
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG3	13	0.62
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	6	0.62
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	6	0.62
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD2	5	0.62
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD3	5	0.62
(1,4907)	1:20:A:TRP:HE1	1:78:A:LEU:HB2	20	0.62
(1,4907)	1:20:A:TRP:HE1	1:78:A:LEU:HB3	20	0.62
(1,3544)	1:97:A:ASP:HB3	1:99:A:SER:HA	9	0.62
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB2	14	0.62
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB3	14	0.62
(1,2905)	1:126:A:LEU:HD11	1:199:A:TYR:HD1	16	0.62
(1,2905)	1:126:A:LEU:HD11	1:199:A:TYR:HD2	16	0.62
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD1	2	0.62
(1,2892)	1:175:A:ILE:HD13	1:176:A:TYR:HD2	2	0.62
(1,2884)	1:61:A:GLU:HG2	1:3:A:GLU:HA	7	0.62
(1,2826)	1:59:A:ILE:HB	1:61:A:GLU:HG2	18	0.62
(1,2826)	1:59:A:ILE:HB	1:61:A:GLU:HG3	18	0.62
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG21	6	0.62
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG22	6	0.62
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG23	6	0.62
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG11	8	0.62
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG12	8	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG13	8	0.62
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG21	8	0.62
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG22	8	0.62
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG23	8	0.62
(1,2606)	1:64:A:ILE:HD13	1:78:A:LEU:HA	15	0.62
(1,2554)	1:175:A:ILE:HD12	1:192:A:VAL:HA	5	0.62
(1,2541)	1:142:A:VAL:HB	1:148:A:LEU:HA	6	0.62
(1,2539)	1:54:A:ILE:HD12	1:11:A:VAL:HA	10	0.62
(1,2534)	1:101:A:ILE:HG22	1:140:A:PRO:HA	2	0.62
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD1	15	0.62
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD2	15	0.62
(1,2459)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	16	0.62
(1,2457)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	16	0.62
(1,2429)	1:181:A:ILE:HD13	1:180:A:GLY:H	1	0.62
(1,2429)	1:181:A:ILE:HD11	1:180:A:GLY:H	7	0.62
(1,2379)	1:24:A:LEU:HD12	1:46:A:PHE:H	16	0.62
(1,2373)	1:26:A:ILE:HD12	1:43:A:VAL:H	16	0.62
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	16	0.61
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	16	0.61
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	16	0.61
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	16	0.61
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	16	0.61
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	16	0.61
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG12	5	0.61
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG13	5	0.61
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	12	0.61
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	12	0.61
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	16	0.61
(1,5247)	1:40:A:GLN:HE21	1:55:A:ALA:HA	5	0.61
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	14	0.61
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	14	0.61
(1,4965)	1:84:A:PHE:H	1:88:A:ARG:HE	2	0.61
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	10	0.61
(1,3436)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	10	0.61
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	10	0.61
(1,3435)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	10	0.61
(1,2866)	1:210:A:ALA:HA	1:5:A:LEU:HB2	17	0.61
(1,2866)	1:210:A:ALA:HA	1:5:A:LEU:HB3	17	0.61
(1,2696)	1:181:A:ILE:HB	1:183:A:ILE:HB	5	0.61
(1,2657)	1:12:A:VAL:HG22	1:60:A:LYS:HE2	10	0.61
(1,2657)	1:12:A:VAL:HG22	1:60:A:LYS:HE3	10	0.61
(1,2578)	1:64:A:ILE:HD13	1:62:A:VAL:HA	19	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2571)	1:130:A:MET:HE2	1:198:A:LYS:HA	15	0.61
(1,2571)	1:130:A:MET:HE1	1:136:A:PRO:HA	17	0.61
(1,2429)	1:181:A:ILE:HD12	1:180:A:GLY:H	6	0.61
(1,2418)	1:200:A:LEU:HD13	1:199:A:TYR:H	3	0.61
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	19	0.6
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	19	0.6
(1,5128)	1:197:A:ARG:H	1:198:A:LYS:HD2	17	0.6
(1,5128)	1:197:A:ARG:H	1:198:A:LYS:HD3	17	0.6
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	17	0.6
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	17	0.6
(1,3287)	1:53:A:SER:HB3	1:37:A:LYS:HD2	5	0.6
(1,3287)	1:53:A:SER:HB3	1:37:A:LYS:HD3	5	0.6
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	9	0.6
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	9	0.6
(1,2903)	1:11:A:VAL:HG23	1:54:A:ILE:HB	6	0.6
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB2	3	0.6
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB3	3	0.6
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB2	16	0.6
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB3	16	0.6
(1,2669)	1:85:A:LEU:HD12	1:8:A:VAL:HB	17	0.6
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB2	7	0.6
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB3	7	0.6
(1,2549)	1:36:A:VAL:HG12	1:37:A:LYS:HA	6	0.6
(1,2541)	1:142:A:VAL:HB	1:148:A:LEU:HA	13	0.6
(1,2539)	1:54:A:ILE:HD12	1:11:A:VAL:HA	9	0.6
(1,2536)	1:181:A:ILE:HD12	1:179:A:LEU:HA	5	0.6
(1,2534)	1:101:A:ILE:HG23	1:140:A:PRO:HA	19	0.6
(1,2530)	1:36:A:VAL:HG12	1:37:A:LYS:HA	6	0.6
(1,2461)	1:64:A:ILE:HD11	1:66:A:ASN:H	5	0.6
(1,2429)	1:181:A:ILE:HD12	1:180:A:GLY:H	19	0.6
(1,2429)	1:181:A:ILE:HD11	1:180:A:GLY:H	20	0.6
(1,2260)	1:101:A:ILE:HA	1:100:A:GLU:HG2	11	0.6
(1,2260)	1:101:A:ILE:HA	1:100:A:GLU:HG3	11	0.6
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB2	15	0.6
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB3	15	0.6
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB2	3	0.6
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB3	3	0.6
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG2	12	0.6
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG3	12	0.6
(1,5801)	1:146:A:LYS:HE2	1:182:A:PRO:HG2	20	0.59
(1,5801)	1:146:A:LYS:HE2	1:182:A:PRO:HG3	20	0.59
(1,5665)	1:50:A:LYS:HB3	1:133:A:ARG:H	14	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5490)	1:63:A:ASP:H	1:61:A:GLU:HB2	19	0.59
(1,5490)	1:63:A:ASP:H	1:61:A:GLU:HB3	19	0.59
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	10	0.59
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	10	0.59
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	10	0.59
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	10	0.59
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	10	0.59
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	10	0.59
(1,5373)	1:134:A:GLY:H	1:44:A:ARG:HD2	18	0.59
(1,5373)	1:134:A:GLY:H	1:44:A:ARG:HD3	18	0.59
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	12	0.59
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	12	0.59
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	8	0.59
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	8	0.59
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	13	0.59
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	13	0.59
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	13	0.59
(1,3016)	1:157:A:VAL:HG21	1:156:A:LEU:HA	1	0.59
(1,3016)	1:157:A:VAL:HG22	1:156:A:LEU:HA	18	0.59
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	5	0.59
(1,2866)	1:210:A:ALA:HA	1:5:A:LEU:HB2	2	0.59
(1,2866)	1:210:A:ALA:HA	1:5:A:LEU:HB3	2	0.59
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG11	19	0.59
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG12	19	0.59
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG13	19	0.59
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG21	19	0.59
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG22	19	0.59
(1,2804)	1:171:A:VAL:HG12	1:157:A:VAL:HG23	19	0.59
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG11	19	0.59
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG12	19	0.59
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG13	19	0.59
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG21	19	0.59
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG22	19	0.59
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG23	19	0.59
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	2	0.59
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	2	0.59
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	4	0.59
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	4	0.59
(1,2696)	1:181:A:ILE:HB	1:183:A:ILE:HB	7	0.59
(1,2685)	1:67:A:LEU:HD11	1:71:A:GLU:HB2	20	0.59
(1,2685)	1:67:A:LEU:HD11	1:71:A:GLU:HB3	20	0.59
(1,2596)	1:90:A:VAL:HG22	1:85:A:LEU:HA	11	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2578)	1:64:A:ILE:HD13	1:62:A:VAL:HA	1	0.59
(1,2448)	1:130:A:MET:HE1	1:200:A:LEU:H	6	0.59
(1,2429)	1:181:A:ILE:HD11	1:180:A:GLY:H	5	0.59
(1,2375)	1:60:A:LYS:HD2	1:61:A:GLU:H	4	0.59
(1,2373)	1:26:A:ILE:HD11	1:44:A:ARG:H	13	0.59
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB2	20	0.58
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB3	20	0.58
(1,5697)	1:139:A:LYS:HD3	1:138:A:ASN:HD21	11	0.58
(1,5697)	1:139:A:LYS:HD3	1:138:A:ASN:HD22	11	0.58
(1,5697)	1:124:A:GLN:HB2	1:121:A:ASN:HD21	15	0.58
(1,5697)	1:124:A:GLN:HB2	1:121:A:ASN:HD22	15	0.58
(1,5679)	1:139:A:LYS:HD2	1:138:A:ASN:HD21	15	0.58
(1,5679)	1:139:A:LYS:HD2	1:138:A:ASN:HD22	15	0.58
(1,5679)	1:139:A:LYS:HD3	1:138:A:ASN:HD21	15	0.58
(1,5679)	1:139:A:LYS:HD3	1:138:A:ASN:HD22	15	0.58
(1,5625)	1:146:A:LYS:HG2	1:145:A:TYR:H	3	0.58
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	2	0.58
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	2	0.58
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	6	0.58
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	6	0.58
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB2	20	0.58
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB3	20	0.58
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	16	0.58
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	16	0.58
(1,5386)	1:200:A:LEU:H	1:196:A:TYR:HE1	17	0.58
(1,5386)	1:200:A:LEU:H	1:196:A:TYR:HE2	17	0.58
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG11	18	0.58
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG12	18	0.58
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG13	18	0.58
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG21	18	0.58
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG22	18	0.58
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG23	18	0.58
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD11	9	0.58
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD12	9	0.58
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD13	9	0.58
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD21	9	0.58
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD22	9	0.58
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD23	9	0.58
(1,3505)	1:197:A:ARG:HG2	1:197:A:ARG:HA	11	0.58
(1,3399)	1:198:A:LYS:HD2	1:139:A:LYS:HB2	9	0.58
(1,3399)	1:198:A:LYS:HD2	1:139:A:LYS:HB3	9	0.58
(1,3338)	1:100:A:GLU:HB2	1:101:A:ILE:HG12	8	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3338)	1:100:A:GLU:HB2	1:101:A:ILE:HG13	8	0.58
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG2	2	0.58
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG3	2	0.58
(1,3014)	1:175:A:ILE:HG23	1:156:A:LEU:HA	3	0.58
(1,3014)	1:175:A:ILE:HG23	1:156:A:LEU:HA	5	0.58
(1,3014)	1:175:A:ILE:HG23	1:156:A:LEU:HA	7	0.58
(1,3012)	1:173:A:LYS:HB3	1:174:A:GLN:HA	1	0.58
(1,2903)	1:11:A:VAL:HG12	1:54:A:ILE:HB	10	0.58
(1,2884)	1:61:A:GLU:HG3	1:3:A:GLU:HA	18	0.58
(1,2843)	1:181:A:ILE:HD13	1:182:A:PRO:HG2	2	0.58
(1,2843)	1:181:A:ILE:HD13	1:182:A:PRO:HG3	2	0.58
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB2	20	0.58
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB3	20	0.58
(1,2549)	1:36:A:VAL:HG11	1:37:A:LYS:HA	14	0.58
(1,2538)	1:183:A:ILE:HD13	1:184:A:LEU:HA	7	0.58
(1,2536)	1:181:A:ILE:HD12	1:179:A:LEU:HA	10	0.58
(1,2536)	1:181:A:ILE:HD12	1:179:A:LEU:HA	12	0.58
(1,2535)	1:101:A:ILE:HD11	1:96:A:MET:HA	11	0.58
(1,2530)	1:36:A:VAL:HG11	1:37:A:LYS:HA	14	0.58
(1,2429)	1:181:A:ILE:HD12	1:180:A:GLY:H	11	0.58
(1,2429)	1:181:A:ILE:HD13	1:180:A:GLY:H	14	0.58
(1,2429)	1:181:A:ILE:HD11	1:180:A:GLY:H	18	0.58
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	6	0.58
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	6	0.58
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	9	0.58
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	9	0.58
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	15	0.58
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	15	0.58
(1,5788)	1:98:A:ILE:HD13	1:121:A:ASN:HA	16	0.57
(1,5786)	1:115:A:ASP:HA	1:117:A:GLU:H	9	0.57
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	10	0.57
(1,5665)	1:34:A:ILE:HG13	1:33:A:ASP:H	17	0.57
(1,5128)	1:197:A:ARG:H	1:198:A:LYS:HD2	19	0.57
(1,5128)	1:197:A:ARG:H	1:198:A:LYS:HD3	19	0.57
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG2	9	0.57
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG3	9	0.57
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	1	0.57
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	1	0.57
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE2	14	0.57
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE3	14	0.57
(1,3339)	1:7:A:LYS:HB3	1:5:A:LEU:HG	1	0.57
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	14	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	1	0.57
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	1	0.57
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD11	8	0.57
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD12	8	0.57
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD13	8	0.57
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG21	19	0.57
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG22	19	0.57
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG23	19	0.57
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD11	3	0.57
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD12	3	0.57
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD13	3	0.57
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD21	3	0.57
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD22	3	0.57
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD23	3	0.57
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD11	8	0.57
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD12	8	0.57
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD13	8	0.57
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD21	8	0.57
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD22	8	0.57
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD23	8	0.57
(1,2708)	1:137:A:ILE:HD13	1:140:A:PRO:HB2	17	0.57
(1,2708)	1:137:A:ILE:HD13	1:140:A:PRO:HB3	17	0.57
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB2	20	0.57
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB3	20	0.57
(1,2571)	1:130:A:MET:HE3	1:136:A:PRO:HA	20	0.57
(1,2536)	1:181:A:ILE:HD12	1:179:A:LEU:HA	7	0.57
(1,2536)	1:181:A:ILE:HD13	1:179:A:LEU:HA	9	0.57
(1,2536)	1:181:A:ILE:HD12	1:179:A:LEU:HA	20	0.57
(1,2474)	1:101:A:ILE:HD13	1:101:A:ILE:H	5	0.57
(1,2471)	1:12:A:VAL:HG22	1:20:A:TRP:HD1	11	0.57
(1,2429)	1:181:A:ILE:HD12	1:180:A:GLY:H	15	0.57
(1,2400)	1:34:A:ILE:HD13	1:32:A:ASP:H	6	0.57
(1,5801)	1:146:A:LYS:HE2	1:182:A:PRO:HG2	2	0.56
(1,5801)	1:146:A:LYS:HE2	1:182:A:PRO:HG3	2	0.56
(1,5786)	1:115:A:ASP:HA	1:117:A:GLU:H	1	0.56
(1,5697)	1:139:A:LYS:HD2	1:138:A:ASN:HD21	17	0.56
(1,5697)	1:139:A:LYS:HD2	1:138:A:ASN:HD22	17	0.56
(1,5557)	1:124:A:GLN:HB3	1:95:A:LYS:H	14	0.56
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	4	0.56
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	4	0.56
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	8	0.56
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	8	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	8	0.56
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	8	0.56
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	8	0.56
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	8	0.56
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	8	0.56
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	8	0.56
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG12	18	0.56
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG13	18	0.56
(1,5312)	1:20:A:TRP:HE1	1:11:A:VAL:H	13	0.56
(1,5233)	1:1:A:ASN:HD21	1:61:A:GLU:HG2	10	0.56
(1,5233)	1:1:A:ASN:HD21	1:61:A:GLU:HG3	10	0.56
(1,5020)	1:85:A:LEU:H	1:46:A:PHE:HD1	17	0.56
(1,5020)	1:85:A:LEU:H	1:46:A:PHE:HD2	17	0.56
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	10	0.56
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	10	0.56
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	2	0.56
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	2	0.56
(1,3436)	1:12:A:VAL:HG23	1:60:A:LYS:HE2	3	0.56
(1,3436)	1:12:A:VAL:HG23	1:60:A:LYS:HE3	3	0.56
(1,3435)	1:12:A:VAL:HG23	1:60:A:LYS:HE2	3	0.56
(1,3435)	1:12:A:VAL:HG23	1:60:A:LYS:HE3	3	0.56
(1,3427)	1:184:A:LEU:HD11	1:182:A:PRO:HB2	16	0.56
(1,3427)	1:184:A:LEU:HD11	1:182:A:PRO:HB3	16	0.56
(1,3378)	1:173:A:LYS:HG3	1:183:A:ILE:HB	19	0.56
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	7	0.56
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	7	0.56
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	7	0.56
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	19	0.56
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	19	0.56
(1,3016)	1:157:A:VAL:HG22	1:156:A:LEU:HA	9	0.56
(1,3016)	1:157:A:VAL:HG23	1:156:A:LEU:HA	16	0.56
(1,3012)	1:173:A:LYS:HB3	1:174:A:GLN:HA	6	0.56
(1,2947)	1:30:A:CYS:HB2	1:29:A:SER:HB2	1	0.56
(1,2947)	1:30:A:CYS:HB2	1:29:A:SER:HB3	1	0.56
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	17	0.56
(1,2826)	1:59:A:ILE:HB	1:61:A:GLU:HG2	19	0.56
(1,2826)	1:59:A:ILE:HB	1:61:A:GLU:HG3	19	0.56
(1,2717)	1:130:A:MET:HE2	1:137:A:ILE:HB	1	0.56
(1,2657)	1:12:A:VAL:HG23	1:60:A:LYS:HE2	3	0.56
(1,2657)	1:12:A:VAL:HG23	1:60:A:LYS:HE3	3	0.56
(1,2539)	1:54:A:ILE:HD11	1:14:A:ALA:HA	14	0.56
(1,2534)	1:101:A:ILE:HG22	1:140:A:PRO:HA	9	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2468)	1:84:A:PHE:HE2	1:88:A:ARG:HB2	3	0.56
(1,2468)	1:84:A:PHE:HE2	1:88:A:ARG:HB3	3	0.56
(1,2461)	1:64:A:ILE:HD13	1:66:A:ASN:H	16	0.56
(1,2459)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	13	0.56
(1,2457)	1:90:A:VAL:HG23	1:94:A:TRP:HZ3	13	0.56
(1,2429)	1:181:A:ILE:HD11	1:180:A:GLY:H	10	0.56
(1,2383)	1:43:A:VAL:HG23	1:52:A:TYR:H	18	0.56
(1,2238)	1:207:A:CYS:HA	1:213:A:GLN:HE21	5	0.56
(1,2238)	1:207:A:CYS:HA	1:213:A:GLN:HE22	5	0.56
(1,2238)	1:207:A:CYS:HA	1:213:A:GLN:HE21	11	0.56
(1,2238)	1:207:A:CYS:HA	1:213:A:GLN:HE22	11	0.56
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	17	0.56
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	17	0.56
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	18	0.56
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	18	0.56
(1,5850)	1:113:A:GLU:HG3	1:113:A:GLU:H	6	0.55
(1,5804)	1:167:A:ASP:HB2	1:168:A:SER:HB2	6	0.55
(1,5804)	1:167:A:ASP:HB2	1:168:A:SER:HB3	6	0.55
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB2	3	0.55
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB3	3	0.55
(1,5795)	1:167:A:ASP:HB2	1:168:A:SER:HB2	6	0.55
(1,5795)	1:167:A:ASP:HB2	1:168:A:SER:HB3	6	0.55
(1,5681)	1:44:A:ARG:HE	1:50:A:LYS:H	14	0.55
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	15	0.55
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	15	0.55
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	15	0.55
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	15	0.55
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	15	0.55
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	15	0.55
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB1	3	0.55
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB2	3	0.55
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB3	3	0.55
(1,5318)	1:36:A:VAL:H	1:37:A:LYS:HG2	3	0.55
(1,5318)	1:36:A:VAL:H	1:37:A:LYS:HG3	3	0.55
(1,5290)	1:73:A:SER:H	1:79:A:GLN:HG2	3	0.55
(1,5290)	1:73:A:SER:H	1:79:A:GLN:HG3	3	0.55
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	13	0.55
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	13	0.55
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	11	0.55
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	11	0.55
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	14	0.55
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	14	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	14	0.55
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD2	19	0.55
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD3	19	0.55
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG2	18	0.55
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG3	18	0.55
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	6	0.55
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	6	0.55
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	6	0.55
(1,3053)	1:55:A:ALA:HB1	1:40:A:GLN:HA	9	0.55
(1,3016)	1:157:A:VAL:HG23	1:156:A:LEU:HA	2	0.55
(1,3016)	1:157:A:VAL:HG12	1:156:A:LEU:HA	15	0.55
(1,3012)	1:173:A:LYS:HB3	1:174:A:GLN:HA	9	0.55
(1,2848)	1:11:A:VAL:HG23	1:44:A:ARG:H	12	0.55
(1,2848)	1:11:A:VAL:HG23	1:44:A:ARG:H	16	0.55
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	18	0.55
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	18	0.55
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD11	2	0.55
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD12	2	0.55
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD13	2	0.55
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD21	2	0.55
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD22	2	0.55
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD23	2	0.55
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG11	15	0.55
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG12	15	0.55
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG13	15	0.55
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG21	15	0.55
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG22	15	0.55
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG23	15	0.55
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG11	20	0.55
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG12	20	0.55
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG13	20	0.55
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG21	20	0.55
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG22	20	0.55
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG23	20	0.55
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB2	1	0.55
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB3	1	0.55
(1,2578)	1:64:A:ILE:HD13	1:62:A:VAL:HA	11	0.55
(1,2571)	1:130:A:MET:HE1	1:136:A:PRO:HA	5	0.55
(1,2534)	1:101:A:ILE:HG23	1:105:A:SER:HA	4	0.55
(1,2481)	1:187:A:ALA:HB3	1:191:A:ASN:HD21	15	0.55
(1,2481)	1:187:A:ALA:HB3	1:191:A:ASN:HD22	15	0.55
(1,2442)	1:101:A:ILE:HD13	1:100:A:GLU:H	15	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2429)	1:181:A:ILE:HD13	1:145:A:TYR:H	16	0.55
(1,2426)	1:101:A:ILE:HG23	1:103:A:GLU:H	9	0.55
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	8	0.55
(1,2383)	1:43:A:VAL:HG22	1:52:A:TYR:H	3	0.55
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG21	11	0.55
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG22	11	0.55
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG23	11	0.55
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	2	0.55
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	2	0.55
(1,113)	1:176:A:TYR:HD2	1:182:A:PRO:HA	2	0.55
(1,5861)	1:116:A:PRO:HG3	1:117:A:GLU:H	12	0.54
(1,5625)	1:143:A:LEU:HG	1:145:A:TYR:H	8	0.54
(1,5559)	1:24:A:LEU:HD21	1:8:A:VAL:H	4	0.54
(1,5553)	1:148:A:LEU:HG	1:142:A:VAL:H	4	0.54
(1,5430)	1:24:A:LEU:H	1:52:A:TYR:HE1	12	0.54
(1,5430)	1:24:A:LEU:H	1:52:A:TYR:HE2	12	0.54
(1,5375)	1:202:A:GLY:H	1:204:A:GLU:HB2	3	0.54
(1,5375)	1:202:A:GLY:H	1:204:A:GLU:HB3	3	0.54
(1,5322)	1:149:A:ASN:H	1:146:A:LYS:HG2	12	0.54
(1,5322)	1:149:A:ASN:H	1:146:A:LYS:HG3	12	0.54
(1,5237)	1:145:A:TYR:H	1:143:A:LEU:HG	8	0.54
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	14	0.54
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	17	0.54
(1,5053)	1:78:A:LEU:H	1:75:A:LYS:HD2	8	0.54
(1,5053)	1:78:A:LEU:H	1:75:A:LYS:HD3	8	0.54
(1,3053)	1:55:A:ALA:HB1	1:40:A:GLN:HA	5	0.54
(1,3053)	1:55:A:ALA:HB2	1:40:A:GLN:HA	12	0.54
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	8	0.54
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG12	9	0.54
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG13	9	0.54
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	7	0.54
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG21	4	0.54
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG22	4	0.54
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG23	4	0.54
(1,2708)	1:137:A:ILE:HD11	1:140:A:PRO:HB2	14	0.54
(1,2708)	1:137:A:ILE:HD11	1:140:A:PRO:HB3	14	0.54
(1,2479)	1:194:A:THR:HG23	1:199:A:TYR:HD1	11	0.54
(1,2479)	1:194:A:THR:HG23	1:199:A:TYR:HD2	11	0.54
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	6	0.54
(1,2375)	1:60:A:LYS:HD3	1:11:A:VAL:H	10	0.54
(1,173)	1:146:A:LYS:H	1:145:A:TYR:HD1	4	0.54
(1,173)	1:146:A:LYS:H	1:145:A:TYR:HD2	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	8	0.54
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	8	0.54
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	13	0.54
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	13	0.54
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	20	0.54
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	20	0.54
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD21	14	0.54
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD22	14	0.54
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB2	2	0.53
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB3	2	0.53
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB2	7	0.53
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB3	7	0.53
(1,5788)	1:98:A:ILE:HD12	1:105:A:SER:HA	6	0.53
(1,5788)	1:98:A:ILE:HD13	1:105:A:SER:HA	18	0.53
(1,5547)	1:100:A:GLU:HG3	1:100:A:GLU:H	12	0.53
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	14	0.53
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	14	0.53
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	14	0.53
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	14	0.53
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	14	0.53
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	14	0.53
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG12	2	0.53
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG13	2	0.53
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD11	10	0.53
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD12	10	0.53
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD13	10	0.53
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD21	10	0.53
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD22	10	0.53
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD23	10	0.53
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG11	15	0.53
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG12	15	0.53
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG13	15	0.53
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG21	15	0.53
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG22	15	0.53
(1,5362)	1:40:A:GLN:HE21	1:36:A:VAL:HG23	15	0.53
(1,5252)	1:88:A:ARG:HE	1:46:A:PHE:HB2	9	0.53
(1,5252)	1:88:A:ARG:HE	1:46:A:PHE:HB3	9	0.53
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	6	0.53
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	15	0.53
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB2	16	0.53
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB3	16	0.53
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	16	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	16	0.53
(1,3439)	1:102:A:LEU:HD21	1:147:A:ASP:HB2	11	0.53
(1,3439)	1:102:A:LEU:HD21	1:147:A:ASP:HB3	11	0.53
(1,3439)	1:102:A:LEU:HD11	1:147:A:ASP:HB2	14	0.53
(1,3439)	1:102:A:LEU:HD11	1:147:A:ASP:HB3	14	0.53
(1,3330)	1:100:A:GLU:HG2	1:101:A:ILE:HG12	17	0.53
(1,3330)	1:100:A:GLU:HG2	1:101:A:ILE:HG13	17	0.53
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	8	0.53
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD2	20	0.53
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD3	20	0.53
(1,3014)	1:175:A:ILE:HG21	1:156:A:LEU:HA	9	0.53
(1,3014)	1:175:A:ILE:HG21	1:156:A:LEU:HA	12	0.53
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB2	19	0.53
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB3	19	0.53
(1,2903)	1:11:A:VAL:HG13	1:54:A:ILE:HB	13	0.53
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	8	0.53
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	2	0.53
(1,2578)	1:64:A:ILE:HD11	1:62:A:VAL:HA	8	0.53
(1,2575)	1:64:A:ILE:HG21	1:82:A:SER:HA	18	0.53
(1,2538)	1:183:A:ILE:HD12	1:184:A:LEU:HA	17	0.53
(1,2531)	1:142:A:VAL:HG21	1:143:A:LEU:HA	12	0.53
(1,2489)	1:87:A:THR:HG23	1:89:A:VAL:H	20	0.53
(1,2442)	1:101:A:ILE:HD12	1:100:A:GLU:H	13	0.53
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	13	0.53
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	18	0.53
(1,2373)	1:26:A:ILE:HD13	1:43:A:VAL:H	3	0.53
(1,5842)	1:222:A:LEU:H	1:221:A:GLU:HG2	6	0.52
(1,5842)	1:222:A:LEU:H	1:221:A:GLU:HG3	6	0.52
(1,5785)	1:222:A:LEU:H	1:221:A:GLU:HG2	6	0.52
(1,5785)	1:222:A:LEU:H	1:221:A:GLU:HG3	6	0.52
(1,5665)	1:50:A:LYS:HB2	1:133:A:ARG:H	11	0.52
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD21	8	0.52
(1,5654)	1:27:A:SER:HA	1:31:A:ASN:HD22	8	0.52
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	6	0.52
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	6	0.52
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	6	0.52
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	6	0.52
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	6	0.52
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	6	0.52
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	6	0.52
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	6	0.52
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	16	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	16	0.52
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	9	0.52
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	9	0.52
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB2	13	0.52
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB3	13	0.52
(1,5020)	1:85:A:LEU:H	1:88:A:ARG:HE	19	0.52
(1,3436)	1:12:A:VAL:HG12	1:60:A:LYS:HE2	1	0.52
(1,3436)	1:12:A:VAL:HG12	1:60:A:LYS:HE3	1	0.52
(1,3435)	1:12:A:VAL:HG12	1:60:A:LYS:HE2	1	0.52
(1,3435)	1:12:A:VAL:HG12	1:60:A:LYS:HE3	1	0.52
(1,3339)	1:123:A:LEU:HB3	1:150:A:LEU:HG	8	0.52
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD11	6	0.52
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD12	6	0.52
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD13	6	0.52
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD21	6	0.52
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD22	6	0.52
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD23	6	0.52
(1,3053)	1:55:A:ALA:HB1	1:40:A:GLN:HA	6	0.52
(1,3014)	1:175:A:ILE:HG22	1:156:A:LEU:HA	10	0.52
(1,3014)	1:175:A:ILE:HG22	1:156:A:LEU:HA	17	0.52
(1,3014)	1:175:A:ILE:HG21	1:156:A:LEU:HA	20	0.52
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD11	9	0.52
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD12	9	0.52
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD13	9	0.52
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD21	9	0.52
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD22	9	0.52
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD23	9	0.52
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD11	20	0.52
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD12	20	0.52
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD13	20	0.52
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD21	20	0.52
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD22	20	0.52
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD23	20	0.52
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB2	15	0.52
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB3	15	0.52
(1,2575)	1:64:A:ILE:HG22	1:78:A:LEU:HA	11	0.52
(1,2575)	1:64:A:ILE:HG23	1:78:A:LEU:HA	19	0.52
(1,2541)	1:142:A:VAL:HB	1:148:A:LEU:HA	20	0.52
(1,2479)	1:194:A:THR:HG21	1:199:A:TYR:HD1	14	0.52
(1,2479)	1:194:A:THR:HG21	1:199:A:TYR:HD2	14	0.52
(1,2462)	1:197:A:ARG:HD3	1:201:A:TYR:HD1	12	0.52
(1,2462)	1:197:A:ARG:HD3	1:201:A:TYR:HD2	12	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2400)	1:34:A:ILE:HD11	1:52:A:TYR:H	12	0.52
(1,2375)	1:60:A:LYS:HD3	1:61:A:GLU:H	2	0.52
(1,168)	1:190:A:TYR:HE1	1:191:A:ASN:HD21	7	0.52
(1,168)	1:190:A:TYR:HE1	1:191:A:ASN:HD22	7	0.52
(1,5861)	1:116:A:PRO:HG2	1:117:A:GLU:H	9	0.51
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB2	4	0.51
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB3	4	0.51
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB2	11	0.51
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB3	11	0.51
(1,5549)	1:204:A:GLU:HB3	1:201:A:TYR:H	10	0.51
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB2	3	0.51
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB3	3	0.51
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	14	0.51
(1,5247)	1:40:A:GLN:HE21	1:37:A:LYS:HA	14	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD11	2	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD12	2	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD13	2	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD21	2	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD22	2	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD23	2	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD11	16	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD12	16	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD13	16	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD21	16	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD22	16	0.51
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD23	16	0.51
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	4	0.51
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	20	0.51
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	18	0.51
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	18	0.51
(1,4965)	1:84:A:PHE:H	1:88:A:ARG:HE	7	0.51
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	3	0.51
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	3	0.51
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	3	0.51
(1,3312)	1:158:A:TYR:HB2	1:157:A:VAL:HB	4	0.51
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD2	20	0.51
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD3	20	0.51
(1,3053)	1:55:A:ALA:HB3	1:40:A:GLN:HA	1	0.51
(1,3053)	1:55:A:ALA:HB2	1:40:A:GLN:HA	3	0.51
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	7	0.51
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	20	0.51
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	20	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2905)	1:126:A:LEU:HD13	1:199:A:TYR:HD1	2	0.51
(1,2905)	1:126:A:LEU:HD13	1:199:A:TYR:HD2	2	0.51
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD11	20	0.51
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD12	20	0.51
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD13	20	0.51
(1,2848)	1:11:A:VAL:HG22	1:44:A:ARG:H	15	0.51
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD11	20	0.51
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD12	20	0.51
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD13	20	0.51
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD21	20	0.51
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD22	20	0.51
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD23	20	0.51
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG11	13	0.51
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG12	13	0.51
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG13	13	0.51
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG21	13	0.51
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG22	13	0.51
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG23	13	0.51
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG11	18	0.51
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG12	18	0.51
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG13	18	0.51
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG21	18	0.51
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG22	18	0.51
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG23	18	0.51
(1,2649)	1:64:A:ILE:HD12	1:63:A:ASP:HB2	9	0.51
(1,2649)	1:64:A:ILE:HD12	1:63:A:ASP:HB3	9	0.51
(1,2549)	1:36:A:VAL:HG11	1:37:A:LYS:HA	15	0.51
(1,2539)	1:54:A:ILE:HD12	1:14:A:ALA:HA	2	0.51
(1,2536)	1:181:A:ILE:HD11	1:179:A:LEU:HA	1	0.51
(1,2531)	1:142:A:VAL:HG23	1:143:A:LEU:HA	7	0.51
(1,2531)	1:142:A:VAL:HG13	1:147:A:ASP:HA	20	0.51
(1,2530)	1:36:A:VAL:HG11	1:37:A:LYS:HA	15	0.51
(1,2442)	1:101:A:ILE:HD11	1:100:A:GLU:H	10	0.51
(1,2418)	1:200:A:LEU:HD21	1:199:A:TYR:H	14	0.51
(1,2379)	1:24:A:LEU:HD11	1:44:A:ARG:H	3	0.51
(1,2373)	1:26:A:ILE:HD11	1:43:A:VAL:H	11	0.51
(1,2373)	1:26:A:ILE:HD13	1:43:A:VAL:H	17	0.51
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB2	14	0.51
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB3	14	0.51
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE1	1	0.51
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE2	1	0.51
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	3	0.51
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	14	0.51
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	14	0.51
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	19	0.51
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	19	0.51
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD21	13	0.51
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD22	13	0.51
(1,5797)	1:71:A:GLU:HA	1:68:A:PRO:HD2	5	0.5
(1,5797)	1:71:A:GLU:HA	1:68:A:PRO:HD3	5	0.5
(1,5797)	1:71:A:GLU:HA	1:68:A:PRO:HD2	8	0.5
(1,5797)	1:71:A:GLU:HA	1:68:A:PRO:HD3	8	0.5
(1,5602)	1:34:A:ILE:HG21	1:53:A:SER:H	14	0.5
(1,5558)	1:12:A:VAL:HG12	1:17:A:ARG:H	11	0.5
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE2	17	0.5
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE3	17	0.5
(1,5466)	1:47:A:ILE:H	1:77:A:GLY:HA2	12	0.5
(1,5466)	1:47:A:ILE:H	1:77:A:GLY:HA3	12	0.5
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG12	15	0.5
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG13	15	0.5
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	11	0.5
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	11	0.5
(1,5333)	1:221:A:GLU:H	1:222:A:LEU:HB2	6	0.5
(1,5333)	1:221:A:GLU:H	1:222:A:LEU:HB3	6	0.5
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	18	0.5
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	8	0.5
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD2	16	0.5
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD3	16	0.5
(1,3433)	1:4:A:LEU:HD21	1:56:A:ARG:HD2	20	0.5
(1,3433)	1:4:A:LEU:HD21	1:56:A:ARG:HD3	20	0.5
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	13	0.5
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	13	0.5
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG2	7	0.5
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG3	7	0.5
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	18	0.5
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	18	0.5
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	18	0.5
(1,3014)	1:175:A:ILE:HG22	1:156:A:LEU:HA	8	0.5
(1,3014)	1:175:A:ILE:HG21	1:156:A:LEU:HA	13	0.5
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	4	0.5
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	11	0.5
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	1	0.5
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2828)	1:137:A:ILE:HB	1:101:A:ILE:HA	12	0.5
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG11	17	0.5
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG12	17	0.5
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG13	17	0.5
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG21	17	0.5
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG22	17	0.5
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG23	17	0.5
(1,2532)	1:183:A:ILE:HG23	1:182:A:PRO:HA	10	0.5
(1,2489)	1:87:A:THR:HG23	1:84:A:PHE:HD1	18	0.5
(1,2489)	1:87:A:THR:HG23	1:84:A:PHE:HD2	18	0.5
(1,2481)	1:187:A:ALA:HB3	1:191:A:ASN:HD21	8	0.5
(1,2481)	1:187:A:ALA:HB3	1:191:A:ASN:HD22	8	0.5
(1,2471)	1:12:A:VAL:HG23	1:20:A:TRP:HD1	3	0.5
(1,2442)	1:101:A:ILE:HD11	1:100:A:GLU:H	18	0.5
(1,2429)	1:181:A:ILE:HD13	1:180:A:GLY:H	3	0.5
(1,2429)	1:181:A:ILE:HD13	1:180:A:GLY:H	8	0.5
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	17	0.5
(1,2238)	1:207:A:CYS:HA	1:213:A:GLN:HE21	15	0.5
(1,2238)	1:207:A:CYS:HA	1:213:A:GLN:HE22	15	0.5
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	5	0.5
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	5	0.5
(1,132)	1:154:A:PHE:HD1	1:158:A:TYR:HB2	20	0.5
(1,132)	1:154:A:PHE:HD1	1:158:A:TYR:HB3	20	0.5
(1,5861)	1:116:A:PRO:HG3	1:117:A:GLU:H	4	0.49
(1,5681)	1:94:A:TRP:HZ3	1:94:A:TRP:H	9	0.49
(1,5386)	1:200:A:LEU:H	1:196:A:TYR:HE1	8	0.49
(1,5386)	1:200:A:LEU:H	1:196:A:TYR:HE2	8	0.49
(1,5318)	1:36:A:VAL:H	1:34:A:ILE:HB	13	0.49
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB2	13	0.49
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB3	13	0.49
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	16	0.49
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	16	0.49
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	16	0.49
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	18	0.49
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB2	7	0.49
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB3	7	0.49
(1,4985)	1:19:A:GLU:H	1:19:A:GLU:HG2	15	0.49
(1,4985)	1:19:A:GLU:H	1:19:A:GLU:HG3	15	0.49
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	19	0.49
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	19	0.49
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	19	0.49
(1,4907)	1:20:A:TRP:HE1	1:78:A:LEU:HB2	9	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4907)	1:20:A:TRP:HE1	1:78:A:LEU:HB3	9	0.49
(1,3339)	1:123:A:LEU:HB3	1:150:A:LEU:HG	13	0.49
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	1	0.49
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	1	0.49
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	1	0.49
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	1	0.49
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	1	0.49
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	1	0.49
(1,3014)	1:175:A:ILE:HG23	1:156:A:LEU:HA	11	0.49
(1,3014)	1:175:A:ILE:HG21	1:156:A:LEU:HA	18	0.49
(1,3014)	1:175:A:ILE:HG21	1:156:A:LEU:HA	19	0.49
(1,2975)	1:179:A:LEU:HD21	1:176:A:TYR:HA	8	0.49
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB2	10	0.49
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB3	10	0.49
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG12	8	0.49
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG13	8	0.49
(1,2848)	1:11:A:VAL:HG21	1:44:A:ARG:H	9	0.49
(1,2745)	1:137:A:ILE:HD12	1:126:A:LEU:HB2	15	0.49
(1,2745)	1:137:A:ILE:HD12	1:126:A:LEU:HB3	15	0.49
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB2	9	0.49
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB3	9	0.49
(1,2548)	1:150:A:LEU:HD12	1:141:A:PRO:HA	5	0.49
(1,2534)	1:101:A:ILE:HG23	1:140:A:PRO:HA	12	0.49
(1,2429)	1:181:A:ILE:HD11	1:180:A:GLY:H	2	0.49
(1,2415)	1:19:A:GLU:H	1:19:A:GLU:HG2	15	0.49
(1,2415)	1:19:A:GLU:H	1:19:A:GLU:HG3	15	0.49
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	7	0.49
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	7	0.49
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB2	17	0.48
(1,5803)	1:18:A:THR:HG22	1:16:A:GLU:HB3	17	0.48
(1,5578)	1:153:A:LEU:HA	1:157:A:VAL:H	7	0.48
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	11	0.48
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	11	0.48
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	11	0.48
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	11	0.48
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	11	0.48
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	11	0.48
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB1	8	0.48
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB2	8	0.48
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB3	8	0.48
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD11	10	0.48
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD12	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD13	10	0.48
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD21	10	0.48
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD22	10	0.48
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD23	10	0.48
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD11	11	0.48
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD12	11	0.48
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD13	11	0.48
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD21	11	0.48
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD22	11	0.48
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD23	11	0.48
(1,5128)	1:197:A:ARG:H	1:200:A:LEU:HG	14	0.48
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB2	10	0.48
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB3	10	0.48
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB2	10	0.48
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB3	10	0.48
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	3	0.48
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	3	0.48
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	3	0.48
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	12	0.48
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	12	0.48
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	12	0.48
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	1	0.48
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	1	0.48
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	1	0.48
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	1	0.48
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	1	0.48
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	1	0.48
(1,3210)	1:15:A:THR:HA	1:17:A:ARG:HD2	20	0.48
(1,3210)	1:15:A:THR:HA	1:17:A:ARG:HD3	20	0.48
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD2	11	0.48
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD3	11	0.48
(1,3014)	1:175:A:ILE:HG23	1:156:A:LEU:HA	6	0.48
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	20	0.48
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	3	0.48
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD11	14	0.48
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD12	14	0.48
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD13	14	0.48
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD21	14	0.48
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD22	14	0.48
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD23	14	0.48
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB2	8	0.48
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB3	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2596)	1:90:A:VAL:HG21	1:85:A:LEU:HA	17	0.48
(1,2535)	1:101:A:ILE:HD11	1:97:A:ASP:HA	10	0.48
(1,2532)	1:183:A:ILE:HG21	1:184:A:LEU:HA	15	0.48
(1,2468)	1:84:A:PHE:HE1	1:88:A:ARG:HG2	19	0.48
(1,2468)	1:84:A:PHE:HE1	1:88:A:ARG:HG3	19	0.48
(1,2425)	1:54:A:ILE:HG23	1:12:A:VAL:H	12	0.48
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	10	0.48
(1,5559)	1:24:A:LEU:HD11	1:8:A:VAL:H	9	0.47
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	13	0.47
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	13	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	13	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	13	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	13	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	13	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	13	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	13	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	19	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	19	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	19	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	19	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	19	0.47
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	19	0.47
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	8	0.47
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	8	0.47
(1,5416)	1:10:A:SER:H	1:22:A:PRO:HB2	7	0.47
(1,5416)	1:10:A:SER:H	1:22:A:PRO:HB3	7	0.47
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	19	0.47
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	19	0.47
(1,5233)	1:1:A:ASN:HD22	1:61:A:GLU:HG2	3	0.47
(1,5233)	1:1:A:ASN:HD22	1:61:A:GLU:HG3	3	0.47
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB2	18	0.47
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB3	18	0.47
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	3	0.47
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	5	0.47
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	15	0.47
(1,3433)	1:4:A:LEU:HD23	1:56:A:ARG:HD2	17	0.47
(1,3433)	1:4:A:LEU:HD23	1:56:A:ARG:HD3	17	0.47
(1,3312)	1:158:A:TYR:HB2	1:157:A:VAL:HB	3	0.47
(1,3139)	1:101:A:ILE:H	1:97:A:ASP:HB2	13	0.47
(1,3139)	1:101:A:ILE:H	1:97:A:ASP:HB3	13	0.47
(1,3053)	1:55:A:ALA:HB2	1:40:A:GLN:HA	7	0.47
(1,3053)	1:55:A:ALA:HB3	1:40:A:GLN:HA	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3053)	1:55:A:ALA:HB2	1:40:A:GLN:HA	13	0.47
(1,3053)	1:55:A:ALA:HB1	1:40:A:GLN:HA	18	0.47
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD2	7	0.47
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD3	7	0.47
(1,3016)	1:157:A:VAL:HG22	1:156:A:LEU:HA	8	0.47
(1,3016)	1:157:A:VAL:HG22	1:156:A:LEU:HA	14	0.47
(1,3014)	1:175:A:ILE:HG21	1:156:A:LEU:HA	1	0.47
(1,3014)	1:175:A:ILE:HG22	1:156:A:LEU:HA	4	0.47
(1,3014)	1:175:A:ILE:HG21	1:156:A:LEU:HA	16	0.47
(1,2975)	1:65:A:LEU:HD22	1:82:A:SER:HA	5	0.47
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB2	11	0.47
(1,2970)	1:68:A:PRO:HG2	1:70:A:SER:HB3	11	0.47
(1,2908)	1:137:A:ILE:HD11	1:199:A:TYR:H	2	0.47
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	6	0.47
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	12	0.47
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	12	0.47
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	12	0.47
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	12	0.47
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	12	0.47
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	12	0.47
(1,2699)	1:8:A:VAL:HG21	1:85:A:LEU:HG	1	0.47
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB2	17	0.47
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB3	17	0.47
(1,2573)	1:187:A:ALA:HB3	1:186:A:SER:HB2	5	0.47
(1,2573)	1:187:A:ALA:HB3	1:186:A:SER:HB3	5	0.47
(1,2573)	1:187:A:ALA:HB2	1:186:A:SER:HB2	18	0.47
(1,2573)	1:187:A:ALA:HB2	1:186:A:SER:HB3	18	0.47
(1,2502)	1:42:A:LEU:HG	1:27:A:SER:HA	1	0.47
(1,2462)	1:197:A:ARG:HD2	1:196:A:TYR:HE1	9	0.47
(1,2462)	1:197:A:ARG:HD2	1:196:A:TYR:HE2	9	0.47
(1,2426)	1:101:A:ILE:HG22	1:103:A:GLU:H	11	0.47
(1,2418)	1:200:A:LEU:HD21	1:199:A:TYR:H	5	0.47
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	1	0.47
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	1	0.47
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	10	0.47
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	10	0.47
(1,5848)	1:113:A:GLU:HB3	1:114:A:LEU:HG	5	0.46
(1,5803)	1:18:A:THR:HG21	1:16:A:GLU:HB2	1	0.46
(1,5803)	1:18:A:THR:HG21	1:16:A:GLU:HB3	1	0.46
(1,5801)	1:146:A:LYS:HE2	1:182:A:PRO:HG2	6	0.46
(1,5801)	1:146:A:LYS:HE2	1:182:A:PRO:HG3	6	0.46
(1,5679)	1:139:A:LYS:HB2	1:138:A:ASN:HD21	19	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5679)	1:139:A:LYS:HB2	1:138:A:ASN:HD22	19	0.46
(1,5679)	1:139:A:LYS:HB3	1:138:A:ASN:HD21	19	0.46
(1,5679)	1:139:A:LYS:HB3	1:138:A:ASN:HD22	19	0.46
(1,5642)	1:187:A:ALA:HB3	1:191:A:ASN:HD21	20	0.46
(1,5642)	1:187:A:ALA:HB3	1:191:A:ASN:HD22	20	0.46
(1,5556)	1:197:A:ARG:HB3	1:201:A:TYR:H	15	0.46
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	5	0.46
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	5	0.46
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	19	0.46
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	19	0.46
(1,5396)	1:124:A:GLN:H	1:98:A:ILE:HG12	19	0.46
(1,5396)	1:124:A:GLN:H	1:98:A:ILE:HG13	19	0.46
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	6	0.46
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	2	0.46
(1,5233)	1:1:A:ASN:HD22	1:61:A:GLU:HG2	13	0.46
(1,5233)	1:1:A:ASN:HD22	1:61:A:GLU:HG3	13	0.46
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	19	0.46
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	19	0.46
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	1	0.46
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	16	0.46
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	3	0.46
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	3	0.46
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG2	8	0.46
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG3	8	0.46
(1,3442)	1:59:A:ILE:HG21	1:61:A:GLU:HG2	19	0.46
(1,3442)	1:59:A:ILE:HG21	1:61:A:GLU:HG3	19	0.46
(1,3442)	1:59:A:ILE:HG22	1:61:A:GLU:HG2	19	0.46
(1,3442)	1:59:A:ILE:HG22	1:61:A:GLU:HG3	19	0.46
(1,3442)	1:59:A:ILE:HG23	1:61:A:GLU:HG2	19	0.46
(1,3442)	1:59:A:ILE:HG23	1:61:A:GLU:HG3	19	0.46
(1,3287)	1:53:A:SER:HB2	1:37:A:LYS:HD2	15	0.46
(1,3287)	1:53:A:SER:HB2	1:37:A:LYS:HD3	15	0.46
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	8	0.46
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	8	0.46
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	8	0.46
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	8	0.46
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	8	0.46
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	8	0.46
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG2	5	0.46
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG3	5	0.46
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG2	8	0.46
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG3	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	10	0.46
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	10	0.46
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	10	0.46
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	18	0.46
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	9	0.46
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	9	0.46
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	11	0.46
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD11	7	0.46
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD12	7	0.46
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD13	7	0.46
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD21	7	0.46
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD22	7	0.46
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD23	7	0.46
(1,2745)	1:137:A:ILE:HD12	1:126:A:LEU:HB2	8	0.46
(1,2745)	1:137:A:ILE:HD12	1:126:A:LEU:HB3	8	0.46
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG11	3	0.46
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG12	3	0.46
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG13	3	0.46
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG21	3	0.46
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG22	3	0.46
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG23	3	0.46
(1,2717)	1:130:A:MET:HE1	1:133:A:ARG:HG2	15	0.46
(1,2717)	1:130:A:MET:HE1	1:133:A:ARG:HG3	15	0.46
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB2	14	0.46
(1,2696)	1:181:A:ILE:HB	1:182:A:PRO:HB3	14	0.46
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB2	15	0.46
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB3	15	0.46
(1,2636)	1:65:A:LEU:HD11	1:63:A:ASP:HB2	12	0.46
(1,2636)	1:65:A:LEU:HD11	1:63:A:ASP:HB3	12	0.46
(1,2548)	1:150:A:LEU:HD22	1:141:A:PRO:HA	11	0.46
(1,2532)	1:183:A:ILE:HG21	1:182:A:PRO:HA	12	0.46
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD11	10	0.46
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD12	10	0.46
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD13	10	0.46
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD21	10	0.46
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD22	10	0.46
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD23	10	0.46
(1,2399)	1:96:A:MET:HE1	1:137:A:ILE:H	17	0.46
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	2	0.46
(1,2379)	1:24:A:LEU:HD12	1:46:A:PHE:H	14	0.46
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	16	0.46
(1,2373)	1:26:A:ILE:HD13	1:43:A:VAL:H	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE1	20	0.46
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE2	20	0.46
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD1	11	0.46
(1,173)	1:190:A:TYR:H	1:190:A:TYR:HD2	11	0.46
(1,173)	1:191:A:ASN:HD22	1:190:A:TYR:HD1	16	0.46
(1,173)	1:191:A:ASN:HD22	1:190:A:TYR:HD2	16	0.46
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG21	20	0.45
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG22	20	0.45
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG23	20	0.45
(1,5788)	1:98:A:ILE:HD11	1:105:A:SER:HA	14	0.45
(1,5681)	1:94:A:TRP:HZ3	1:94:A:TRP:H	5	0.45
(1,5681)	1:44:A:ARG:HE	1:50:A:LYS:H	15	0.45
(1,5642)	1:187:A:ALA:HB1	1:191:A:ASN:HD21	13	0.45
(1,5642)	1:187:A:ALA:HB1	1:191:A:ASN:HD22	13	0.45
(1,5559)	1:24:A:LEU:HD22	1:8:A:VAL:H	16	0.45
(1,5428)	1:23:A:ALA:H	1:46:A:PHE:HD1	14	0.45
(1,5428)	1:23:A:ALA:H	1:46:A:PHE:HD2	14	0.45
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	8	0.45
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	8	0.45
(1,5366)	1:79:A:GLN:HE22	1:82:A:SER:HB2	4	0.45
(1,5366)	1:79:A:GLN:HE22	1:82:A:SER:HB3	4	0.45
(1,5318)	1:36:A:VAL:H	1:37:A:LYS:HG2	12	0.45
(1,5318)	1:36:A:VAL:H	1:37:A:LYS:HG3	12	0.45
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	5	0.45
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB2	5	0.45
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB3	5	0.45
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	7	0.45
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	14	0.45
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	18	0.45
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	10	0.45
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	10	0.45
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	10	0.45
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	10	0.45
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	10	0.45
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	10	0.45
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	10	0.45
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	10	0.45
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	10	0.45
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	10	0.45
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	10	0.45
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	10	0.45
(1,3431)	1:83:A:ILE:HG21	1:87:A:THR:HG21	13	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3431)	1:83:A:ILE:HG21	1:87:A:THR:HG22	13	0.45
(1,3431)	1:83:A:ILE:HG21	1:87:A:THR:HG23	13	0.45
(1,3379)	1:75:A:LYS:HG2	1:19:A:GLU:HG2	4	0.45
(1,3379)	1:75:A:LYS:HG2	1:19:A:GLU:HG3	4	0.45
(1,3200)	1:184:A:LEU:HA	1:183:A:ILE:HG12	19	0.45
(1,3200)	1:184:A:LEU:HA	1:183:A:ILE:HG13	19	0.45
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG2	9	0.45
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG3	9	0.45
(1,3053)	1:55:A:ALA:HB1	1:40:A:GLN:HA	11	0.45
(1,3051)	1:34:A:ILE:HG22	1:53:A:SER:HA	15	0.45
(1,3012)	1:160:A:GLN:HG3	1:156:A:LEU:HA	19	0.45
(1,2975)	1:65:A:LEU:HD22	1:82:A:SER:HA	17	0.45
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	18	0.45
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	18	0.45
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	12	0.45
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG11	1	0.45
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG12	1	0.45
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG13	1	0.45
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG21	1	0.45
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG22	1	0.45
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG23	1	0.45
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD11	6	0.45
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD12	6	0.45
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD13	6	0.45
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD21	6	0.45
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD22	6	0.45
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD23	6	0.45
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	4	0.45
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	4	0.45
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	4	0.45
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	4	0.45
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	4	0.45
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	4	0.45
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD11	6	0.45
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD12	6	0.45
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD13	6	0.45
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD21	6	0.45
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD22	6	0.45
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD23	6	0.45
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD11	10	0.45
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD12	10	0.45
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD13	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD21	10	0.45
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD22	10	0.45
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD23	10	0.45
(1,2699)	1:8:A:VAL:HG12	1:85:A:LEU:HB2	11	0.45
(1,2699)	1:8:A:VAL:HG12	1:85:A:LEU:HB3	11	0.45
(1,2699)	1:8:A:VAL:HG22	1:85:A:LEU:HG	20	0.45
(1,2682)	1:62:A:VAL:HB	1:9:A:VAL:HB	14	0.45
(1,2671)	1:18:A:THR:HG22	1:16:A:GLU:HG2	17	0.45
(1,2671)	1:18:A:THR:HG22	1:16:A:GLU:HG3	17	0.45
(1,2660)	1:65:A:LEU:HD13	1:63:A:ASP:HB2	17	0.45
(1,2660)	1:65:A:LEU:HD13	1:63:A:ASP:HB3	17	0.45
(1,2571)	1:130:A:MET:HE3	1:136:A:PRO:HA	2	0.45
(1,2532)	1:183:A:ILE:HG21	1:184:A:LEU:HA	2	0.45
(1,2532)	1:183:A:ILE:HG21	1:182:A:PRO:HA	13	0.45
(1,2531)	1:142:A:VAL:HG21	1:143:A:LEU:HA	8	0.45
(1,2529)	1:5:A:LEU:HD11	1:2:A:ASP:HA	2	0.45
(1,2481)	1:187:A:ALA:HB2	1:191:A:ASN:HD21	9	0.45
(1,2481)	1:187:A:ALA:HB2	1:191:A:ASN:HD22	9	0.45
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD1	3	0.45
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD2	3	0.45
(1,2429)	1:181:A:ILE:HD11	1:180:A:GLY:H	12	0.45
(1,2403)	1:3:A:GLU:HB2	1:4:A:LEU:H	18	0.45
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB2	10	0.45
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB3	10	0.45
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG21	3	0.45
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG22	3	0.45
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG23	3	0.45
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB2	14	0.45
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB3	14	0.45
(1,5861)	1:116:A:PRO:HG2	1:117:A:GLU:H	20	0.44
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB2	19	0.44
(1,5803)	1:18:A:THR:HG23	1:16:A:GLU:HB3	19	0.44
(1,5678)	1:137:A:ILE:HD11	1:130:A:MET:H	19	0.44
(1,5642)	1:187:A:ALA:HB1	1:191:A:ASN:HD21	5	0.44
(1,5642)	1:187:A:ALA:HB1	1:191:A:ASN:HD22	5	0.44
(1,5642)	1:187:A:ALA:HB2	1:191:A:ASN:HD21	7	0.44
(1,5642)	1:187:A:ALA:HB2	1:191:A:ASN:HD22	7	0.44
(1,5642)	1:143:A:LEU:HG	1:191:A:ASN:HD21	11	0.44
(1,5642)	1:143:A:LEU:HG	1:191:A:ASN:HD22	11	0.44
(1,5557)	1:124:A:GLN:HB3	1:95:A:LYS:H	8	0.44
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE2	3	0.44
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE3	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	4	0.44
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	4	0.44
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	4	0.44
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	4	0.44
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	4	0.44
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	4	0.44
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	12	0.44
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	12	0.44
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	12	0.44
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	12	0.44
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	12	0.44
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	12	0.44
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB2	15	0.44
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB3	15	0.44
(1,5266)	1:211:A:ASN:HD21	1:210:A:ALA:HB1	17	0.44
(1,5266)	1:211:A:ASN:HD21	1:210:A:ALA:HB2	17	0.44
(1,5266)	1:211:A:ASN:HD21	1:210:A:ALA:HB3	17	0.44
(1,5233)	1:1:A:ASN:HD21	1:61:A:GLU:HG2	6	0.44
(1,5233)	1:1:A:ASN:HD21	1:61:A:GLU:HG3	6	0.44
(1,5128)	1:197:A:ARG:H	1:198:A:LYS:HD2	13	0.44
(1,5128)	1:197:A:ARG:H	1:198:A:LYS:HD3	13	0.44
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	9	0.44
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	12	0.44
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG2	4	0.44
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG3	4	0.44
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	4	0.44
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	4	0.44
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	1	0.44
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	1	0.44
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	2	0.44
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	2	0.44
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	2	0.44
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	2	0.44
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	2	0.44
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	2	0.44
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	2	0.44
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	2	0.44
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	2	0.44
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	2	0.44
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	2	0.44
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	2	0.44
(1,3442)	1:59:A:ILE:HG21	1:61:A:GLU:HG2	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3442)	1:59:A:ILE:HG21	1:61:A:GLU:HG3	6	0.44
(1,3442)	1:59:A:ILE:HG22	1:61:A:GLU:HG2	6	0.44
(1,3442)	1:59:A:ILE:HG22	1:61:A:GLU:HG3	6	0.44
(1,3442)	1:59:A:ILE:HG23	1:61:A:GLU:HG2	6	0.44
(1,3442)	1:59:A:ILE:HG23	1:61:A:GLU:HG3	6	0.44
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	8	0.44
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	8	0.44
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	8	0.44
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD11	11	0.44
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD12	11	0.44
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD13	11	0.44
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD21	11	0.44
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD22	11	0.44
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD23	11	0.44
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	6	0.44
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	6	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG2	2	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG3	2	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG2	7	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG3	7	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG2	10	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG3	10	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG2	12	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG3	12	0.44
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG2	14	0.44
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG3	14	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG2	16	0.44
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG3	16	0.44
(1,3014)	1:175:A:ILE:HG23	1:156:A:LEU:HA	2	0.44
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	2	0.44
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	12	0.44
(1,2908)	1:137:A:ILE:HD11	1:130:A:MET:H	19	0.44
(1,2903)	1:11:A:VAL:HG11	1:54:A:ILE:HB	15	0.44
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG11	16	0.44
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG12	16	0.44
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG13	16	0.44
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG21	16	0.44
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG22	16	0.44
(1,2873)	1:10:A:SER:HA	1:9:A:VAL:HG23	16	0.44
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD11	6	0.44
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD12	6	0.44
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD13	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2842)	1:181:A:ILE:HD13	1:176:A:TYR:HB2	17	0.44
(1,2842)	1:181:A:ILE:HD13	1:176:A:TYR:HB3	17	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD11	1	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD12	1	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD13	1	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD21	1	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD22	1	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD23	1	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD11	17	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD12	17	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD13	17	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD21	17	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD22	17	0.44
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD23	17	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	3	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	3	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	3	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	3	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	3	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	3	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	11	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	11	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	11	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	11	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	11	0.44
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	11	0.44
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD11	14	0.44
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD12	14	0.44
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD13	14	0.44
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD21	14	0.44
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD22	14	0.44
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD23	14	0.44
(1,2745)	1:137:A:ILE:HD11	1:126:A:LEU:HB2	5	0.44
(1,2745)	1:137:A:ILE:HD11	1:126:A:LEU:HB3	5	0.44
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB2	6	0.44
(1,2708)	1:137:A:ILE:HD12	1:140:A:PRO:HB3	6	0.44
(1,2699)	1:8:A:VAL:HG22	1:85:A:LEU:HG	2	0.44
(1,2699)	1:8:A:VAL:HG22	1:85:A:LEU:HG	5	0.44
(1,2699)	1:8:A:VAL:HG13	1:85:A:LEU:HB2	12	0.44
(1,2699)	1:8:A:VAL:HG13	1:85:A:LEU:HB3	12	0.44
(1,2660)	1:65:A:LEU:HD13	1:63:A:ASP:HB2	14	0.44
(1,2660)	1:65:A:LEU:HD13	1:63:A:ASP:HB3	14	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2578)	1:64:A:ILE:HD13	1:62:A:VAL:HA	14	0.44
(1,2571)	1:130:A:MET:HE2	1:136:A:PRO:HA	3	0.44
(1,2571)	1:130:A:MET:HE1	1:198:A:LYS:HA	4	0.44
(1,2571)	1:130:A:MET:HE3	1:198:A:LYS:HA	14	0.44
(1,2548)	1:150:A:LEU:HD22	1:141:A:PRO:HA	18	0.44
(1,2539)	1:54:A:ILE:HD13	1:14:A:ALA:HA	19	0.44
(1,2375)	1:60:A:LYS:HD2	1:61:A:GLU:H	9	0.44
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	17	0.44
(1,172)	1:122:A:PHE:HE2	1:126:A:LEU:HG	18	0.44
(1,113)	1:176:A:TYR:HD1	1:182:A:PRO:HA	13	0.44
(1,5804)	1:167:A:ASP:HB2	1:168:A:SER:HB2	1	0.43
(1,5804)	1:167:A:ASP:HB2	1:168:A:SER:HB3	1	0.43
(1,5795)	1:167:A:ASP:HB2	1:168:A:SER:HB2	1	0.43
(1,5795)	1:167:A:ASP:HB2	1:168:A:SER:HB3	1	0.43
(1,5681)	1:94:A:TRP:HZ3	1:94:A:TRP:H	3	0.43
(1,5665)	1:200:A:LEU:HB3	1:205:A:GLU:H	19	0.43
(1,5602)	1:34:A:ILE:HG23	1:53:A:SER:H	12	0.43
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	20	0.43
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	1	0.43
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	1	0.43
(1,5331)	1:75:A:LYS:H	1:71:A:GLU:HG2	20	0.43
(1,5331)	1:75:A:LYS:H	1:71:A:GLU:HG3	20	0.43
(1,5313)	1:20:A:TRP:HE1	1:71:A:GLU:HG2	13	0.43
(1,5313)	1:20:A:TRP:HE1	1:71:A:GLU:HG3	13	0.43
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB2	12	0.43
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB3	12	0.43
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	10	0.43
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	10	0.43
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	10	0.43
(1,5128)	1:197:A:ARG:H	1:200:A:LEU:HG	12	0.43
(1,5081)	1:88:A:ARG:H	1:89:A:VAL:HA	3	0.43
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG2	18	0.43
(1,5054)	1:78:A:LEU:H	1:75:A:LYS:HG3	18	0.43
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG2	1	0.43
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG3	1	0.43
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	6	0.43
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	6	0.43
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG2	10	0.43
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG3	10	0.43
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	11	0.43
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	13	0.43
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	13	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	13	0.43
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	5	0.43
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	5	0.43
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	5	0.43
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	5	0.43
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	5	0.43
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	5	0.43
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	5	0.43
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	5	0.43
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	5	0.43
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	5	0.43
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	5	0.43
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	5	0.43
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG2	6	0.43
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG3	6	0.43
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG2	6	0.43
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG3	6	0.43
(1,3340)	1:19:A:GLU:HB2	1:75:A:LYS:HG2	16	0.43
(1,3340)	1:19:A:GLU:HB2	1:75:A:LYS:HG3	16	0.43
(1,3340)	1:19:A:GLU:HB3	1:75:A:LYS:HG2	16	0.43
(1,3340)	1:19:A:GLU:HB3	1:75:A:LYS:HG3	16	0.43
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	14	0.43
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	14	0.43
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	14	0.43
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	14	0.43
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	3	0.43
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	3	0.43
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG2	1	0.43
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG3	1	0.43
(1,3053)	1:55:A:ALA:HB1	1:40:A:GLN:HA	8	0.43
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	10	0.43
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD2	16	0.43
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD3	16	0.43
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD2	17	0.43
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD3	17	0.43
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	10	0.43
(1,2835)	1:126:A:LEU:HD12	1:130:A:MET:H	8	0.43
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG21	9	0.43
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG22	9	0.43
(1,2783)	1:61:A:GLU:HG3	1:59:A:ILE:HG23	9	0.43
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD11	1	0.43
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD12	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD13	1	0.43
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD21	1	0.43
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD22	1	0.43
(1,2744)	1:195:A:ALA:HB2	1:153:A:LEU:HD23	1	0.43
(1,2660)	1:65:A:LEU:HD13	1:63:A:ASP:HB2	3	0.43
(1,2660)	1:65:A:LEU:HD13	1:63:A:ASP:HB3	3	0.43
(1,2577)	1:166:A:ILE:HD11	1:160:A:GLN:HA	9	0.43
(1,2577)	1:166:A:ILE:HD13	1:160:A:GLN:HA	20	0.43
(1,2575)	1:64:A:ILE:HG22	1:78:A:LEU:HA	8	0.43
(1,2571)	1:130:A:MET:HE3	1:198:A:LYS:HA	16	0.43
(1,2539)	1:54:A:ILE:HD12	1:11:A:VAL:HA	18	0.43
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD1	7	0.43
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD2	7	0.43
(1,2422)	1:126:A:LEU:HD12	1:130:A:MET:H	8	0.43
(1,2379)	1:24:A:LEU:HD23	1:44:A:ARG:H	15	0.43
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB2	18	0.43
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB3	18	0.43
(1,2256)	1:89:A:VAL:HA	1:88:A:ARG:H	3	0.43
(1,5861)	1:116:A:PRO:HG3	1:117:A:GLU:H	7	0.42
(1,5850)	1:113:A:GLU:HG2	1:114:A:LEU:H	13	0.42
(1,5788)	1:98:A:ILE:HD12	1:105:A:SER:HA	15	0.42
(1,5625)	1:146:A:LYS:HG2	1:145:A:TYR:H	5	0.42
(1,5578)	1:153:A:LEU:HA	1:157:A:VAL:H	14	0.42
(1,5558)	1:12:A:VAL:HG11	1:17:A:ARG:H	15	0.42
(1,5554)	1:128:A:LYS:HB2	1:129:A:PHE:H	16	0.42
(1,5554)	1:128:A:LYS:HB2	1:129:A:PHE:H	19	0.42
(1,5534)	1:78:A:LEU:HB3	1:81:A:ALA:H	12	0.42
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE2	18	0.42
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE3	18	0.42
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	9	0.42
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	9	0.42
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	9	0.42
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	9	0.42
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	9	0.42
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	9	0.42
(1,5417)	1:10:A:SER:H	1:3:A:GLU:HB2	7	0.42
(1,5417)	1:10:A:SER:H	1:3:A:GLU:HB3	7	0.42
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	8	0.42
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	8	0.42
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	12	0.42
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	13	0.42
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG2	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG3	2	0.42
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	15	0.42
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	15	0.42
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG2	2	0.42
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG3	2	0.42
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	1	0.42
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	16	0.42
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	16	0.42
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	16	0.42
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD2	15	0.42
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD3	15	0.42
(1,3448)	1:101:A:ILE:HG13	1:96:A:MET:HG2	20	0.42
(1,3448)	1:101:A:ILE:HG13	1:96:A:MET:HG3	20	0.42
(1,3433)	1:12:A:VAL:HG23	1:17:A:ARG:HD2	11	0.42
(1,3433)	1:12:A:VAL:HG23	1:17:A:ARG:HD3	11	0.42
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	19	0.42
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	19	0.42
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	19	0.42
(1,3317)	1:39:A:ASP:HB2	1:38:A:LYS:HG2	4	0.42
(1,3317)	1:39:A:ASP:HB2	1:38:A:LYS:HG3	4	0.42
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD2	13	0.42
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD3	13	0.42
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	14	0.42
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	14	0.42
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	14	0.42
(1,3051)	1:34:A:ILE:HG23	1:53:A:SER:HA	13	0.42
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	20	0.42
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD2	1	0.42
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD3	1	0.42
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	3	0.42
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	13	0.42
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD11	13	0.42
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD12	13	0.42
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD13	13	0.42
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	1	0.42
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	20	0.42
(1,2848)	1:11:A:VAL:HG21	1:44:A:ARG:H	3	0.42
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	7	0.42
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	7	0.42
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD11	2	0.42
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD12	2	0.42
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD13	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD21	2	0.42
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD22	2	0.42
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD23	2	0.42
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG21	18	0.42
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG22	18	0.42
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG23	18	0.42
(1,2717)	1:130:A:MET:HE3	1:133:A:ARG:HG2	3	0.42
(1,2717)	1:130:A:MET:HE3	1:133:A:ARG:HG3	3	0.42
(1,2532)	1:183:A:ILE:HG22	1:184:A:LEU:HA	18	0.42
(1,2489)	1:87:A:THR:HG23	1:84:A:PHE:HD1	14	0.42
(1,2489)	1:87:A:THR:HG23	1:84:A:PHE:HD2	14	0.42
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD1	18	0.42
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD2	18	0.42
(1,2471)	1:12:A:VAL:HG22	1:20:A:TRP:HD1	15	0.42
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG2	2	0.42
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG3	2	0.42
(1,2389)	1:42:A:LEU:HG	1:52:A:TYR:H	4	0.42
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	9	0.42
(1,173)	1:191:A:ASN:HD21	1:190:A:TYR:HD1	12	0.42
(1,173)	1:191:A:ASN:HD21	1:190:A:TYR:HD2	12	0.42
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD21	6	0.42
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD22	6	0.42
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD21	20	0.42
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD22	20	0.42
(1,5803)	1:18:A:THR:HG21	1:16:A:GLU:HB2	5	0.41
(1,5803)	1:18:A:THR:HG21	1:16:A:GLU:HB3	5	0.41
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	3	0.41
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	3	0.41
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	17	0.41
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	17	0.41
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	17	0.41
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	10	0.41
(1,4975)	1:75:A:LYS:H	1:73:A:SER:HA	10	0.41
(1,4975)	1:75:A:LYS:H	1:73:A:SER:HA	20	0.41
(1,3544)	1:97:A:ASP:HB3	1:99:A:SER:HA	14	0.41
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB2	3	0.41
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB3	3	0.41
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB2	3	0.41
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB3	3	0.41
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	13	0.41
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	13	0.41
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	13	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	13	0.41
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	13	0.41
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	13	0.41
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	13	0.41
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	13	0.41
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	13	0.41
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	13	0.41
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	13	0.41
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	13	0.41
(1,3398)	1:15:A:THR:HG21	1:16:A:GLU:HG2	4	0.41
(1,3398)	1:15:A:THR:HG21	1:16:A:GLU:HG3	4	0.41
(1,3398)	1:15:A:THR:HG22	1:16:A:GLU:HG2	4	0.41
(1,3398)	1:15:A:THR:HG22	1:16:A:GLU:HG3	4	0.41
(1,3398)	1:15:A:THR:HG23	1:16:A:GLU:HG2	4	0.41
(1,3398)	1:15:A:THR:HG23	1:16:A:GLU:HG3	4	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	5	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	5	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	5	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	5	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	5	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	5	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	12	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	12	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	12	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	12	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	12	0.41
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	12	0.41
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG2	11	0.41
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG3	11	0.41
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD2	3	0.41
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD3	3	0.41
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD2	10	0.41
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD3	10	0.41
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	17	0.41
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	17	0.41
(1,2905)	1:126:A:LEU:HD11	1:199:A:TYR:HD1	10	0.41
(1,2905)	1:126:A:LEU:HD11	1:199:A:TYR:HD2	10	0.41
(1,2866)	1:210:A:ALA:HA	1:5:A:LEU:HB2	10	0.41
(1,2866)	1:210:A:ALA:HA	1:5:A:LEU:HB3	10	0.41
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	19	0.41
(1,2848)	1:11:A:VAL:HG23	1:44:A:ARG:H	17	0.41
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB2	19	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2843)	1:181:A:ILE:HD13	1:153:A:LEU:HB3	19	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	5	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	5	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	5	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	5	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	5	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	5	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	16	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	16	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	16	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	16	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	16	0.41
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	16	0.41
(1,2745)	1:137:A:ILE:HD11	1:126:A:LEU:HB2	20	0.41
(1,2745)	1:137:A:ILE:HD11	1:126:A:LEU:HB3	20	0.41
(1,2577)	1:166:A:ILE:HD13	1:160:A:GLN:HA	16	0.41
(1,2549)	1:36:A:VAL:HG13	1:37:A:LYS:HA	17	0.41
(1,2532)	1:183:A:ILE:HG21	1:182:A:PRO:HA	20	0.41
(1,2530)	1:36:A:VAL:HG13	1:37:A:LYS:HA	17	0.41
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD1	11	0.41
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD2	11	0.41
(1,2459)	1:90:A:VAL:HG21	1:94:A:TRP:HZ3	3	0.41
(1,2457)	1:90:A:VAL:HG21	1:94:A:TRP:HZ3	3	0.41
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	1	0.41
(1,2383)	1:43:A:VAL:HG23	1:52:A:TYR:H	17	0.41
(1,5803)	1:152:A:LYS:HD2	1:113:A:GLU:HB2	16	0.4
(1,5803)	1:152:A:LYS:HD2	1:113:A:GLU:HB3	16	0.4
(1,5697)	1:124:A:GLN:HB2	1:121:A:ASN:HD21	3	0.4
(1,5697)	1:124:A:GLN:HB2	1:121:A:ASN:HD22	3	0.4
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	13	0.4
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	9	0.4
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	9	0.4
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	17	0.4
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	17	0.4
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD2	3	0.4
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD3	3	0.4
(1,5366)	1:79:A:GLN:HE22	1:82:A:SER:HB2	3	0.4
(1,5366)	1:79:A:GLN:HE22	1:82:A:SER:HB3	3	0.4
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	20	0.4
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	20	0.4
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB1	10	0.4
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB2	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB3	10	0.4
(1,5314)	1:20:A:TRP:HE1	1:75:A:LYS:HG2	20	0.4
(1,5314)	1:20:A:TRP:HE1	1:75:A:LYS:HG3	20	0.4
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	16	0.4
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	16	0.4
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB2	12	0.4
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB3	12	0.4
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	12	0.4
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	12	0.4
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG2	20	0.4
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG3	20	0.4
(1,4985)	1:19:A:GLU:H	1:19:A:GLU:HG2	18	0.4
(1,4985)	1:19:A:GLU:H	1:19:A:GLU:HG3	18	0.4
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	11	0.4
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	11	0.4
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	11	0.4
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	15	0.4
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	15	0.4
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	15	0.4
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	19	0.4
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	19	0.4
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	19	0.4
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	19	0.4
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	19	0.4
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	19	0.4
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	11	0.4
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	11	0.4
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	11	0.4
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	11	0.4
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	5	0.4
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	5	0.4
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	9	0.4
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	9	0.4
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	9	0.4
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	14	0.4
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	15	0.4
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	14	0.4
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	15	0.4
(1,2841)	1:166:A:ILE:HD12	1:157:A:VAL:H	14	0.4
(1,2835)	1:126:A:LEU:HD22	1:130:A:MET:H	18	0.4
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD11	9	0.4
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD12	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD13	9	0.4
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD21	9	0.4
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD22	9	0.4
(1,2759)	1:71:A:GLU:HB3	1:78:A:LEU:HD23	9	0.4
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	18	0.4
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	18	0.4
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	18	0.4
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	18	0.4
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	18	0.4
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	18	0.4
(1,2745)	1:137:A:ILE:HD12	1:126:A:LEU:HB2	14	0.4
(1,2745)	1:137:A:ILE:HD12	1:126:A:LEU:HB3	14	0.4
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG2	9	0.4
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG3	9	0.4
(1,2665)	1:47:A:ILE:HD11	1:76:A:PRO:HB2	9	0.4
(1,2665)	1:47:A:ILE:HD11	1:76:A:PRO:HB3	9	0.4
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB2	8	0.4
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB3	8	0.4
(1,2632)	1:198:A:LYS:HD2	1:199:A:TYR:HB2	10	0.4
(1,2632)	1:198:A:LYS:HD2	1:199:A:TYR:HB3	10	0.4
(1,2578)	1:64:A:ILE:HD11	1:62:A:VAL:HA	6	0.4
(1,2564)	1:157:A:VAL:HG12	1:153:A:LEU:HA	19	0.4
(1,2549)	1:36:A:VAL:HG12	1:37:A:LYS:HA	2	0.4
(1,2549)	1:36:A:VAL:HG13	1:37:A:LYS:HA	9	0.4
(1,2549)	1:36:A:VAL:HG13	1:37:A:LYS:HA	10	0.4
(1,2536)	1:181:A:ILE:HD13	1:179:A:LEU:HA	15	0.4
(1,2534)	1:101:A:ILE:HG22	1:105:A:SER:HA	11	0.4
(1,2532)	1:183:A:ILE:HG21	1:182:A:PRO:HA	1	0.4
(1,2530)	1:36:A:VAL:HG12	1:37:A:LYS:HA	2	0.4
(1,2530)	1:36:A:VAL:HG13	1:37:A:LYS:HA	9	0.4
(1,2530)	1:36:A:VAL:HG13	1:37:A:LYS:HA	10	0.4
(1,2502)	1:42:A:LEU:HG	1:27:A:SER:HA	3	0.4
(1,2474)	1:101:A:ILE:HD13	1:127:A:TYR:HD1	18	0.4
(1,2474)	1:101:A:ILE:HD13	1:127:A:TYR:HD2	18	0.4
(1,2466)	1:60:A:LYS:HD2	1:17:A:ARG:HE	16	0.4
(1,2442)	1:101:A:ILE:HD11	1:100:A:GLU:H	1	0.4
(1,2442)	1:101:A:ILE:HD12	1:100:A:GLU:H	9	0.4
(1,2442)	1:101:A:ILE:HD11	1:100:A:GLU:H	17	0.4
(1,2422)	1:126:A:LEU:HD22	1:130:A:MET:H	18	0.4
(1,2415)	1:19:A:GLU:H	1:19:A:GLU:HG2	18	0.4
(1,2415)	1:19:A:GLU:H	1:19:A:GLU:HG3	18	0.4
(1,2389)	1:42:A:LEU:HG	1:52:A:TYR:H	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2375)	1:60:A:LYS:HD2	1:61:A:GLU:H	18	0.4
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD21	4	0.4
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD22	4	0.4
(1,128)	1:51:A:PHE:HD2	1:133:A:ARG:HB2	14	0.4
(1,128)	1:51:A:PHE:HD2	1:133:A:ARG:HB3	14	0.4
(1,113)	1:176:A:TYR:HD1	1:182:A:PRO:HA	4	0.4
(1,5791)	1:102:A:LEU:HB3	1:105:A:SER:HB2	3	0.39
(1,5791)	1:102:A:LEU:HB3	1:105:A:SER:HB3	3	0.39
(1,5790)	1:102:A:LEU:HB3	1:105:A:SER:HB2	3	0.39
(1,5790)	1:102:A:LEU:HB3	1:105:A:SER:HB3	3	0.39
(1,5786)	1:115:A:ASP:HA	1:117:A:GLU:H	10	0.39
(1,5697)	1:139:A:LYS:HD3	1:138:A:ASN:HD21	9	0.39
(1,5697)	1:139:A:LYS:HD3	1:138:A:ASN:HD22	9	0.39
(1,5642)	1:187:A:ALA:HB2	1:191:A:ASN:HD21	3	0.39
(1,5642)	1:187:A:ALA:HB2	1:191:A:ASN:HD22	3	0.39
(1,5642)	1:187:A:ALA:HB3	1:191:A:ASN:HD21	14	0.39
(1,5642)	1:187:A:ALA:HB3	1:191:A:ASN:HD22	14	0.39
(1,5602)	1:34:A:ILE:HG23	1:53:A:SER:H	2	0.39
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	3	0.39
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	3	0.39
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	3	0.39
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	3	0.39
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	3	0.39
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	3	0.39
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB2	14	0.39
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB3	14	0.39
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	10	0.39
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD21	2	0.39
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD22	2	0.39
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	12	0.39
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	12	0.39
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	20	0.39
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	20	0.39
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	20	0.39
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	11	0.39
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG2	1	0.39
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG3	1	0.39
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	7	0.39
(1,3544)	1:97:A:ASP:HB3	1:99:A:SER:HA	5	0.39
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB2	10	0.39
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB3	10	0.39
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	1	0.39
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	1	0.39
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	1	0.39
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	19	0.39
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	19	0.39
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	19	0.39
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	19	0.39
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD2	12	0.39
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD3	12	0.39
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	13	0.39
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	13	0.39
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	13	0.39
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD2	12	0.39
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD3	12	0.39
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD2	18	0.39
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD3	18	0.39
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	2	0.39
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	2	0.39
(1,2917)	1:196:A:TYR:HA	1:201:A:TYR:H	1	0.39
(1,2917)	1:196:A:TYR:HA	1:195:A:ALA:H	17	0.39
(1,2872)	1:100:A:GLU:HB3	1:101:A:ILE:HD11	4	0.39
(1,2872)	1:100:A:GLU:HB3	1:101:A:ILE:HD12	4	0.39
(1,2872)	1:100:A:GLU:HB3	1:101:A:ILE:HD13	4	0.39
(1,2841)	1:166:A:ILE:HD12	1:157:A:VAL:H	2	0.39
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD11	1	0.39
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD12	1	0.39
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD13	1	0.39
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD21	1	0.39
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD22	1	0.39
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD23	1	0.39
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD11	5	0.39
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD12	5	0.39
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD13	5	0.39
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD21	5	0.39
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD22	5	0.39
(1,2770)	1:101:A:ILE:HD12	1:123:A:LEU:HD23	5	0.39
(1,2745)	1:137:A:ILE:HD13	1:126:A:LEU:HB2	11	0.39
(1,2745)	1:137:A:ILE:HD13	1:126:A:LEU:HB3	11	0.39
(1,2701)	1:90:A:VAL:HG12	1:85:A:LEU:HB2	14	0.39
(1,2701)	1:90:A:VAL:HG12	1:85:A:LEU:HB3	14	0.39
(1,2700)	1:90:A:VAL:HG12	1:85:A:LEU:HB2	14	0.39
(1,2700)	1:90:A:VAL:HG12	1:85:A:LEU:HB3	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2682)	1:62:A:VAL:HB	1:9:A:VAL:HB	9	0.39
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB2	14	0.39
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB3	14	0.39
(1,2636)	1:65:A:LEU:HD22	1:63:A:ASP:HB2	15	0.39
(1,2636)	1:65:A:LEU:HD22	1:63:A:ASP:HB3	15	0.39
(1,2578)	1:64:A:ILE:HD12	1:62:A:VAL:HA	2	0.39
(1,2573)	1:187:A:ALA:HB1	1:186:A:SER:HB2	9	0.39
(1,2573)	1:187:A:ALA:HB1	1:186:A:SER:HB3	9	0.39
(1,2532)	1:183:A:ILE:HG22	1:182:A:PRO:HA	6	0.39
(1,2532)	1:183:A:ILE:HG22	1:182:A:PRO:HA	19	0.39
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD1	18	0.39
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD2	18	0.39
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD1	16	0.39
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD2	16	0.39
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD11	17	0.39
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD12	17	0.39
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD13	17	0.39
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD21	17	0.39
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD22	17	0.39
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD23	17	0.39
(1,2460)	1:64:A:ILE:HG23	1:20:A:TRP:HZ2	11	0.39
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG2	1	0.39
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG3	1	0.39
(1,2375)	1:60:A:LYS:HD2	1:61:A:GLU:H	6	0.39
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG21	2	0.39
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG22	2	0.39
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG23	2	0.39
(1,2255)	1:105:A:SER:HB2	1:101:A:ILE:HG21	19	0.39
(1,2255)	1:105:A:SER:HB2	1:101:A:ILE:HG22	19	0.39
(1,2255)	1:105:A:SER:HB2	1:101:A:ILE:HG23	19	0.39
(1,172)	1:122:A:PHE:HE2	1:126:A:LEU:HG	16	0.39
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD21	12	0.39
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD22	12	0.39
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG2	3	0.39
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG3	3	0.39
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG21	3	0.38
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG22	3	0.38
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG23	3	0.38
(1,5678)	1:137:A:ILE:HD11	1:130:A:MET:H	12	0.38
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	17	0.38
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	17	0.38
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB2	16	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB3	16	0.38
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	11	0.38
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	11	0.38
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG2	3	0.38
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG3	3	0.38
(1,5266)	1:211:A:ASN:HD21	1:210:A:ALA:HB1	10	0.38
(1,5266)	1:211:A:ASN:HD21	1:210:A:ALA:HB2	10	0.38
(1,5266)	1:211:A:ASN:HD21	1:210:A:ALA:HB3	10	0.38
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG2	7	0.38
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG3	7	0.38
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	7	0.38
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	7	0.38
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	7	0.38
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	20	0.38
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	20	0.38
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	14	0.38
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	14	0.38
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	14	0.38
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	2	0.38
(1,5020)	1:85:A:LEU:H	1:88:A:ARG:HE	2	0.38
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	11	0.38
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	11	0.38
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	11	0.38
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	12	0.38
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	12	0.38
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	12	0.38
(1,3544)	1:97:A:ASP:HB3	1:99:A:SER:HA	15	0.38
(1,3544)	1:97:A:ASP:HB3	1:99:A:SER:HA	18	0.38
(1,3477)	1:83:A:ILE:H	1:65:A:LEU:HB2	17	0.38
(1,3477)	1:83:A:ILE:H	1:65:A:LEU:HB3	17	0.38
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	4	0.38
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	4	0.38
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	4	0.38
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	4	0.38
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	4	0.38
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	4	0.38
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	4	0.38
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	4	0.38
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	4	0.38
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	4	0.38
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	4	0.38
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3274)	1:22:A:PRO:HD2	1:47:A:ILE:HG12	9	0.38
(1,3274)	1:22:A:PRO:HD2	1:47:A:ILE:HG13	9	0.38
(1,3270)	1:182:A:PRO:HD2	1:146:A:LYS:HD2	15	0.38
(1,3270)	1:182:A:PRO:HD2	1:146:A:LYS:HD3	15	0.38
(1,3217)	1:98:A:ILE:HA	1:96:A:MET:HG2	16	0.38
(1,3217)	1:98:A:ILE:HA	1:96:A:MET:HG3	16	0.38
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	4	0.38
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	4	0.38
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	4	0.38
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	4	0.38
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	13	0.38
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	13	0.38
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	13	0.38
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	13	0.38
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	20	0.38
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	20	0.38
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	20	0.38
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	20	0.38
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	7	0.38
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	7	0.38
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	7	0.38
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG2	15	0.38
(1,3082)	1:173:A:LYS:H	1:173:A:LYS:HG3	15	0.38
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD2	4	0.38
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD3	4	0.38
(1,3014)	1:175:A:ILE:HG21	1:156:A:LEU:HA	14	0.38
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	16	0.38
(1,2975)	1:179:A:LEU:HD12	1:176:A:TYR:HA	3	0.38
(1,2908)	1:137:A:ILE:HD11	1:130:A:MET:H	12	0.38
(1,2841)	1:166:A:ILE:HD11	1:157:A:VAL:H	9	0.38
(1,2835)	1:126:A:LEU:HD22	1:130:A:MET:H	16	0.38
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	5	0.38
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG11	20	0.38
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG12	20	0.38
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG13	20	0.38
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG21	20	0.38
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG22	20	0.38
(1,2783)	1:61:A:GLU:HG3	1:9:A:VAL:HG23	20	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	1	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	1	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	1	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	1	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	1	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	2	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	2	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	2	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	2	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	2	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	2	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	8	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	8	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	8	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	8	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	8	0.38
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	8	0.38
(1,2699)	1:8:A:VAL:HG22	1:85:A:LEU:HG	9	0.38
(1,2699)	1:8:A:VAL:HG23	1:85:A:LEU:HG	16	0.38
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG2	7	0.38
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG3	7	0.38
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB2	1	0.38
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB3	1	0.38
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB2	3	0.38
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB3	3	0.38
(1,2636)	1:65:A:LEU:HD11	1:66:A:ASN:HB2	10	0.38
(1,2636)	1:65:A:LEU:HD11	1:66:A:ASN:HB3	10	0.38
(1,2636)	1:65:A:LEU:HD13	1:63:A:ASP:HB2	19	0.38
(1,2636)	1:65:A:LEU:HD13	1:63:A:ASP:HB3	19	0.38
(1,2577)	1:166:A:ILE:HD13	1:160:A:GLN:HA	6	0.38
(1,2539)	1:54:A:ILE:HD11	1:14:A:ALA:HA	5	0.38
(1,2532)	1:183:A:ILE:HG22	1:184:A:LEU:HA	8	0.38
(1,2531)	1:142:A:VAL:HG13	1:147:A:ASP:HA	2	0.38
(1,2531)	1:142:A:VAL:HG22	1:143:A:LEU:HA	4	0.38
(1,2531)	1:142:A:VAL:HG23	1:143:A:LEU:HA	19	0.38
(1,2529)	1:5:A:LEU:HD13	1:2:A:ASP:HA	6	0.38
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	15	0.38
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD1	16	0.38
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD2	16	0.38
(1,2479)	1:194:A:THR:HG23	1:199:A:TYR:HD1	8	0.38
(1,2479)	1:194:A:THR:HG23	1:199:A:TYR:HD2	8	0.38
(1,2422)	1:126:A:LEU:HD22	1:130:A:MET:H	16	0.38
(1,2403)	1:3:A:GLU:HB3	1:4:A:LEU:H	11	0.38
(1,2375)	1:60:A:LYS:HD2	1:61:A:GLU:H	7	0.38
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	10	0.38
(1,2306)	1:81:A:ALA:HA	1:78:A:LEU:HA	13	0.38
(1,2289)	1:119:A:ARG:HA	1:117:A:GLU:H	3	0.38
(1,172)	1:122:A:PHE:HE1	1:126:A:LEU:HG	2	0.38
(1,113)	1:176:A:TYR:HD1	1:182:A:PRO:HA	8	0.38
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	2	0.37
(1,5522)	1:9:A:VAL:HG22	1:23:A:ALA:H	2	0.37
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	7	0.37
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD2	14	0.37
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD3	14	0.37
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	7	0.37
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	7	0.37
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	13	0.37
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	13	0.37
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	15	0.37
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	15	0.37
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG11	15	0.37
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG12	15	0.37
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG13	15	0.37
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG21	15	0.37
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG22	15	0.37
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG23	15	0.37
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD11	18	0.37
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD12	18	0.37
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD13	18	0.37
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD21	18	0.37
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD22	18	0.37
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD23	18	0.37
(1,5053)	1:78:A:LEU:H	1:64:A:ILE:HG12	15	0.37
(1,5053)	1:78:A:LEU:H	1:64:A:ILE:HG13	15	0.37
(1,5020)	1:85:A:LEU:H	1:88:A:ARG:HE	1	0.37
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG2	19	0.37
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG3	19	0.37
(1,4965)	1:84:A:PHE:H	1:88:A:ARG:HE	12	0.37
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	15	0.37
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	15	0.37
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	15	0.37
(1,3477)	1:83:A:ILE:H	1:65:A:LEU:HB2	8	0.37
(1,3477)	1:83:A:ILE:H	1:65:A:LEU:HB3	8	0.37
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB2	19	0.37
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB3	19	0.37
(1,3443)	1:101:A:ILE:HG13	1:96:A:MET:HB2	14	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3443)	1:101:A:ILE:HG13	1:96:A:MET:HB3	14	0.37
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE2	18	0.37
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE3	18	0.37
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE2	18	0.37
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE3	18	0.37
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE2	18	0.37
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE3	18	0.37
(1,3340)	1:19:A:GLU:HB2	1:75:A:LYS:HG2	11	0.37
(1,3340)	1:19:A:GLU:HB2	1:75:A:LYS:HG3	11	0.37
(1,3340)	1:19:A:GLU:HB3	1:75:A:LYS:HG2	11	0.37
(1,3340)	1:19:A:GLU:HB3	1:75:A:LYS:HG3	11	0.37
(1,3312)	1:58:A:ASP:HB2	1:57:A:LYS:HB2	5	0.37
(1,3312)	1:58:A:ASP:HB2	1:57:A:LYS:HB3	5	0.37
(1,3312)	1:158:A:TYR:HB2	1:157:A:VAL:HB	15	0.37
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD11	14	0.37
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD12	14	0.37
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD13	14	0.37
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD21	14	0.37
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD22	14	0.37
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD23	14	0.37
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	15	0.37
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	15	0.37
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	15	0.37
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	15	0.37
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG2	9	0.37
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG3	9	0.37
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	6	0.37
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	6	0.37
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	6	0.37
(1,2947)	1:133:A:ARG:HD3	1:136:A:PRO:HA	2	0.37
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	16	0.37
(1,2849)	1:67:A:LEU:HG	1:66:A:ASN:H	19	0.37
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD11	6	0.37
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD12	6	0.37
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD13	6	0.37
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD21	6	0.37
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD22	6	0.37
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD23	6	0.37
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG21	10	0.37
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG22	10	0.37
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG23	10	0.37
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG11	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG12	7	0.37
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG13	7	0.37
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG21	7	0.37
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG22	7	0.37
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG23	7	0.37
(1,2708)	1:137:A:ILE:HD12	1:139:A:LYS:HB2	18	0.37
(1,2708)	1:137:A:ILE:HD12	1:139:A:LYS:HB3	18	0.37
(1,2632)	1:198:A:LYS:HD3	1:199:A:TYR:HB2	2	0.37
(1,2632)	1:198:A:LYS:HD3	1:199:A:TYR:HB3	2	0.37
(1,2529)	1:5:A:LEU:HD13	1:2:A:ASP:HA	13	0.37
(1,2479)	1:194:A:THR:HG21	1:199:A:TYR:HD1	10	0.37
(1,2479)	1:194:A:THR:HG21	1:199:A:TYR:HD2	10	0.37
(1,2474)	1:101:A:ILE:HD11	1:127:A:TYR:HD1	9	0.37
(1,2474)	1:101:A:ILE:HD11	1:127:A:TYR:HD2	9	0.37
(1,2466)	1:60:A:LYS:HD3	1:20:A:TRP:HD1	17	0.37
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG2	19	0.37
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG3	19	0.37
(1,5842)	1:222:A:LEU:H	1:221:A:GLU:HG2	10	0.36
(1,5842)	1:222:A:LEU:H	1:221:A:GLU:HG3	10	0.36
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG21	14	0.36
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG22	14	0.36
(1,5810)	1:61:A:GLU:HB2	1:59:A:ILE:HG23	14	0.36
(1,5785)	1:222:A:LEU:H	1:221:A:GLU:HG2	10	0.36
(1,5785)	1:222:A:LEU:H	1:221:A:GLU:HG3	10	0.36
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD21	13	0.36
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD22	13	0.36
(1,5625)	1:143:A:LEU:HG	1:145:A:TYR:H	12	0.36
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	11	0.36
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	11	0.36
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE2	15	0.36
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE3	15	0.36
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG12	10	0.36
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG13	10	0.36
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	7	0.36
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	7	0.36
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	14	0.36
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	14	0.36
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	15	0.36
(1,5356)	1:48:A:ASP:H	1:44:A:ARG:HG2	15	0.36
(1,5356)	1:48:A:ASP:H	1:44:A:ARG:HG3	15	0.36
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	8	0.36
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5237)	1:145:A:TYR:H	1:143:A:LEU:HG	12	0.36
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG2	14	0.36
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG3	14	0.36
(1,5226)	1:82:A:SER:H	1:79:A:GLN:HA	18	0.36
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	1	0.36
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	1	0.36
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	13	0.36
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	13	0.36
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	14	0.36
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	14	0.36
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	8	0.36
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	8	0.36
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	8	0.36
(1,5139)	1:80:A:LYS:H	1:47:A:ILE:HD11	13	0.36
(1,5139)	1:80:A:LYS:H	1:47:A:ILE:HD12	13	0.36
(1,5139)	1:80:A:LYS:H	1:47:A:ILE:HD13	13	0.36
(1,5088)	1:172:A:TRP:H	1:173:A:LYS:HA	19	0.36
(1,5070)	1:40:A:GLN:H	1:56:A:ARG:H	20	0.36
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	15	0.36
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE2	10	0.36
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE3	10	0.36
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD11	1	0.36
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD12	1	0.36
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD13	1	0.36
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD21	1	0.36
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD22	1	0.36
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD23	1	0.36
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD11	9	0.36
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD12	9	0.36
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD13	9	0.36
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD21	9	0.36
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD22	9	0.36
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD23	9	0.36
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	3	0.36
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	3	0.36
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	3	0.36
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	3	0.36
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	17	0.36
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	17	0.36
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	17	0.36
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	17	0.36
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	8	0.36
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	8	0.36
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG21	14	0.36
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG22	14	0.36
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG23	14	0.36
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	14	0.36
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	14	0.36
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	15	0.36
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	15	0.36
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	11	0.36
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	11	0.36
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	11	0.36
(1,3053)	1:55:A:ALA:HB3	1:40:A:GLN:HA	14	0.36
(1,2998)	1:204:A:GLU:HB2	1:197:A:ARG:HA	14	0.36
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG12	16	0.36
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG13	16	0.36
(1,2837)	1:34:A:ILE:HG12	1:51:A:PHE:HA	15	0.36
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	11	0.36
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	11	0.36
(1,2745)	1:137:A:ILE:HD13	1:126:A:LEU:HB2	4	0.36
(1,2745)	1:137:A:ILE:HD13	1:126:A:LEU:HB3	4	0.36
(1,2606)	1:64:A:ILE:HD12	1:78:A:LEU:HA	4	0.36
(1,2578)	1:64:A:ILE:HD11	1:62:A:VAL:HA	13	0.36
(1,2549)	1:36:A:VAL:HG13	1:37:A:LYS:HA	5	0.36
(1,2549)	1:36:A:VAL:HG13	1:37:A:LYS:HA	7	0.36
(1,2539)	1:54:A:ILE:HD12	1:14:A:ALA:HA	8	0.36
(1,2530)	1:36:A:VAL:HG13	1:37:A:LYS:HA	5	0.36
(1,2530)	1:36:A:VAL:HG13	1:37:A:LYS:HA	7	0.36
(1,2529)	1:5:A:LEU:HD12	1:2:A:ASP:HA	17	0.36
(1,2482)	1:175:A:ILE:HD11	1:172:A:TRP:HZ2	2	0.36
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD1	10	0.36
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD2	10	0.36
(1,2479)	1:194:A:THR:HG23	1:190:A:TYR:HD1	2	0.36
(1,2479)	1:194:A:THR:HG23	1:190:A:TYR:HD2	2	0.36
(1,2479)	1:194:A:THR:HG22	1:190:A:TYR:HD1	13	0.36
(1,2479)	1:194:A:THR:HG22	1:190:A:TYR:HD2	13	0.36
(1,2411)	1:88:A:ARG:HD2	1:88:A:ARG:H	20	0.36
(1,2403)	1:3:A:GLU:HB2	1:4:A:LEU:H	12	0.36
(1,2400)	1:34:A:ILE:HD11	1:52:A:TYR:H	18	0.36
(1,2375)	1:60:A:LYS:HD2	1:61:A:GLU:H	15	0.36
(1,5679)	1:139:A:LYS:HD2	1:138:A:ASN:HD21	11	0.35
(1,5679)	1:139:A:LYS:HD2	1:138:A:ASN:HD22	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5679)	1:139:A:LYS:HD3	1:138:A:ASN:HD21	11	0.35
(1,5679)	1:139:A:LYS:HD3	1:138:A:ASN:HD22	11	0.35
(1,5679)	1:139:A:LYS:HD2	1:138:A:ASN:HD21	17	0.35
(1,5679)	1:139:A:LYS:HD2	1:138:A:ASN:HD22	17	0.35
(1,5679)	1:139:A:LYS:HD3	1:138:A:ASN:HD21	17	0.35
(1,5679)	1:139:A:LYS:HD3	1:138:A:ASN:HD22	17	0.35
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	15	0.35
(1,5572)	1:94:A:TRP:HD1	1:94:A:TRP:H	12	0.35
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	17	0.35
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	17	0.35
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	17	0.35
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	17	0.35
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	17	0.35
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	17	0.35
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	7	0.35
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	7	0.35
(1,5396)	1:124:A:GLN:H	1:98:A:ILE:HG12	7	0.35
(1,5396)	1:124:A:GLN:H	1:98:A:ILE:HG13	7	0.35
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	14	0.35
(1,5373)	1:134:A:GLY:H	1:133:A:ARG:HD2	17	0.35
(1,5373)	1:134:A:GLY:H	1:133:A:ARG:HD3	17	0.35
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	7	0.35
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	7	0.35
(1,5333)	1:221:A:GLU:H	1:222:A:LEU:HG	12	0.35
(1,5252)	1:88:A:ARG:HE	1:88:A:ARG:HA	2	0.35
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	5	0.35
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	5	0.35
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	15	0.35
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	15	0.35
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	15	0.35
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	16	0.35
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	16	0.35
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG2	11	0.35
(1,4996)	1:75:A:LYS:H	1:76:A:PRO:HG3	11	0.35
(1,4965)	1:84:A:PHE:H	1:88:A:ARG:HE	14	0.35
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	10	0.35
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	10	0.35
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	10	0.35
(1,3270)	1:182:A:PRO:HD2	1:146:A:LYS:HD2	10	0.35
(1,3270)	1:182:A:PRO:HD2	1:146:A:LYS:HD3	10	0.35
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	13	0.35
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	13	0.35
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	11	0.35
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	11	0.35
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	11	0.35
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	4	0.35
(1,2903)	1:11:A:VAL:HG13	1:54:A:ILE:HB	1	0.35
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD11	14	0.35
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD12	14	0.35
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD13	14	0.35
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	7	0.35
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	4	0.35
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	11	0.35
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD11	19	0.35
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD12	19	0.35
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD13	19	0.35
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD21	19	0.35
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD22	19	0.35
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD23	19	0.35
(1,2660)	1:65:A:LEU:HD13	1:63:A:ASP:HB2	20	0.35
(1,2660)	1:65:A:LEU:HD13	1:63:A:ASP:HB3	20	0.35
(1,2532)	1:183:A:ILE:HG23	1:182:A:PRO:HA	5	0.35
(1,2531)	1:142:A:VAL:HG21	1:143:A:LEU:HA	18	0.35
(1,2502)	1:42:A:LEU:HG	1:53:A:SER:HA	17	0.35
(1,2485)	1:34:A:ILE:HG12	1:51:A:PHE:HD1	15	0.35
(1,2485)	1:34:A:ILE:HG12	1:51:A:PHE:HD2	15	0.35
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD1	17	0.35
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD2	17	0.35
(1,2403)	1:3:A:GLU:HB2	1:4:A:LEU:H	2	0.35
(1,2375)	1:60:A:LYS:HD2	1:61:A:GLU:H	5	0.35
(1,2375)	1:60:A:LYS:HD2	1:61:A:GLU:H	20	0.35
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	7	0.35
(1,2314)	1:88:A:ARG:HA	1:88:A:ARG:HE	2	0.35
(1,2238)	1:207:A:CYS:HA	1:213:A:GLN:HE21	7	0.35
(1,2238)	1:207:A:CYS:HA	1:213:A:GLN:HE22	7	0.35
(1,113)	1:176:A:TYR:HD2	1:182:A:PRO:HA	6	0.35
(1,5821)	1:108:A:LYS:HB2	1:108:A:LYS:H	7	0.34
(1,5663)	1:38:A:LYS:HG3	1:40:A:GLN:H	6	0.34
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	16	0.34
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	18	0.34
(1,5490)	1:63:A:ASP:H	1:67:A:LEU:HG	14	0.34
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	4	0.34
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD2	7	0.34
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD3	7	0.34
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	16	0.34
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	6	0.34
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	6	0.34
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	2	0.34
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	2	0.34
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	9	0.34
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	9	0.34
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	6	0.34
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	7	0.34
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	7	0.34
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	9	0.34
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	9	0.34
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB2	3	0.34
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB3	3	0.34
(1,5166)	1:159:A:HIS:H	1:157:A:VAL:HB	15	0.34
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG2	5	0.34
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG3	5	0.34
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	2	0.34
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	7	0.34
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	7	0.34
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	7	0.34
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD2	14	0.34
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD3	14	0.34
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	2	0.34
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	2	0.34
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	2	0.34
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	10	0.34
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	10	0.34
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	10	0.34
(1,3259)	1:80:A:LYS:HA	1:80:A:LYS:HE2	12	0.34
(1,3259)	1:80:A:LYS:HA	1:80:A:LYS:HE3	12	0.34
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	17	0.34
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	17	0.34
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	17	0.34
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	17	0.34
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	17	0.34
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	17	0.34
(1,3221)	1:170:A:ALA:HA	1:173:A:LYS:HD2	11	0.34
(1,3221)	1:170:A:ALA:HA	1:173:A:LYS:HD3	11	0.34
(1,3177)	1:122:A:PHE:HD1	1:203:A:PHE:HB2	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3177)	1:122:A:PHE:HD1	1:203:A:PHE:HB3	6	0.34
(1,3177)	1:122:A:PHE:HD2	1:203:A:PHE:HB2	6	0.34
(1,3177)	1:122:A:PHE:HD2	1:203:A:PHE:HB3	6	0.34
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB2	10	0.34
(1,3177)	1:203:A:PHE:HE1	1:203:A:PHE:HB3	10	0.34
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB2	10	0.34
(1,3177)	1:203:A:PHE:HE2	1:203:A:PHE:HB3	10	0.34
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	17	0.34
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	17	0.34
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	8	0.34
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	8	0.34
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	8	0.34
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	16	0.34
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	16	0.34
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	16	0.34
(1,3096)	1:19:A:GLU:H	1:16:A:GLU:HG2	5	0.34
(1,3096)	1:19:A:GLU:H	1:16:A:GLU:HG3	5	0.34
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG2	17	0.34
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG3	17	0.34
(1,3053)	1:55:A:ALA:HB1	1:40:A:GLN:HA	16	0.34
(1,2908)	1:137:A:ILE:HD13	1:199:A:TYR:H	13	0.34
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD11	16	0.34
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD12	16	0.34
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD13	16	0.34
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD21	16	0.34
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD22	16	0.34
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD23	16	0.34
(1,2726)	1:61:A:GLU:HG3	1:60:A:LYS:HB2	18	0.34
(1,2726)	1:61:A:GLU:HG3	1:60:A:LYS:HB3	18	0.34
(1,2682)	1:62:A:VAL:HB	1:9:A:VAL:HB	15	0.34
(1,2578)	1:64:A:ILE:HD11	1:62:A:VAL:HA	15	0.34
(1,2575)	1:64:A:ILE:HG21	1:78:A:LEU:HA	3	0.34
(1,2549)	1:36:A:VAL:HG13	1:37:A:LYS:HA	1	0.34
(1,2549)	1:36:A:VAL:HG11	1:37:A:LYS:HA	3	0.34
(1,2530)	1:36:A:VAL:HG13	1:37:A:LYS:HA	1	0.34
(1,2530)	1:36:A:VAL:HG11	1:37:A:LYS:HA	3	0.34
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD1	14	0.34
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD2	14	0.34
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG2	5	0.34
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG3	5	0.34
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	14	0.34
(1,2373)	1:26:A:ILE:HD13	1:43:A:VAL:H	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG21	7	0.34
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG22	7	0.34
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG23	7	0.34
(1,5803)	1:152:A:LYS:HD2	1:113:A:GLU:HB2	13	0.33
(1,5803)	1:152:A:LYS:HD2	1:113:A:GLU:HB3	13	0.33
(1,5788)	1:98:A:ILE:HD11	1:105:A:SER:HA	11	0.33
(1,5554)	1:128:A:LYS:HB3	1:129:A:PHE:H	7	0.33
(1,5522)	1:9:A:VAL:HG23	1:23:A:ALA:H	18	0.33
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	14	0.33
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	14	0.33
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	15	0.33
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	15	0.33
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG12	17	0.33
(1,5450)	1:124:A:GLN:H	1:101:A:ILE:HG13	17	0.33
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	5	0.33
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	3	0.33
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	3	0.33
(1,5331)	1:75:A:LYS:H	1:71:A:GLU:HG2	10	0.33
(1,5331)	1:75:A:LYS:H	1:71:A:GLU:HG3	10	0.33
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	20	0.33
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG11	15	0.33
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG12	15	0.33
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG13	15	0.33
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG21	15	0.33
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG22	15	0.33
(1,5267)	1:160:A:GLN:HE21	1:157:A:VAL:HG23	15	0.33
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	10	0.33
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	10	0.33
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	15	0.33
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	15	0.33
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	5	0.33
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	5	0.33
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	5	0.33
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD11	15	0.33
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD12	15	0.33
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD13	15	0.33
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD21	15	0.33
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD22	15	0.33
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD23	15	0.33
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	4	0.33
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	4	0.33
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	13	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	13	0.33
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	13	0.33
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	8	0.33
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	16	0.33
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	16	0.33
(1,4939)	1:3:A:GLU:H	1:2:A:ASP:H	14	0.33
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD2	4	0.33
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD3	4	0.33
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	10	0.33
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	10	0.33
(1,3544)	1:97:A:ASP:HB3	1:99:A:SER:HA	20	0.33
(1,3429)	1:181:A:ILE:HG21	1:182:A:PRO:HG2	16	0.33
(1,3429)	1:181:A:ILE:HG21	1:182:A:PRO:HG3	16	0.33
(1,3429)	1:181:A:ILE:HG22	1:182:A:PRO:HG2	16	0.33
(1,3429)	1:181:A:ILE:HG22	1:182:A:PRO:HG3	16	0.33
(1,3429)	1:181:A:ILE:HG23	1:182:A:PRO:HG2	16	0.33
(1,3429)	1:181:A:ILE:HG23	1:182:A:PRO:HG3	16	0.33
(1,3340)	1:76:A:PRO:HG2	1:75:A:LYS:HG2	15	0.33
(1,3340)	1:76:A:PRO:HG2	1:75:A:LYS:HG3	15	0.33
(1,3340)	1:76:A:PRO:HG3	1:75:A:LYS:HG2	15	0.33
(1,3340)	1:76:A:PRO:HG3	1:75:A:LYS:HG3	15	0.33
(1,3330)	1:90:A:VAL:HB	1:91:A:PRO:HG2	7	0.33
(1,3330)	1:90:A:VAL:HB	1:91:A:PRO:HG3	7	0.33
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	4	0.33
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	4	0.33
(1,3259)	1:80:A:LYS:HA	1:80:A:LYS:HE2	7	0.33
(1,3259)	1:80:A:LYS:HA	1:80:A:LYS:HE3	7	0.33
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG21	2	0.33
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG22	2	0.33
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG23	2	0.33
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	1	0.33
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	1	0.33
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	4	0.33
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	4	0.33
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	12	0.33
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	12	0.33
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	12	0.33
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	14	0.33
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	14	0.33
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	14	0.33
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	17	0.33
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	17	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	17	0.33
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG2	20	0.33
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG3	20	0.33
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	1	0.33
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	1	0.33
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	1	0.33
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	2	0.33
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	2	0.33
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	2	0.33
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	2	0.33
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	2	0.33
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	2	0.33
(1,3053)	1:55:A:ALA:HB1	1:40:A:GLN:HA	17	0.33
(1,3051)	1:34:A:ILE:HG22	1:53:A:SER:HA	1	0.33
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	18	0.33
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	10	0.33
(1,2947)	1:133:A:ARG:HD2	1:136:A:PRO:HA	13	0.33
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	19	0.33
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	18	0.33
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD11	10	0.33
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD12	10	0.33
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD13	10	0.33
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD21	10	0.33
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD22	10	0.33
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD23	10	0.33
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG11	11	0.33
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG12	11	0.33
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG13	11	0.33
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG21	11	0.33
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG22	11	0.33
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG23	11	0.33
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB2	16	0.33
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB3	16	0.33
(1,2669)	1:85:A:LEU:HD12	1:8:A:VAL:HB	15	0.33
(1,2596)	1:90:A:VAL:HG13	1:85:A:LEU:HA	13	0.33
(1,2577)	1:166:A:ILE:HD11	1:160:A:GLN:HA	4	0.33
(1,2571)	1:130:A:MET:HE3	1:136:A:PRO:HA	6	0.33
(1,2532)	1:183:A:ILE:HG21	1:184:A:LEU:HA	4	0.33
(1,2532)	1:183:A:ILE:HG23	1:182:A:PRO:HA	16	0.33
(1,2481)	1:187:A:ALA:HB1	1:190:A:TYR:HD1	5	0.33
(1,2481)	1:187:A:ALA:HB1	1:190:A:TYR:HD2	5	0.33
(1,2479)	1:194:A:THR:HG22	1:190:A:TYR:HD1	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:194:A:THR:HG22	1:190:A:TYR:HD2	6	0.33
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD1	9	0.33
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD2	9	0.33
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD1	2	0.33
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD2	2	0.33
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	18	0.33
(1,2375)	1:60:A:LYS:HD2	1:61:A:GLU:H	8	0.33
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	19	0.33
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB2	5	0.33
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB3	5	0.33
(1,2238)	1:207:A:CYS:HA	1:211:A:ASN:HD21	3	0.33
(1,2238)	1:207:A:CYS:HA	1:211:A:ASN:HD22	3	0.33
(1,172)	1:122:A:PHE:HE1	1:200:A:LEU:HB2	7	0.33
(1,172)	1:122:A:PHE:HE1	1:200:A:LEU:HB3	7	0.33
(1,120)	1:199:A:TYR:HE1	1:137:A:ILE:HG12	9	0.33
(1,120)	1:199:A:TYR:HE1	1:137:A:ILE:HG13	9	0.33
(1,5849)	1:113:A:GLU:HG3	1:113:A:GLU:HA	20	0.32
(1,5821)	1:108:A:LYS:HB2	1:109:A:ASP:H	9	0.32
(1,5572)	1:94:A:TRP:HD1	1:94:A:TRP:H	3	0.32
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	5	0.32
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	5	0.32
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	7	0.32
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	7	0.32
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	8	0.32
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	8	0.32
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	19	0.32
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	19	0.32
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	5	0.32
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	5	0.32
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD11	11	0.32
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD12	11	0.32
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD13	11	0.32
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD21	11	0.32
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD22	11	0.32
(1,5362)	1:40:A:GLN:HE21	1:42:A:LEU:HD23	11	0.32
(1,5356)	1:48:A:ASP:H	1:44:A:ARG:HG2	9	0.32
(1,5356)	1:48:A:ASP:H	1:44:A:ARG:HG3	9	0.32
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	3	0.32
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	3	0.32
(1,5333)	1:221:A:GLU:H	1:222:A:LEU:HB2	11	0.32
(1,5333)	1:221:A:GLU:H	1:222:A:LEU:HB3	11	0.32
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG11	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG12	4	0.32
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG13	4	0.32
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG21	4	0.32
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG22	4	0.32
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG23	4	0.32
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG2	3	0.32
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG3	3	0.32
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	16	0.32
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	16	0.32
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	16	0.32
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	3	0.32
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	3	0.32
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	4	0.32
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	4	0.32
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	4	0.32
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	6	0.32
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	6	0.32
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	6	0.32
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	9	0.32
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	9	0.32
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	9	0.32
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG11	14	0.32
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG12	14	0.32
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG13	14	0.32
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG21	14	0.32
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG22	14	0.32
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG23	14	0.32
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	19	0.32
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	19	0.32
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	16	0.32
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	16	0.32
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	16	0.32
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	2	0.32
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	2	0.32
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	2	0.32
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	6	0.32
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	6	0.32
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	6	0.32
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	14	0.32
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	14	0.32
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	14	0.32
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	6	0.32
(1,3544)	1:97:A:ASP:HB3	1:99:A:SER:HA	7	0.32
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	17	0.32
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	17	0.32
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	17	0.32
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	17	0.32
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	17	0.32
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	17	0.32
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	17	0.32
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	17	0.32
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	17	0.32
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	17	0.32
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	17	0.32
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	17	0.32
(1,3439)	1:102:A:LEU:HD22	1:147:A:ASP:HB2	16	0.32
(1,3439)	1:102:A:LEU:HD22	1:147:A:ASP:HB3	16	0.32
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE2	20	0.32
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE3	20	0.32
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE2	20	0.32
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE3	20	0.32
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE2	20	0.32
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE3	20	0.32
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	19	0.32
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	19	0.32
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	19	0.32
(1,3287)	1:140:A:PRO:HD3	1:139:A:LYS:HD2	4	0.32
(1,3287)	1:140:A:PRO:HD3	1:139:A:LYS:HD3	4	0.32
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD2	20	0.32
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD3	20	0.32
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD11	2	0.32
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD12	2	0.32
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD13	2	0.32
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD21	2	0.32
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD22	2	0.32
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD23	2	0.32
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD11	18	0.32
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD12	18	0.32
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD13	18	0.32
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD21	18	0.32
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD22	18	0.32
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD23	18	0.32
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	4	0.32
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	4	0.32
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	9	0.32
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	9	0.32
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	9	0.32
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	16	0.32
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	16	0.32
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	16	0.32
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	18	0.32
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	18	0.32
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	18	0.32
(1,3051)	1:43:A:VAL:HG23	1:53:A:SER:HA	8	0.32
(1,3012)	1:160:A:GLN:HG2	1:156:A:LEU:HA	17	0.32
(1,2998)	1:204:A:GLU:HB3	1:197:A:ARG:HA	11	0.32
(1,2959)	1:84:A:PHE:HE1	1:84:A:PHE:HA	15	0.32
(1,2947)	1:133:A:ARG:HD2	1:136:A:PRO:HA	7	0.32
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD11	10	0.32
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD12	10	0.32
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD13	10	0.32
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD21	10	0.32
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD22	10	0.32
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD23	10	0.32
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG11	12	0.32
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG12	12	0.32
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG13	12	0.32
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG21	12	0.32
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG22	12	0.32
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG23	12	0.32
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG21	6	0.32
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG22	6	0.32
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG23	6	0.32
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD11	2	0.32
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD12	2	0.32
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD13	2	0.32
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD21	2	0.32
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD22	2	0.32
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD23	2	0.32
(1,2609)	1:5:A:LEU:HD11	1:6:A:GLY:HA2	15	0.32
(1,2609)	1:5:A:LEU:HD11	1:6:A:GLY:HA3	15	0.32
(1,2591)	1:133:A:ARG:HG3	1:134:A:GLY:HA2	7	0.32
(1,2591)	1:133:A:ARG:HG3	1:134:A:GLY:HA3	7	0.32
(1,2578)	1:64:A:ILE:HD13	1:62:A:VAL:HA	16	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2571)	1:130:A:MET:HE3	1:198:A:LYS:HA	11	0.32
(1,2549)	1:36:A:VAL:HG12	1:37:A:LYS:HA	4	0.32
(1,2538)	1:183:A:ILE:HD11	1:184:A:LEU:HA	9	0.32
(1,2536)	1:181:A:ILE:HD11	1:179:A:LEU:HA	14	0.32
(1,2534)	1:101:A:ILE:HG22	1:105:A:SER:HA	20	0.32
(1,2532)	1:183:A:ILE:HG21	1:182:A:PRO:HA	9	0.32
(1,2530)	1:36:A:VAL:HG12	1:37:A:LYS:HA	4	0.32
(1,2481)	1:187:A:ALA:HB1	1:190:A:TYR:HD1	19	0.32
(1,2481)	1:187:A:ALA:HB1	1:190:A:TYR:HD2	19	0.32
(1,2479)	1:194:A:THR:HG23	1:190:A:TYR:HD1	17	0.32
(1,2479)	1:194:A:THR:HG23	1:190:A:TYR:HD2	17	0.32
(1,2479)	1:194:A:THR:HG23	1:199:A:TYR:HD1	20	0.32
(1,2479)	1:194:A:THR:HG23	1:199:A:TYR:HD2	20	0.32
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD1	11	0.32
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD2	11	0.32
(1,2443)	1:83:A:ILE:HD12	1:83:A:ILE:H	17	0.32
(1,2411)	1:88:A:ARG:HD2	1:88:A:ARG:H	12	0.32
(1,2403)	1:3:A:GLU:HB2	1:4:A:LEU:H	20	0.32
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	3	0.32
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB2	8	0.32
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB3	8	0.32
(1,113)	1:176:A:TYR:HD2	1:182:A:PRO:HA	10	0.32
(1,113)	1:176:A:TYR:HD1	1:182:A:PRO:HA	20	0.32
(1,5849)	1:113:A:GLU:HG3	1:113:A:GLU:HA	19	0.31
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG21	18	0.31
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG22	18	0.31
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG23	18	0.31
(1,5697)	1:139:A:LYS:HD3	1:138:A:ASN:HD21	1	0.31
(1,5697)	1:139:A:LYS:HD3	1:138:A:ASN:HD22	1	0.31
(1,5697)	1:124:A:GLN:HB3	1:121:A:ASN:HD21	16	0.31
(1,5697)	1:124:A:GLN:HB3	1:121:A:ASN:HD22	16	0.31
(1,5679)	1:139:A:LYS:HB2	1:138:A:ASN:HD21	16	0.31
(1,5679)	1:139:A:LYS:HB2	1:138:A:ASN:HD22	16	0.31
(1,5679)	1:139:A:LYS:HB3	1:138:A:ASN:HD21	16	0.31
(1,5679)	1:139:A:LYS:HB3	1:138:A:ASN:HD22	16	0.31
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	8	0.31
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	15	0.31
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	15	0.31
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	7	0.31
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	7	0.31
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	7	0.31
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	7	0.31
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	7	0.31
(1,5404)	1:89:A:VAL:H	1:89:A:VAL:HB	5	0.31
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	6	0.31
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	6	0.31
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB1	6	0.31
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB2	6	0.31
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB3	6	0.31
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	4	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	2	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	2	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	2	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	10	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	10	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	10	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	11	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	11	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	11	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	20	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	20	0.31
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	20	0.31
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB2	5	0.31
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB3	5	0.31
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	5	0.31
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	5	0.31
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	5	0.31
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	17	0.31
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	17	0.31
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	17	0.31
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	4	0.31
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	8	0.31
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	16	0.31
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	16	0.31
(1,3516)	1:80:A:LYS:HD2	1:46:A:PHE:HB2	20	0.31
(1,3516)	1:80:A:LYS:HD2	1:46:A:PHE:HB3	20	0.31
(1,3516)	1:80:A:LYS:HD3	1:46:A:PHE:HB2	20	0.31
(1,3516)	1:80:A:LYS:HD3	1:46:A:PHE:HB3	20	0.31
(1,3505)	1:197:A:ARG:HG3	1:197:A:ARG:HA	3	0.31
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	11	0.31
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	3	0.31
(1,3442)	1:59:A:ILE:HG21	1:61:A:GLU:HG2	9	0.31
(1,3442)	1:59:A:ILE:HG21	1:61:A:GLU:HG3	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3442)	1:59:A:ILE:HG22	1:61:A:GLU:HG2	9	0.31
(1,3442)	1:59:A:ILE:HG22	1:61:A:GLU:HG3	9	0.31
(1,3442)	1:59:A:ILE:HG23	1:61:A:GLU:HG2	9	0.31
(1,3442)	1:59:A:ILE:HG23	1:61:A:GLU:HG3	9	0.31
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	12	0.31
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	12	0.31
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	12	0.31
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	12	0.31
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	12	0.31
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	12	0.31
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	12	0.31
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	12	0.31
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	12	0.31
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	12	0.31
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	12	0.31
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	12	0.31
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE2	18	0.31
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE3	18	0.31
(1,3398)	1:15:A:THR:HG21	1:16:A:GLU:HG2	20	0.31
(1,3398)	1:15:A:THR:HG21	1:16:A:GLU:HG3	20	0.31
(1,3398)	1:15:A:THR:HG22	1:16:A:GLU:HG2	20	0.31
(1,3398)	1:15:A:THR:HG22	1:16:A:GLU:HG3	20	0.31
(1,3398)	1:15:A:THR:HG23	1:16:A:GLU:HG2	20	0.31
(1,3398)	1:15:A:THR:HG23	1:16:A:GLU:HG3	20	0.31
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	11	0.31
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	11	0.31
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	11	0.31
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD11	20	0.31
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD12	20	0.31
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD13	20	0.31
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD21	20	0.31
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD22	20	0.31
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD23	20	0.31
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	5	0.31
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	5	0.31
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	5	0.31
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD2	1	0.31
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD3	1	0.31
(1,3177)	1:122:A:PHE:HD1	1:203:A:PHE:HB2	5	0.31
(1,3177)	1:122:A:PHE:HD1	1:203:A:PHE:HB3	5	0.31
(1,3177)	1:122:A:PHE:HD2	1:203:A:PHE:HB2	5	0.31
(1,3177)	1:122:A:PHE:HD2	1:203:A:PHE:HB3	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3161)	1:133:A:ARG:HE	1:135:A:THR:HG21	11	0.31
(1,3161)	1:133:A:ARG:HE	1:135:A:THR:HG22	11	0.31
(1,3161)	1:133:A:ARG:HE	1:135:A:THR:HG23	11	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	2	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	2	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	2	0.31
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG21	4	0.31
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG22	4	0.31
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG23	4	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	10	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	10	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	10	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	11	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	11	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	11	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	20	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	20	0.31
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	20	0.31
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	10	0.31
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	10	0.31
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	10	0.31
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG2	13	0.31
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG3	13	0.31
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	5	0.31
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	5	0.31
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	5	0.31
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	7	0.31
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	7	0.31
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	7	0.31
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	10	0.31
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	10	0.31
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	10	0.31
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG2	20	0.31
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG3	20	0.31
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG2	2	0.31
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG3	2	0.31
(1,2975)	1:179:A:LEU:HD13	1:176:A:TYR:HA	11	0.31
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB2	5	0.31
(1,2843)	1:181:A:ILE:HD12	1:153:A:LEU:HB3	5	0.31
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	6	0.31
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	6	0.31
(1,2828)	1:137:A:ILE:HB	1:101:A:ILE:HA	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG21	15	0.31
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG22	15	0.31
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG23	15	0.31
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG11	9	0.31
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG12	9	0.31
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG13	9	0.31
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG21	9	0.31
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG22	9	0.31
(1,2744)	1:195:A:ALA:HB2	1:192:A:VAL:HG23	9	0.31
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG11	17	0.31
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG12	17	0.31
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG13	17	0.31
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG21	17	0.31
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG22	17	0.31
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG23	17	0.31
(1,2575)	1:64:A:ILE:HG23	1:78:A:LEU:HA	6	0.31
(1,2575)	1:64:A:ILE:HG23	1:78:A:LEU:HA	10	0.31
(1,2532)	1:183:A:ILE:HG23	1:182:A:PRO:HA	7	0.31
(1,2532)	1:183:A:ILE:HG23	1:184:A:LEU:HA	11	0.31
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	10	0.31
(1,2489)	1:87:A:THR:HG22	1:84:A:PHE:HD1	2	0.31
(1,2489)	1:87:A:THR:HG22	1:84:A:PHE:HD2	2	0.31
(1,2429)	1:181:A:ILE:HD13	1:180:A:GLY:H	13	0.31
(1,2403)	1:3:A:GLU:HB2	1:4:A:LEU:H	9	0.31
(1,2385)	1:34:A:ILE:HB	1:53:A:SER:H	13	0.31
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	15	0.31
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	16	0.31
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	15	0.31
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	19	0.31
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG21	13	0.31
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG22	13	0.31
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG23	13	0.31
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE1	2	0.31
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE2	2	0.31
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE1	4	0.31
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE2	4	0.31
(1,183)	1:50:A:LYS:H	1:52:A:TYR:HE1	19	0.31
(1,183)	1:50:A:LYS:H	1:52:A:TYR:HE2	19	0.31
(1,113)	1:176:A:TYR:HD2	1:182:A:PRO:HA	5	0.31
(1,113)	1:176:A:TYR:HD2	1:182:A:PRO:HA	19	0.31
(1,5821)	1:108:A:LYS:HB2	1:108:A:LYS:H	15	0.3
(1,5679)	1:139:A:LYS:HB2	1:138:A:ASN:HD21	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5679)	1:139:A:LYS:HB2	1:138:A:ASN:HD22	3	0.3
(1,5679)	1:139:A:LYS:HB3	1:138:A:ASN:HD21	3	0.3
(1,5679)	1:139:A:LYS:HB3	1:138:A:ASN:HD22	3	0.3
(1,5663)	1:160:A:GLN:HB2	1:157:A:VAL:H	17	0.3
(1,5578)	1:153:A:LEU:HA	1:157:A:VAL:H	11	0.3
(1,5547)	1:100:A:GLU:HG3	1:100:A:GLU:H	15	0.3
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	6	0.3
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	6	0.3
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	11	0.3
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	11	0.3
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD2	4	0.3
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD3	4	0.3
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	20	0.3
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	20	0.3
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	10	0.3
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	10	0.3
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	16	0.3
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	16	0.3
(1,5322)	1:149:A:ASN:H	1:146:A:LYS:HG2	5	0.3
(1,5322)	1:149:A:ASN:H	1:146:A:LYS:HG3	5	0.3
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	7	0.3
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	7	0.3
(1,5318)	1:36:A:VAL:H	1:37:A:LYS:HG2	15	0.3
(1,5318)	1:36:A:VAL:H	1:37:A:LYS:HG3	15	0.3
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	7	0.3
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	7	0.3
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	7	0.3
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	7	0.3
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	7	0.3
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	7	0.3
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	8	0.3
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	8	0.3
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB2	6	0.3
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB3	6	0.3
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	6	0.3
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	6	0.3
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	6	0.3
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	19	0.3
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	19	0.3
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	19	0.3
(1,5149)	1:105:A:SER:H	1:103:A:GLU:HA	3	0.3
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	3	0.3
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	3	0.3
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	15	0.3
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	15	0.3
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	15	0.3
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG2	19	0.3
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG3	19	0.3
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	10	0.3
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	17	0.3
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	9	0.3
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	9	0.3
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	9	0.3
(1,3524)	1:58:A:ASP:H	1:57:A:LYS:HE2	9	0.3
(1,3524)	1:58:A:ASP:H	1:57:A:LYS:HE3	9	0.3
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	6	0.3
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	15	0.3
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	15	0.3
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	15	0.3
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	17	0.3
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	17	0.3
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	17	0.3
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB2	5	0.3
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB3	5	0.3
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	20	0.3
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	20	0.3
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	20	0.3
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	20	0.3
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	20	0.3
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	20	0.3
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	8	0.3
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	8	0.3
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	10	0.3
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	10	0.3
(1,3177)	1:122:A:PHE:HD1	1:203:A:PHE:HB2	8	0.3
(1,3177)	1:122:A:PHE:HD1	1:203:A:PHE:HB3	8	0.3
(1,3177)	1:122:A:PHE:HD2	1:203:A:PHE:HB2	8	0.3
(1,3177)	1:122:A:PHE:HD2	1:203:A:PHE:HB3	8	0.3
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG21	16	0.3
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG22	16	0.3
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG23	16	0.3
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	6	0.3
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	6	0.3
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG21	15	0.3
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG22	15	0.3
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG23	15	0.3
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	19	0.3
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	19	0.3
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	19	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	6	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	6	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	6	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	13	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	13	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	13	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	19	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	19	0.3
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	19	0.3
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG2	16	0.3
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG3	16	0.3
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD2	14	0.3
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD3	14	0.3
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	14	0.3
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	14	0.3
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	14	0.3
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	14	0.3
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	14	0.3
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	14	0.3
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	14	0.3
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	14	0.3
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	14	0.3
(1,3053)	1:55:A:ALA:HB3	1:40:A:GLN:HA	15	0.3
(1,2917)	1:196:A:TYR:HA	1:195:A:ALA:H	20	0.3
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	15	0.3
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	15	0.3
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG21	9	0.3
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG22	9	0.3
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG23	9	0.3
(1,2682)	1:62:A:VAL:HB	1:9:A:VAL:HB	16	0.3
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG2	12	0.3
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG3	12	0.3
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB2	11	0.3
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB3	11	0.3
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB2	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB3	20	0.3
(1,2577)	1:166:A:ILE:HD13	1:160:A:GLN:HA	11	0.3
(1,2535)	1:101:A:ILE:HD11	1:97:A:ASP:HA	17	0.3
(1,2532)	1:183:A:ILE:HG22	1:182:A:PRO:HA	17	0.3
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	5	0.3
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	17	0.3
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD1	1	0.3
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD2	1	0.3
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD1	6	0.3
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD2	6	0.3
(1,2474)	1:101:A:ILE:HD13	1:127:A:TYR:HD1	17	0.3
(1,2474)	1:101:A:ILE:HD13	1:127:A:TYR:HD2	17	0.3
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	3	0.3
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	8	0.3
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	6	0.3
(1,2372)	1:96:A:MET:HE1	1:127:A:TYR:H	7	0.3
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	15	0.3
(1,183)	1:50:A:LYS:H	1:52:A:TYR:HE1	16	0.3
(1,183)	1:50:A:LYS:H	1:52:A:TYR:HE2	16	0.3
(1,113)	1:176:A:TYR:HD1	1:182:A:PRO:HA	1	0.3
(1,113)	1:176:A:TYR:HD1	1:182:A:PRO:HA	16	0.3
(1,5681)	1:44:A:ARG:HE	1:50:A:LYS:H	2	0.29
(1,5602)	1:34:A:ILE:HG23	1:53:A:SER:H	5	0.29
(1,5602)	1:34:A:ILE:HG22	1:53:A:SER:H	15	0.29
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	3	0.29
(1,5572)	1:94:A:TRP:HD1	1:94:A:TRP:H	15	0.29
(1,5558)	1:12:A:VAL:HG12	1:17:A:ARG:H	6	0.29
(1,5534)	1:78:A:LEU:HB3	1:81:A:ALA:H	11	0.29
(1,5522)	1:9:A:VAL:HG22	1:23:A:ALA:H	12	0.29
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	11	0.29
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	11	0.29
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	10	0.29
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	10	0.29
(1,5436)	1:31:A:ASN:H	1:27:A:SER:HA	16	0.29
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	13	0.29
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	19	0.29
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	19	0.29
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB2	11	0.29
(1,5366)	1:79:A:GLN:HE21	1:82:A:SER:HB3	11	0.29
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	12	0.29
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	12	0.29
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	15	0.29
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	15	0.29
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	15	0.29
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	15	0.29
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	15	0.29
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	19	0.29
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	19	0.29
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	19	0.29
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	19	0.29
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	19	0.29
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	19	0.29
(1,5290)	1:73:A:SER:H	1:69:A:GLU:HG2	4	0.29
(1,5290)	1:73:A:SER:H	1:69:A:GLU:HG3	4	0.29
(1,5247)	1:40:A:GLN:HE21	1:55:A:ALA:HA	4	0.29
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	2	0.29
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	2	0.29
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	2	0.29
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB2	1	0.29
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB3	1	0.29
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB2	13	0.29
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB3	13	0.29
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB2	17	0.29
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB3	17	0.29
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	17	0.29
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	17	0.29
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	17	0.29
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	9	0.29
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	4	0.29
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	4	0.29
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	9	0.29
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	9	0.29
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	10	0.29
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	10	0.29
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	10	0.29
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	17	0.29
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	17	0.29
(1,3502)	1:22:A:PRO:HB2	1:21:A:TYR:HA	11	0.29
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	7	0.29
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	9	0.29
(1,3339)	1:123:A:LEU:HB3	1:150:A:LEU:HG	2	0.29
(1,3270)	1:80:A:LYS:HA	1:83:A:ILE:HG12	8	0.29
(1,3270)	1:80:A:LYS:HA	1:83:A:ILE:HG13	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3270)	1:182:A:PRO:HD2	1:146:A:LYS:HD2	18	0.29
(1,3270)	1:182:A:PRO:HD2	1:146:A:LYS:HD3	18	0.29
(1,3200)	1:184:A:LEU:HA	1:183:A:ILE:HG12	2	0.29
(1,3200)	1:184:A:LEU:HA	1:183:A:ILE:HG13	2	0.29
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG21	7	0.29
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG22	7	0.29
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG23	7	0.29
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG21	12	0.29
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG22	12	0.29
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG23	12	0.29
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	17	0.29
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	17	0.29
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	17	0.29
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	12	0.29
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	12	0.29
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	2	0.29
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	2	0.29
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	2	0.29
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	2	0.29
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	2	0.29
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	2	0.29
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	4	0.29
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	4	0.29
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	4	0.29
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	16	0.29
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	16	0.29
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	16	0.29
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG2	6	0.29
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG3	6	0.29
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG2	16	0.29
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG3	16	0.29
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	9	0.29
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	9	0.29
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	9	0.29
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	9	0.29
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	9	0.29
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	9	0.29
(1,3051)	1:34:A:ILE:HG23	1:53:A:SER:HA	6	0.29
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD2	8	0.29
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD3	8	0.29
(1,2975)	1:179:A:LEU:HD11	1:176:A:TYR:HA	9	0.29
(1,2975)	1:179:A:LEU:HD11	1:176:A:TYR:HA	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2975)	1:179:A:LEU:HD13	1:176:A:TYR:HA	19	0.29
(1,2917)	1:196:A:TYR:HA	1:195:A:ALA:H	3	0.29
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD11	14	0.29
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD12	14	0.29
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD13	14	0.29
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	2	0.29
(1,2842)	1:181:A:ILE:HD13	1:176:A:TYR:HB2	1	0.29
(1,2842)	1:181:A:ILE:HD13	1:176:A:TYR:HB3	1	0.29
(1,2841)	1:166:A:ILE:HD12	1:157:A:VAL:H	18	0.29
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD11	8	0.29
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD12	8	0.29
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD13	8	0.29
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD21	8	0.29
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD22	8	0.29
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD23	8	0.29
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD11	16	0.29
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD12	16	0.29
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD13	16	0.29
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD21	16	0.29
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD22	16	0.29
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD23	16	0.29
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB2	10	0.29
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB3	10	0.29
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB2	16	0.29
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB3	16	0.29
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB2	18	0.29
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB3	18	0.29
(1,2578)	1:64:A:ILE:HD11	1:62:A:VAL:HA	5	0.29
(1,2573)	1:187:A:ALA:HB2	1:186:A:SER:HB2	17	0.29
(1,2573)	1:187:A:ALA:HB2	1:186:A:SER:HB3	17	0.29
(1,2535)	1:101:A:ILE:HD12	1:96:A:MET:HA	8	0.29
(1,2532)	1:183:A:ILE:HG23	1:184:A:LEU:HA	14	0.29
(1,2489)	1:87:A:THR:HG22	1:84:A:PHE:HD1	5	0.29
(1,2489)	1:87:A:THR:HG22	1:84:A:PHE:HD2	5	0.29
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD1	3	0.29
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD2	3	0.29
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD11	19	0.29
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD12	19	0.29
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD13	19	0.29
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD21	19	0.29
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD22	19	0.29
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD23	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2466)	1:60:A:LYS:HD3	1:17:A:ARG:HE	20	0.29
(1,2403)	1:3:A:GLU:HB2	1:4:A:LEU:H	15	0.29
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	5	0.29
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	2	0.29
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	11	0.29
(1,750)	1:114:A:LEU:H	1:114:A:LEU:HG	18	0.29
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD21	3	0.29
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD22	3	0.29
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	10	0.28
(1,5803)	1:152:A:LYS:HD2	1:113:A:GLU:HB2	12	0.28
(1,5803)	1:152:A:LYS:HD2	1:113:A:GLU:HB3	12	0.28
(1,5602)	1:34:A:ILE:HG23	1:53:A:SER:H	6	0.28
(1,5593)	1:25:A:VAL:HG21	1:4:A:LEU:H	3	0.28
(1,5578)	1:153:A:LEU:HA	1:157:A:VAL:H	19	0.28
(1,5522)	1:9:A:VAL:HG22	1:23:A:ALA:H	5	0.28
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	14	0.28
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	14	0.28
(1,5471)	1:79:A:GLN:HE22	1:72:A:LEU:HB2	4	0.28
(1,5471)	1:79:A:GLN:HE22	1:72:A:LEU:HB3	4	0.28
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD2	15	0.28
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD3	15	0.28
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	2	0.28
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	2	0.28
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	2	0.28
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	2	0.28
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	2	0.28
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	2	0.28
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB2	17	0.28
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB3	17	0.28
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE1	14	0.28
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE2	14	0.28
(1,5428)	1:23:A:ALA:H	1:20:A:TRP:HZ3	13	0.28
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	1	0.28
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	8	0.28
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	10	0.28
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	20	0.28
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	20	0.28
(1,5292)	1:18:A:THR:H	1:19:A:GLU:HG2	13	0.28
(1,5292)	1:18:A:THR:H	1:19:A:GLU:HG3	13	0.28
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	1	0.28
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	1	0.28
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	3	0.28
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	3	0.28
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	3	0.28
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG21	12	0.28
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG22	12	0.28
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG23	12	0.28
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG21	19	0.28
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG22	19	0.28
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG23	19	0.28
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	4	0.28
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	4	0.28
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	4	0.28
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	7	0.28
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	7	0.28
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	7	0.28
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG11	2	0.28
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG12	2	0.28
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG13	2	0.28
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG21	2	0.28
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG22	2	0.28
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG23	2	0.28
(1,5053)	1:78:A:LEU:H	1:75:A:LYS:HD2	1	0.28
(1,5053)	1:78:A:LEU:H	1:75:A:LYS:HD3	1	0.28
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	14	0.28
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	14	0.28
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	6	0.28
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	6	0.28
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	6	0.28
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	19	0.28
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	19	0.28
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	19	0.28
(1,4965)	1:84:A:PHE:H	1:88:A:ARG:HE	20	0.28
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD11	19	0.28
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD12	19	0.28
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD13	19	0.28
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD21	19	0.28
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD22	19	0.28
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD23	19	0.28
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	5	0.28
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	5	0.28
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	5	0.28
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	20	0.28
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	20	0.28
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	13	0.28
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	13	0.28
(1,4471)	1:72:A:LEU:HB2	1:70:A:SER:H	17	0.28
(1,4471)	1:72:A:LEU:HB3	1:70:A:SER:H	17	0.28
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	1	0.28
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	2	0.28
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	13	0.28
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	20	0.28
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	7	0.28
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	7	0.28
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	7	0.28
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	7	0.28
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	7	0.28
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	7	0.28
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	7	0.28
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	7	0.28
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	7	0.28
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	7	0.28
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	7	0.28
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	7	0.28
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	10	0.28
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	10	0.28
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	10	0.28
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	10	0.28
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	10	0.28
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	10	0.28
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	10	0.28
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	10	0.28
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	10	0.28
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	10	0.28
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	10	0.28
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	10	0.28
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	1	0.28
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	1	0.28
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	1	0.28
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	8	0.28
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	8	0.28
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	8	0.28
(1,3338)	1:100:A:GLU:HB2	1:101:A:ILE:HG12	14	0.28
(1,3338)	1:100:A:GLU:HB2	1:101:A:ILE:HG13	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	4	0.28
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	4	0.28
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	4	0.28
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD11	12	0.28
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD12	12	0.28
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD13	12	0.28
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD21	12	0.28
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD22	12	0.28
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD23	12	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	6	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	6	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	6	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	6	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	6	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	6	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	10	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	10	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	10	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	10	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	10	0.28
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	10	0.28
(1,3200)	1:184:A:LEU:HA	1:183:A:ILE:HG12	10	0.28
(1,3200)	1:184:A:LEU:HA	1:183:A:ILE:HG13	10	0.28
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG21	5	0.28
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG22	5	0.28
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG23	5	0.28
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	1	0.28
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	1	0.28
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	1	0.28
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	3	0.28
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	3	0.28
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	3	0.28
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG2	2	0.28
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG3	2	0.28
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG2	6	0.28
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG3	6	0.28
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	2	0.28
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	2	0.28
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	2	0.28
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	3	0.28
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	3	0.28
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	12	0.28
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	12	0.28
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	12	0.28
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	6	0.28
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	6	0.28
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	6	0.28
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	6	0.28
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	6	0.28
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	6	0.28
(1,3051)	1:34:A:ILE:HG23	1:53:A:SER:HA	19	0.28
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD2	14	0.28
(1,3037)	1:181:A:ILE:HB	1:182:A:PRO:HD3	14	0.28
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	14	0.28
(1,2917)	1:196:A:TYR:HA	1:195:A:ALA:H	6	0.28
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD11	11	0.28
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD12	11	0.28
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD13	11	0.28
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	6	0.28
(1,2835)	1:126:A:LEU:HD23	1:130:A:MET:H	9	0.28
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	19	0.28
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	19	0.28
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	19	0.28
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	19	0.28
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	19	0.28
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	19	0.28
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG11	5	0.28
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG12	5	0.28
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG13	5	0.28
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG21	5	0.28
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG22	5	0.28
(1,2744)	1:195:A:ALA:HB1	1:192:A:VAL:HG23	5	0.28
(1,2717)	1:130:A:MET:HE1	1:198:A:LYS:HB2	4	0.28
(1,2717)	1:130:A:MET:HE1	1:198:A:LYS:HB3	4	0.28
(1,2717)	1:130:A:MET:HE3	1:198:A:LYS:HB2	14	0.28
(1,2717)	1:130:A:MET:HE3	1:198:A:LYS:HB3	14	0.28
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB2	12	0.28
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB3	12	0.28
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	13	0.28
(1,2502)	1:42:A:LEU:HG	1:27:A:SER:HA	12	0.28
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD1	20	0.28
(1,2481)	1:187:A:ALA:HB3	1:190:A:TYR:HD2	20	0.28
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD1	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:194:A:THR:HG21	1:190:A:TYR:HD2	5	0.28
(1,2479)	1:194:A:THR:HG23	1:190:A:TYR:HD1	16	0.28
(1,2479)	1:194:A:THR:HG23	1:190:A:TYR:HD2	16	0.28
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD11	4	0.28
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD12	4	0.28
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD13	4	0.28
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD21	4	0.28
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD22	4	0.28
(1,2469)	1:84:A:PHE:HE1	1:24:A:LEU:HD23	4	0.28
(1,2443)	1:83:A:ILE:HD11	1:83:A:ILE:H	3	0.28
(1,2443)	1:83:A:ILE:HD12	1:83:A:ILE:H	13	0.28
(1,2422)	1:126:A:LEU:HD23	1:130:A:MET:H	9	0.28
(1,2403)	1:3:A:GLU:HB2	1:4:A:LEU:H	8	0.28
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	7	0.28
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	11	0.28
(1,2375)	1:60:A:LYS:HD2	1:61:A:GLU:H	11	0.28
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	2	0.28
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	6	0.28
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB2	17	0.28
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB3	17	0.28
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG2	2	0.28
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG3	2	0.28
(1,5641)	1:37:A:LYS:HA	1:40:A:GLN:HE21	14	0.27
(1,5641)	1:37:A:LYS:HA	1:40:A:GLN:HE22	14	0.27
(1,5626)	1:64:A:ILE:HG21	1:82:A:SER:H	20	0.27
(1,5592)	1:43:A:VAL:HG11	1:44:A:ARG:H	4	0.27
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	4	0.27
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	13	0.27
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	13	0.27
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	19	0.27
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	19	0.27
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB2	1	0.27
(1,5475)	1:197:A:ARG:H	1:199:A:TYR:HB3	1	0.27
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	18	0.27
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE1	4	0.27
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE2	4	0.27
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	12	0.27
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	12	0.27
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	16	0.27
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	16	0.27
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	7	0.27
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	18	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	18	0.27
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	18	0.27
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	18	0.27
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	18	0.27
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	18	0.27
(1,5292)	1:18:A:THR:H	1:19:A:GLU:HG2	12	0.27
(1,5292)	1:18:A:THR:H	1:19:A:GLU:HG3	12	0.27
(1,5267)	1:160:A:GLN:HE21	1:175:A:ILE:HD11	5	0.27
(1,5267)	1:160:A:GLN:HE21	1:175:A:ILE:HD12	5	0.27
(1,5267)	1:160:A:GLN:HE21	1:175:A:ILE:HD13	5	0.27
(1,5226)	1:82:A:SER:H	1:78:A:LEU:HA	10	0.27
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	4	0.27
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	4	0.27
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG21	13	0.27
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG22	13	0.27
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG23	13	0.27
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	19	0.27
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	19	0.27
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	19	0.27
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	11	0.27
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	11	0.27
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	11	0.27
(1,4994)	1:222:A:LEU:H	1:222:A:LEU:HG	15	0.27
(1,4970)	1:64:A:ILE:H	1:62:A:VAL:HA	20	0.27
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	18	0.27
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	18	0.27
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	12	0.27
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	12	0.27
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	14	0.27
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	14	0.27
(1,3507)	1:67:A:LEU:H	1:65:A:LEU:HB2	14	0.27
(1,3507)	1:67:A:LEU:H	1:65:A:LEU:HB3	14	0.27
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE2	15	0.27
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE3	15	0.27
(1,3433)	1:12:A:VAL:HG12	1:17:A:ARG:HD2	10	0.27
(1,3433)	1:12:A:VAL:HG12	1:17:A:ARG:HD3	10	0.27
(1,3431)	1:36:A:VAL:HG11	1:35:A:THR:HG21	10	0.27
(1,3431)	1:36:A:VAL:HG11	1:35:A:THR:HG22	10	0.27
(1,3431)	1:36:A:VAL:HG11	1:35:A:THR:HG23	10	0.27
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG2	3	0.27
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG3	3	0.27
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG2	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG3	3	0.27
(1,3339)	1:123:A:LEU:HB3	1:150:A:LEU:HG	10	0.27
(1,3330)	1:90:A:VAL:HB	1:91:A:PRO:HG2	3	0.27
(1,3330)	1:90:A:VAL:HB	1:91:A:PRO:HG3	3	0.27
(1,3270)	1:144:A:GLY:HA3	1:146:A:LYS:HD2	5	0.27
(1,3270)	1:144:A:GLY:HA3	1:146:A:LYS:HD3	5	0.27
(1,3221)	1:170:A:ALA:HA	1:173:A:LYS:HD2	8	0.27
(1,3221)	1:170:A:ALA:HA	1:173:A:LYS:HD3	8	0.27
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	11	0.27
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	11	0.27
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	11	0.27
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	18	0.27
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	18	0.27
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	18	0.27
(1,3091)	1:129:A:PHE:H	1:88:A:ARG:HD2	19	0.27
(1,3091)	1:129:A:PHE:H	1:88:A:ARG:HD3	19	0.27
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	17	0.27
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	17	0.27
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	17	0.27
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	20	0.27
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	20	0.27
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	20	0.27
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	8	0.27
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	8	0.27
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	8	0.27
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	17	0.27
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	17	0.27
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	17	0.27
(1,3051)	1:43:A:VAL:HG23	1:53:A:SER:HA	4	0.27
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	6	0.27
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	18	0.27
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	19	0.27
(1,2947)	1:30:A:CYS:HB2	1:29:A:SER:HB2	18	0.27
(1,2947)	1:30:A:CYS:HB2	1:29:A:SER:HB3	18	0.27
(1,2920)	1:54:A:ILE:HD13	1:52:A:TYR:HA	9	0.27
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD11	5	0.27
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD12	5	0.27
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD13	5	0.27
(1,2835)	1:126:A:LEU:HD23	1:130:A:MET:H	2	0.27
(1,2699)	1:8:A:VAL:HG12	1:85:A:LEU:HB2	4	0.27
(1,2699)	1:8:A:VAL:HG12	1:85:A:LEU:HB3	4	0.27
(1,2699)	1:8:A:VAL:HG11	1:85:A:LEU:HB2	19	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2699)	1:8:A:VAL:HG11	1:85:A:LEU:HB3	19	0.27
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB2	3	0.27
(1,2649)	1:64:A:ILE:HD13	1:63:A:ASP:HB3	3	0.27
(1,2607)	1:137:A:ILE:HD13	1:141:A:PRO:HD2	2	0.27
(1,2607)	1:137:A:ILE:HD13	1:141:A:PRO:HD3	2	0.27
(1,2552)	1:101:A:ILE:HG21	1:102:A:LEU:HA	10	0.27
(1,2551)	1:98:A:ILE:HG22	1:98:A:ILE:HA	11	0.27
(1,2535)	1:101:A:ILE:HD12	1:96:A:MET:HA	18	0.27
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD11	17	0.27
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD12	17	0.27
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD13	17	0.27
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD21	17	0.27
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD22	17	0.27
(1,2498)	1:46:A:PHE:HD1	1:85:A:LEU:HD23	17	0.27
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD11	17	0.27
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD12	17	0.27
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD13	17	0.27
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD21	17	0.27
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD22	17	0.27
(1,2497)	1:46:A:PHE:HD1	1:85:A:LEU:HD23	17	0.27
(1,2471)	1:12:A:VAL:HG12	1:17:A:ARG:HE	12	0.27
(1,2422)	1:126:A:LEU:HD23	1:130:A:MET:H	2	0.27
(1,2418)	1:200:A:LEU:HD23	1:199:A:TYR:H	1	0.27
(1,2411)	1:88:A:ARG:HD2	1:88:A:ARG:H	14	0.27
(1,2400)	1:34:A:ILE:HD13	1:52:A:TYR:H	16	0.27
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	8	0.27
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	14	0.27
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB2	1	0.27
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB3	1	0.27
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG21	15	0.27
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG22	15	0.27
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG23	15	0.27
(1,750)	1:114:A:LEU:H	1:114:A:LEU:HG	11	0.27
(1,128)	1:51:A:PHE:HD1	1:133:A:ARG:HB2	5	0.27
(1,128)	1:51:A:PHE:HD1	1:133:A:ARG:HB3	5	0.27
(1,111)	1:20:A:TRP:HZ2	1:67:A:LEU:HB2	14	0.27
(1,111)	1:20:A:TRP:HZ2	1:67:A:LEU:HB3	14	0.27
(1,5842)	1:111:A:GLU:H	1:111:A:GLU:HG2	13	0.26
(1,5842)	1:111:A:GLU:H	1:111:A:GLU:HG3	13	0.26
(1,5807)	1:99:A:SER:H	1:97:A:ASP:HB2	17	0.26
(1,5807)	1:99:A:SER:H	1:97:A:ASP:HB3	17	0.26
(1,5785)	1:111:A:GLU:H	1:111:A:GLU:HG2	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5785)	1:111:A:GLU:H	1:111:A:GLU:HG3	13	0.26
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	9	0.26
(1,5553)	1:148:A:LEU:HG	1:142:A:VAL:H	20	0.26
(1,5522)	1:9:A:VAL:HG21	1:23:A:ALA:H	13	0.26
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD21	16	0.26
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD22	16	0.26
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD2	13	0.26
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD3	13	0.26
(1,5430)	1:24:A:LEU:H	1:52:A:TYR:HE1	11	0.26
(1,5430)	1:24:A:LEU:H	1:52:A:TYR:HE2	11	0.26
(1,5404)	1:89:A:VAL:H	1:89:A:VAL:HB	20	0.26
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	10	0.26
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	10	0.26
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB1	1	0.26
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB2	1	0.26
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB3	1	0.26
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	15	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	8	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	8	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	8	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	8	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	8	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	8	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	9	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	9	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	9	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	9	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	9	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	9	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	16	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	16	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	16	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	16	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	16	0.26
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	16	0.26
(1,5247)	1:40:A:GLN:HE21	1:55:A:ALA:HA	13	0.26
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	11	0.26
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	11	0.26
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	11	0.26
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	6	0.26
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	6	0.26
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB2	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB3	3	0.26
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG21	6	0.26
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG22	6	0.26
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG23	6	0.26
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	14	0.26
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	14	0.26
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	14	0.26
(1,5070)	1:40:A:GLN:H	1:56:A:ARG:H	15	0.26
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD11	8	0.26
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD12	8	0.26
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD13	8	0.26
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG2	9	0.26
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG3	9	0.26
(1,5020)	1:85:A:LEU:H	1:88:A:ARG:HE	4	0.26
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	3	0.26
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	3	0.26
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	3	0.26
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	4	0.26
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	4	0.26
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	4	0.26
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	2	0.26
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	14	0.26
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	8	0.26
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	8	0.26
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	8	0.26
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	17	0.26
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	17	0.26
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	17	0.26
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	18	0.26
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	18	0.26
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	18	0.26
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	18	0.26
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	18	0.26
(1,3544)	1:97:A:ASP:HB3	1:99:A:SER:HA	10	0.26
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB2	7	0.26
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB3	7	0.26
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB2	7	0.26
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB3	7	0.26
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	10	0.26
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	12	0.26
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	18	0.26
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB2	9	0.26
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB3	9	0.26
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	9	0.26
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	9	0.26
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	9	0.26
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	9	0.26
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	9	0.26
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	9	0.26
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	9	0.26
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	9	0.26
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	9	0.26
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	9	0.26
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	9	0.26
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	9	0.26
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	15	0.26
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	15	0.26
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	15	0.26
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	15	0.26
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	15	0.26
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	15	0.26
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	15	0.26
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	15	0.26
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	15	0.26
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	15	0.26
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	15	0.26
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	15	0.26
(1,3439)	1:102:A:LEU:HD23	1:147:A:ASP:HB2	2	0.26
(1,3439)	1:102:A:LEU:HD23	1:147:A:ASP:HB3	2	0.26
(1,3351)	1:61:A:GLU:HB2	1:60:A:LYS:HB2	10	0.26
(1,3351)	1:61:A:GLU:HB2	1:60:A:LYS:HB3	10	0.26
(1,3351)	1:61:A:GLU:HB3	1:60:A:LYS:HB2	10	0.26
(1,3351)	1:61:A:GLU:HB3	1:60:A:LYS:HB3	10	0.26
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	20	0.26
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	20	0.26
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	20	0.26
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	1	0.26
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	1	0.26
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	1	0.26
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD11	3	0.26
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD12	3	0.26
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD13	3	0.26
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD21	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD22	3	0.26
(1,3224)	1:3:A:GLU:HA	1:5:A:LEU:HD23	3	0.26
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	9	0.26
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	9	0.26
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	9	0.26
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	9	0.26
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	9	0.26
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	9	0.26
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	7	0.26
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	7	0.26
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	3	0.26
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	3	0.26
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	3	0.26
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	20	0.26
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	20	0.26
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	20	0.26
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	11	0.26
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	11	0.26
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	11	0.26
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD2	2	0.26
(1,3091)	1:87:A:THR:H	1:88:A:ARG:HD3	2	0.26
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	5	0.26
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	5	0.26
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	5	0.26
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	5	0.26
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	5	0.26
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	5	0.26
(1,3051)	1:34:A:ILE:HG21	1:53:A:SER:HA	16	0.26
(1,2917)	1:196:A:TYR:HA	1:195:A:ALA:H	9	0.26
(1,2905)	1:126:A:LEU:HD12	1:199:A:TYR:HD1	17	0.26
(1,2905)	1:126:A:LEU:HD12	1:199:A:TYR:HD2	17	0.26
(1,2841)	1:166:A:ILE:HD11	1:157:A:VAL:H	1	0.26
(1,2804)	1:171:A:VAL:HG13	1:175:A:ILE:HD11	17	0.26
(1,2804)	1:171:A:VAL:HG13	1:175:A:ILE:HD12	17	0.26
(1,2804)	1:171:A:VAL:HG13	1:175:A:ILE:HD13	17	0.26
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG11	4	0.26
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG12	4	0.26
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG13	4	0.26
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG21	4	0.26
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG22	4	0.26
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG23	4	0.26
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	15	0.26
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	15	0.26
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	15	0.26
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	15	0.26
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	15	0.26
(1,2699)	1:8:A:VAL:HG11	1:85:A:LEU:HB2	8	0.26
(1,2699)	1:8:A:VAL:HG11	1:85:A:LEU:HB3	8	0.26
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB2	3	0.26
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB3	3	0.26
(1,2643)	1:187:A:ALA:HB1	1:190:A:TYR:HB2	13	0.26
(1,2643)	1:187:A:ALA:HB1	1:190:A:TYR:HB3	13	0.26
(1,2577)	1:166:A:ILE:HD12	1:161:A:GLY:HA2	12	0.26
(1,2577)	1:166:A:ILE:HD12	1:161:A:GLY:HA3	12	0.26
(1,2562)	1:72:A:LEU:HG	1:69:A:GLU:HA	2	0.26
(1,2562)	1:72:A:LEU:HG	1:69:A:GLU:HA	3	0.26
(1,2551)	1:98:A:ILE:HG21	1:98:A:ILE:HA	1	0.26
(1,2551)	1:98:A:ILE:HG21	1:98:A:ILE:HA	2	0.26
(1,2551)	1:98:A:ILE:HG22	1:98:A:ILE:HA	14	0.26
(1,2551)	1:98:A:ILE:HG23	1:98:A:ILE:HA	18	0.26
(1,2551)	1:98:A:ILE:HG23	1:98:A:ILE:HA	19	0.26
(1,2489)	1:87:A:THR:HG21	1:84:A:PHE:HD1	8	0.26
(1,2489)	1:87:A:THR:HG21	1:84:A:PHE:HD2	8	0.26
(1,2489)	1:87:A:THR:HG23	1:84:A:PHE:HD1	12	0.26
(1,2489)	1:87:A:THR:HG23	1:84:A:PHE:HD2	12	0.26
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD1	7	0.26
(1,2481)	1:187:A:ALA:HB2	1:190:A:TYR:HD2	7	0.26
(1,2481)	1:187:A:ALA:HB1	1:190:A:TYR:HD1	13	0.26
(1,2481)	1:187:A:ALA:HB1	1:190:A:TYR:HD2	13	0.26
(1,2480)	1:130:A:MET:HE2	1:199:A:TYR:HD1	4	0.26
(1,2480)	1:130:A:MET:HE2	1:199:A:TYR:HD2	4	0.26
(1,2426)	1:101:A:ILE:HG21	1:103:A:GLU:H	14	0.26
(1,2306)	1:81:A:ALA:HA	1:78:A:LEU:HA	12	0.26
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD11	5	0.26
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD12	5	0.26
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD13	5	0.26
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD11	5	0.26
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD12	5	0.26
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD13	5	0.26
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD11	5	0.26
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD12	5	0.26
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD13	5	0.26
(1,750)	1:114:A:LEU:H	1:114:A:LEU:HG	12	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD11	3	0.26
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD12	3	0.26
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD13	3	0.26
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD21	3	0.26
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD22	3	0.26
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD23	3	0.26
(1,113)	1:176:A:TYR:HD1	1:182:A:PRO:HA	11	0.26
(1,113)	1:176:A:TYR:HD1	1:182:A:PRO:HA	14	0.26
(1,5848)	1:113:A:GLU:HB3	1:114:A:LEU:HG	7	0.25
(1,5842)	1:111:A:GLU:H	1:111:A:GLU:HG2	11	0.25
(1,5842)	1:111:A:GLU:H	1:111:A:GLU:HG3	11	0.25
(1,5828)	1:108:A:LYS:H	1:108:A:LYS:HB2	9	0.25
(1,5828)	1:108:A:LYS:H	1:108:A:LYS:HB3	9	0.25
(1,5788)	1:98:A:ILE:HD13	1:105:A:SER:HA	12	0.25
(1,5785)	1:111:A:GLU:H	1:111:A:GLU:HG2	11	0.25
(1,5785)	1:111:A:GLU:H	1:111:A:GLU:HG3	11	0.25
(1,5549)	1:204:A:GLU:HB2	1:201:A:TYR:H	8	0.25
(1,5536)	1:183:A:ILE:HG13	1:188:A:ALA:H	17	0.25
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	7	0.25
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	7	0.25
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	9	0.25
(1,5471)	1:79:A:GLN:HE21	1:72:A:LEU:HB2	1	0.25
(1,5471)	1:79:A:GLN:HE21	1:72:A:LEU:HB3	1	0.25
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB2	16	0.25
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB3	16	0.25
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	9	0.25
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	9	0.25
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	13	0.25
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	13	0.25
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	13	0.25
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	13	0.25
(1,5373)	1:134:A:GLY:H	1:44:A:ARG:HD2	15	0.25
(1,5373)	1:134:A:GLY:H	1:44:A:ARG:HD3	15	0.25
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	17	0.25
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	17	0.25
(1,5331)	1:75:A:LYS:H	1:71:A:GLU:HG2	8	0.25
(1,5331)	1:75:A:LYS:H	1:71:A:GLU:HG3	8	0.25
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	1	0.25
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	1	0.25
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	1	0.25
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	1	0.25
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	1	0.25
(1,5290)	1:73:A:SER:H	1:69:A:GLU:HG2	17	0.25
(1,5290)	1:73:A:SER:H	1:69:A:GLU:HG3	17	0.25
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	2	0.25
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	2	0.25
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB1	11	0.25
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB2	11	0.25
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB3	11	0.25
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	12	0.25
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	12	0.25
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	12	0.25
(1,5151)	1:105:A:SER:H	1:105:A:SER:HB2	14	0.25
(1,5151)	1:105:A:SER:H	1:105:A:SER:HB3	14	0.25
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG21	8	0.25
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG22	8	0.25
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG23	8	0.25
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	18	0.25
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	18	0.25
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	18	0.25
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	18	0.25
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	18	0.25
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	18	0.25
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG11	1	0.25
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG12	1	0.25
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG13	1	0.25
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG21	1	0.25
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG22	1	0.25
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG23	1	0.25
(1,5053)	1:78:A:LEU:H	1:75:A:LYS:HD2	2	0.25
(1,5053)	1:78:A:LEU:H	1:75:A:LYS:HD3	2	0.25
(1,5020)	1:85:A:LEU:H	1:88:A:ARG:HE	16	0.25
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	1	0.25
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	1	0.25
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	1	0.25
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	14	0.25
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	14	0.25
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	14	0.25
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	9	0.25
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	9	0.25
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	12	0.25
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	3	0.25
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	1	0.25
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	1	0.25
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	1	0.25
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	5	0.25
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	5	0.25
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	4	0.25
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	5	0.25
(1,3448)	1:43:A:VAL:HG12	1:41:A:CYS:HB2	7	0.25
(1,3448)	1:43:A:VAL:HG12	1:41:A:CYS:HB3	7	0.25
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	8	0.25
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	8	0.25
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	8	0.25
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	8	0.25
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	8	0.25
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	8	0.25
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	8	0.25
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	8	0.25
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	8	0.25
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	8	0.25
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	8	0.25
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	8	0.25
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE2	17	0.25
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE3	17	0.25
(1,3325)	1:41:A:CYS:HB2	1:59:A:ILE:HD11	7	0.25
(1,3325)	1:41:A:CYS:HB2	1:59:A:ILE:HD12	7	0.25
(1,3325)	1:41:A:CYS:HB2	1:59:A:ILE:HD13	7	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	13	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	13	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	13	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	13	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	13	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	13	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	15	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	15	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	15	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	15	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	15	0.25
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	15	0.25
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	12	0.25
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	12	0.25
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	12	0.25
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	1	0.25
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	1	0.25
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	5	0.25
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	5	0.25
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	5	0.25
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	15	0.25
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	15	0.25
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	15	0.25
(1,3097)	1:177:A:MET:H	1:174:A:GLN:HG2	18	0.25
(1,3097)	1:177:A:MET:H	1:174:A:GLN:HG3	18	0.25
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	9	0.25
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	9	0.25
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	9	0.25
(1,3051)	1:43:A:VAL:HG23	1:53:A:SER:HA	11	0.25
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD2	6	0.25
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD3	6	0.25
(1,2998)	1:204:A:GLU:HB3	1:197:A:ARG:HA	15	0.25
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	4	0.25
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	5	0.25
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	13	0.25
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	16	0.25
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	12	0.25
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	12	0.25
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	16	0.25
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	16	0.25
(1,2958)	1:72:A:LEU:H	1:70:A:SER:HB2	3	0.25
(1,2958)	1:72:A:LEU:H	1:70:A:SER:HB3	3	0.25
(1,2917)	1:196:A:TYR:HA	1:195:A:ALA:H	13	0.25
(1,2917)	1:196:A:TYR:HA	1:201:A:TYR:H	18	0.25
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG12	4	0.25
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG13	4	0.25
(1,2840)	1:22:A:PRO:HA	1:81:A:ALA:HB1	10	0.25
(1,2840)	1:22:A:PRO:HA	1:81:A:ALA:HB2	10	0.25
(1,2840)	1:22:A:PRO:HA	1:81:A:ALA:HB3	10	0.25
(1,2835)	1:126:A:LEU:HD21	1:130:A:MET:H	6	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG11	10	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG12	10	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG13	10	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG21	10	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG22	10	0.25
(1,2804)	1:171:A:VAL:HG11	1:157:A:VAL:HG23	10	0.25
(1,2717)	1:130:A:MET:HE2	1:133:A:ARG:HG2	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2717)	1:130:A:MET:HE2	1:133:A:ARG:HG3	17	0.25
(1,2575)	1:64:A:ILE:HG22	1:78:A:LEU:HA	4	0.25
(1,2575)	1:64:A:ILE:HG21	1:82:A:SER:HA	14	0.25
(1,2571)	1:130:A:MET:HE3	1:198:A:LYS:HA	19	0.25
(1,2554)	1:175:A:ILE:HD13	1:153:A:LEU:HA	15	0.25
(1,2551)	1:98:A:ILE:HG22	1:98:A:ILE:HA	3	0.25
(1,2551)	1:98:A:ILE:HG21	1:98:A:ILE:HA	4	0.25
(1,2551)	1:98:A:ILE:HG21	1:98:A:ILE:HA	6	0.25
(1,2551)	1:98:A:ILE:HG21	1:98:A:ILE:HA	10	0.25
(1,2551)	1:98:A:ILE:HG23	1:98:A:ILE:HA	12	0.25
(1,2551)	1:98:A:ILE:HG22	1:98:A:ILE:HA	20	0.25
(1,2531)	1:142:A:VAL:HG11	1:147:A:ASP:HA	3	0.25
(1,2474)	1:101:A:ILE:HD13	1:127:A:TYR:HD1	1	0.25
(1,2474)	1:101:A:ILE:HD13	1:127:A:TYR:HD2	1	0.25
(1,2428)	1:64:A:ILE:HD13	1:65:A:LEU:H	18	0.25
(1,2425)	1:54:A:ILE:HG23	1:12:A:VAL:H	7	0.25
(1,2422)	1:126:A:LEU:HD21	1:130:A:MET:H	6	0.25
(1,2411)	1:88:A:ARG:HD2	1:88:A:ARG:H	1	0.25
(1,2411)	1:88:A:ARG:HD2	1:88:A:ARG:H	15	0.25
(1,2374)	1:54:A:ILE:HB	1:53:A:SER:H	20	0.25
(1,2289)	1:119:A:ARG:HA	1:117:A:GLU:H	19	0.25
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD11	2	0.25
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD12	2	0.25
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD13	2	0.25
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD11	7	0.25
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD12	7	0.25
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD13	7	0.25
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD11	7	0.25
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD12	7	0.25
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD13	7	0.25
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD11	7	0.25
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD12	7	0.25
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD13	7	0.25
(1,750)	1:114:A:LEU:H	1:114:A:LEU:HG	1	0.25
(1,183)	1:50:A:LYS:H	1:52:A:TYR:HE1	11	0.25
(1,183)	1:50:A:LYS:H	1:52:A:TYR:HE2	11	0.25
(1,168)	1:190:A:TYR:HE1	1:191:A:ASN:HD21	18	0.25
(1,168)	1:190:A:TYR:HE1	1:191:A:ASN:HD22	18	0.25
(1,150)	1:127:A:TYR:HE2	1:141:A:PRO:HG2	5	0.25
(1,150)	1:127:A:TYR:HE2	1:141:A:PRO:HG3	5	0.25
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG2	19	0.25
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG3	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	13	0.24
(1,5811)	1:67:A:LEU:HD21	1:68:A:PRO:HD2	19	0.24
(1,5811)	1:67:A:LEU:HD21	1:68:A:PRO:HD3	19	0.24
(1,5789)	1:108:A:LYS:H	1:107:A:SER:HB2	17	0.24
(1,5789)	1:108:A:LYS:H	1:107:A:SER:HB3	17	0.24
(1,5788)	1:98:A:ILE:HD12	1:105:A:SER:HA	13	0.24
(1,5697)	1:139:A:LYS:HD3	1:138:A:ASN:HD21	20	0.24
(1,5697)	1:139:A:LYS:HD3	1:138:A:ASN:HD22	20	0.24
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD21	8	0.24
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD22	8	0.24
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	10	0.24
(1,5557)	1:124:A:GLN:HB3	1:95:A:LYS:H	13	0.24
(1,5522)	1:9:A:VAL:HG21	1:23:A:ALA:H	11	0.24
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	3	0.24
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	3	0.24
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD21	4	0.24
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD22	4	0.24
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	16	0.24
(1,5428)	1:23:A:ALA:H	1:20:A:TRP:HZ3	2	0.24
(1,5417)	1:10:A:SER:H	1:22:A:PRO:HB2	18	0.24
(1,5417)	1:10:A:SER:H	1:22:A:PRO:HB3	18	0.24
(1,5416)	1:10:A:SER:H	1:22:A:PRO:HB2	18	0.24
(1,5416)	1:10:A:SER:H	1:22:A:PRO:HB3	18	0.24
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE1	1	0.24
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE2	1	0.24
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	20	0.24
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	14	0.24
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	14	0.24
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	18	0.24
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	18	0.24
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	9	0.24
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	2	0.24
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	2	0.24
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	2	0.24
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	2	0.24
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	2	0.24
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	2	0.24
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB2	3	0.24
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB3	3	0.24
(1,5235)	1:70:A:SER:H	1:69:A:GLU:HB2	19	0.24
(1,5235)	1:70:A:SER:H	1:69:A:GLU:HB3	19	0.24
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	6	0.24
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	6	0.24
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	14	0.24
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	14	0.24
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	14	0.24
(1,5145)	1:52:A:TYR:HD2	1:52:A:TYR:H	9	0.24
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	14	0.24
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	14	0.24
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	14	0.24
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG11	19	0.24
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG12	19	0.24
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG13	19	0.24
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG21	19	0.24
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG22	19	0.24
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG23	19	0.24
(1,5128)	1:197:A:ARG:H	1:200:A:LEU:HG	20	0.24
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG11	5	0.24
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG12	5	0.24
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG13	5	0.24
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG21	5	0.24
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG22	5	0.24
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG23	5	0.24
(1,5103)	1:123:A:LEU:H	1:119:A:ARG:HB2	10	0.24
(1,5103)	1:123:A:LEU:H	1:119:A:ARG:HB3	10	0.24
(1,4970)	1:64:A:ILE:H	1:62:A:VAL:HA	7	0.24
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	3	0.24
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	15	0.24
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	4	0.24
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	4	0.24
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	4	0.24
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	4	0.24
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	4	0.24
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	4	0.24
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	4	0.24
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	4	0.24
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	4	0.24
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	4	0.24
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	4	0.24
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	4	0.24
(1,3431)	1:83:A:ILE:HG23	1:87:A:THR:HG21	3	0.24
(1,3431)	1:83:A:ILE:HG23	1:87:A:THR:HG22	3	0.24
(1,3431)	1:83:A:ILE:HG23	1:87:A:THR:HG23	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3402)	1:35:A:THR:HG22	1:36:A:VAL:HB	12	0.24
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	4	0.24
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	4	0.24
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	4	0.24
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	16	0.24
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	16	0.24
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	16	0.24
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	20	0.24
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	20	0.24
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	20	0.24
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	7	0.24
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	7	0.24
(1,3270)	1:144:A:GLY:HA3	1:146:A:LYS:HD2	16	0.24
(1,3270)	1:144:A:GLY:HA3	1:146:A:LYS:HD3	16	0.24
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD2	9	0.24
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD3	9	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD11	4	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD12	4	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD13	4	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD21	4	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD22	4	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD23	4	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD11	15	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD12	15	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD13	15	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD21	15	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD22	15	0.24
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD23	15	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	2	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	2	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	2	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	2	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	2	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	2	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	4	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	4	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	4	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	4	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	4	0.24
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	4	0.24
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG21	5	0.24
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG22	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3154)	1:34:A:ILE:H	1:34:A:ILE:HG23	5	0.24
(1,3144)	1:20:A:TRP:HD1	1:16:A:GLU:HG2	11	0.24
(1,3144)	1:20:A:TRP:HD1	1:16:A:GLU:HG3	11	0.24
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	6	0.24
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	6	0.24
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	6	0.24
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	14	0.24
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	14	0.24
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	14	0.24
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG21	16	0.24
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG22	16	0.24
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG23	16	0.24
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	8	0.24
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	8	0.24
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	8	0.24
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	15	0.24
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	15	0.24
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	15	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	11	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	11	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	11	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	11	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	11	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	11	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	13	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	13	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	13	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	13	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	13	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	13	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	16	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	16	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	16	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	16	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	16	0.24
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	16	0.24
(1,3014)	1:175:A:ILE:HG23	1:156:A:LEU:HA	15	0.24
(1,3011)	1:103:A:GLU:HG3	1:103:A:GLU:HA	3	0.24
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	2	0.24
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	3	0.24
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	12	0.24
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2903)	1:11:A:VAL:HG12	1:54:A:ILE:HB	11	0.24
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD11	15	0.24
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD12	15	0.24
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD13	15	0.24
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD11	18	0.24
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD12	18	0.24
(1,2873)	1:10:A:SER:HA	1:64:A:ILE:HD13	18	0.24
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG21	20	0.24
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG22	20	0.24
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG23	20	0.24
(1,2841)	1:166:A:ILE:HD13	1:157:A:VAL:H	13	0.24
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	13	0.24
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD11	5	0.24
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD12	5	0.24
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD13	5	0.24
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD21	5	0.24
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD22	5	0.24
(1,2824)	1:6:A:GLY:HA2	1:24:A:LEU:HD23	5	0.24
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD11	19	0.24
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD12	19	0.24
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD13	19	0.24
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD21	19	0.24
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD22	19	0.24
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD23	19	0.24
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG21	8	0.24
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG22	8	0.24
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG23	8	0.24
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG21	13	0.24
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG22	13	0.24
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG23	13	0.24
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	6	0.24
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	6	0.24
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	6	0.24
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	6	0.24
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	6	0.24
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	6	0.24
(1,2682)	1:62:A:VAL:HB	1:9:A:VAL:HB	6	0.24
(1,2577)	1:166:A:ILE:HD12	1:160:A:GLN:HA	2	0.24
(1,2577)	1:166:A:ILE:HD13	1:160:A:GLN:HA	10	0.24
(1,2551)	1:98:A:ILE:HG22	1:98:A:ILE:HA	9	0.24
(1,2551)	1:98:A:ILE:HG22	1:98:A:ILE:HA	13	0.24
(1,2551)	1:98:A:ILE:HG22	1:98:A:ILE:HA	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2536)	1:181:A:ILE:HD11	1:179:A:LEU:HA	8	0.24
(1,2535)	1:101:A:ILE:HD13	1:97:A:ASP:HA	3	0.24
(1,2535)	1:101:A:ILE:HD11	1:97:A:ASP:HA	16	0.24
(1,2533)	1:9:A:VAL:HG21	1:25:A:VAL:HA	7	0.24
(1,2418)	1:200:A:LEU:HD21	1:150:A:LEU:H	4	0.24
(1,2403)	1:3:A:GLU:HB2	1:4:A:LEU:H	19	0.24
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB2	7	0.24
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB3	7	0.24
(1,117)	1:52:A:TYR:HD2	1:52:A:TYR:H	9	0.24
(1,113)	1:176:A:TYR:HD1	1:182:A:PRO:HA	15	0.24
(1,5832)	1:108:A:LYS:H	1:108:A:LYS:HB2	7	0.23
(1,5832)	1:108:A:LYS:H	1:108:A:LYS:HB3	7	0.23
(1,5828)	1:108:A:LYS:H	1:108:A:LYS:HB2	7	0.23
(1,5828)	1:108:A:LYS:H	1:108:A:LYS:HB3	7	0.23
(1,5690)	1:65:A:LEU:HA	1:66:A:ASN:HD21	17	0.23
(1,5690)	1:65:A:LEU:HA	1:66:A:ASN:HD22	17	0.23
(1,5681)	1:94:A:TRP:HZ3	1:94:A:TRP:H	10	0.23
(1,5642)	1:187:A:ALA:HB3	1:191:A:ASN:HD21	17	0.23
(1,5642)	1:187:A:ALA:HB3	1:191:A:ASN:HD22	17	0.23
(1,5623)	1:61:A:GLU:HG2	1:1:A:ASN:HD21	10	0.23
(1,5623)	1:61:A:GLU:HG2	1:1:A:ASN:HD22	10	0.23
(1,5623)	1:61:A:GLU:HG3	1:1:A:ASN:HD21	10	0.23
(1,5623)	1:61:A:GLU:HG3	1:1:A:ASN:HD22	10	0.23
(1,5553)	1:148:A:LEU:HG	1:142:A:VAL:H	7	0.23
(1,5553)	1:148:A:LEU:HG	1:142:A:VAL:H	13	0.23
(1,5534)	1:78:A:LEU:HB2	1:81:A:ALA:H	20	0.23
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	1	0.23
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	1	0.23
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	5	0.23
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	5	0.23
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	8	0.23
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	8	0.23
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	16	0.23
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	16	0.23
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD21	19	0.23
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD22	19	0.23
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	12	0.23
(1,5451)	1:126:A:LEU:H	1:128:A:LYS:HB2	10	0.23
(1,5451)	1:126:A:LEU:H	1:128:A:LYS:HB3	10	0.23
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	4	0.23
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	4	0.23
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	12	0.23
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	2	0.23
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	2	0.23
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	14	0.23
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	14	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	4	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	4	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	4	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	4	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	4	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	4	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	10	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	10	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	10	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	10	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	10	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	10	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	20	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	20	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	20	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	20	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	20	0.23
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	20	0.23
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB2	6	0.23
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB3	6	0.23
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB2	8	0.23
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB3	8	0.23
(1,5247)	1:40:A:GLN:HE21	1:55:A:ALA:HA	16	0.23
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	18	0.23
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	18	0.23
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	18	0.23
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	9	0.23
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	9	0.23
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	9	0.23
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG21	20	0.23
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG22	20	0.23
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG23	20	0.23
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	5	0.23
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	5	0.23
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	5	0.23
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	8	0.23
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	8	0.23
(1,5118)	1:7:A:LYS:H	1:5:A:LEU:HG	14	0.23
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD11	2	0.23
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD12	2	0.23
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD13	2	0.23
(1,5052)	1:78:A:LEU:H	1:78:A:LEU:HB2	15	0.23
(1,5052)	1:78:A:LEU:H	1:78:A:LEU:HB3	15	0.23
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	8	0.23
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	8	0.23
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	8	0.23
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	10	0.23
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	10	0.23
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	10	0.23
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	12	0.23
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	12	0.23
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	12	0.23
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	18	0.23
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	19	0.23
(1,3604)	1:149:A:ASN:HB2	1:150:A:LEU:H	15	0.23
(1,3604)	1:149:A:ASN:HB3	1:150:A:LEU:H	15	0.23
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	8	0.23
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	14	0.23
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	17	0.23
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	9	0.23
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	9	0.23
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE2	6	0.23
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE3	6	0.23
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE2	6	0.23
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE3	6	0.23
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE2	6	0.23
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE3	6	0.23
(1,3381)	1:72:A:LEU:HB2	1:79:A:GLN:HG2	7	0.23
(1,3381)	1:72:A:LEU:HB2	1:79:A:GLN:HG3	7	0.23
(1,3381)	1:72:A:LEU:HB3	1:79:A:GLN:HG2	7	0.23
(1,3381)	1:72:A:LEU:HB3	1:79:A:GLN:HG3	7	0.23
(1,3317)	1:39:A:ASP:HB3	1:38:A:LYS:HG2	17	0.23
(1,3317)	1:39:A:ASP:HB3	1:38:A:LYS:HG3	17	0.23
(1,3287)	1:140:A:PRO:HD2	1:139:A:LYS:HD2	18	0.23
(1,3287)	1:140:A:PRO:HD2	1:139:A:LYS:HD3	18	0.23
(1,3217)	1:98:A:ILE:HA	1:96:A:MET:HG2	12	0.23
(1,3217)	1:98:A:ILE:HA	1:96:A:MET:HG3	12	0.23
(1,3200)	1:184:A:LEU:HA	1:183:A:ILE:HG12	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3200)	1:184:A:LEU:HA	1:183:A:ILE:HG13	3	0.23
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	18	0.23
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	18	0.23
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	18	0.23
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD11	9	0.23
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD12	9	0.23
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD13	9	0.23
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD21	9	0.23
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD22	9	0.23
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD23	9	0.23
(1,3097)	1:177:A:MET:H	1:174:A:GLN:HG2	10	0.23
(1,3097)	1:177:A:MET:H	1:174:A:GLN:HG3	10	0.23
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG2	8	0.23
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG3	8	0.23
(1,3051)	1:34:A:ILE:HG22	1:53:A:SER:HA	18	0.23
(1,3048)	1:34:A:ILE:HB	1:51:A:PHE:HA	5	0.23
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD2	19	0.23
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD3	19	0.23
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	8	0.23
(1,2975)	1:179:A:LEU:HD11	1:176:A:TYR:HA	10	0.23
(1,2973)	1:166:A:ILE:HB	1:166:A:ILE:HA	1	0.23
(1,2917)	1:196:A:TYR:HA	1:195:A:ALA:H	19	0.23
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	1	0.23
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	12	0.23
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	18	0.23
(1,2853)	1:34:A:ILE:HB	1:51:A:PHE:HA	5	0.23
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	6	0.23
(1,2826)	1:59:A:ILE:HB	1:61:A:GLU:HG2	7	0.23
(1,2826)	1:59:A:ILE:HB	1:61:A:GLU:HG3	7	0.23
(1,2797)	1:181:A:ILE:HD12	1:143:A:LEU:HD11	19	0.23
(1,2797)	1:181:A:ILE:HD12	1:143:A:LEU:HD12	19	0.23
(1,2797)	1:181:A:ILE:HD12	1:143:A:LEU:HD13	19	0.23
(1,2797)	1:181:A:ILE:HD12	1:143:A:LEU:HD21	19	0.23
(1,2797)	1:181:A:ILE:HD12	1:143:A:LEU:HD22	19	0.23
(1,2797)	1:181:A:ILE:HD12	1:143:A:LEU:HD23	19	0.23
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD11	14	0.23
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD12	14	0.23
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD13	14	0.23
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD21	14	0.23
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD22	14	0.23
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD23	14	0.23
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG21	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG22	16	0.23
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG23	16	0.23
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD11	8	0.23
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD12	8	0.23
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD13	8	0.23
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD21	8	0.23
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD22	8	0.23
(1,2744)	1:195:A:ALA:HB1	1:153:A:LEU:HD23	8	0.23
(1,2726)	1:61:A:GLU:HG3	1:60:A:LYS:HB2	20	0.23
(1,2726)	1:61:A:GLU:HG3	1:60:A:LYS:HB3	20	0.23
(1,2692)	1:195:A:ALA:HB2	1:150:A:LEU:HB2	17	0.23
(1,2692)	1:195:A:ALA:HB2	1:150:A:LEU:HB3	17	0.23
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG2	16	0.23
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG3	16	0.23
(1,2649)	1:64:A:ILE:HD11	1:63:A:ASP:HB2	4	0.23
(1,2649)	1:64:A:ILE:HD11	1:63:A:ASP:HB3	4	0.23
(1,2644)	1:55:A:ALA:HB1	1:57:A:LYS:HE2	5	0.23
(1,2644)	1:55:A:ALA:HB1	1:57:A:LYS:HE3	5	0.23
(1,2644)	1:55:A:ALA:HB2	1:57:A:LYS:HE2	5	0.23
(1,2644)	1:55:A:ALA:HB2	1:57:A:LYS:HE3	5	0.23
(1,2644)	1:55:A:ALA:HB3	1:57:A:LYS:HE2	5	0.23
(1,2644)	1:55:A:ALA:HB3	1:57:A:LYS:HE3	5	0.23
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB2	11	0.23
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB3	11	0.23
(1,2632)	1:198:A:LYS:HD3	1:139:A:LYS:HE2	18	0.23
(1,2632)	1:198:A:LYS:HD3	1:139:A:LYS:HE3	18	0.23
(1,2596)	1:90:A:VAL:HG21	1:85:A:LEU:HA	1	0.23
(1,2562)	1:72:A:LEU:HG	1:69:A:GLU:HA	14	0.23
(1,2552)	1:101:A:ILE:HG23	1:102:A:LEU:HA	17	0.23
(1,2551)	1:98:A:ILE:HG22	1:98:A:ILE:HA	8	0.23
(1,2551)	1:98:A:ILE:HG21	1:98:A:ILE:HA	17	0.23
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	17	0.23
(1,2426)	1:101:A:ILE:HG21	1:103:A:GLU:H	18	0.23
(1,2425)	1:54:A:ILE:HG21	1:12:A:VAL:H	5	0.23
(1,2425)	1:54:A:ILE:HG22	1:12:A:VAL:H	18	0.23
(1,2357)	1:24:A:LEU:HA	1:8:A:VAL:HG11	7	0.23
(1,2357)	1:24:A:LEU:HA	1:8:A:VAL:HG12	7	0.23
(1,2357)	1:24:A:LEU:HA	1:8:A:VAL:HG13	7	0.23
(1,2357)	1:24:A:LEU:HA	1:8:A:VAL:HG21	7	0.23
(1,2357)	1:24:A:LEU:HA	1:8:A:VAL:HG22	7	0.23
(1,2357)	1:24:A:LEU:HA	1:8:A:VAL:HG23	7	0.23
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	12	0.23
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	18	0.23
(1,2238)	1:207:A:CYS:HA	1:211:A:ASN:HD21	13	0.23
(1,2238)	1:207:A:CYS:HA	1:211:A:ASN:HD22	13	0.23
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD11	12	0.23
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD12	12	0.23
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD13	12	0.23
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD11	12	0.23
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD12	12	0.23
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD13	12	0.23
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD11	12	0.23
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD12	12	0.23
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD13	12	0.23
(1,1266)	1:117:A:GLU:HA	1:117:A:GLU:HG2	11	0.23
(1,1266)	1:117:A:GLU:HA	1:117:A:GLU:HG3	11	0.23
(1,336)	1:117:A:GLU:HG2	1:117:A:GLU:HA	11	0.23
(1,336)	1:117:A:GLU:HG3	1:117:A:GLU:HA	11	0.23
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE1	7	0.23
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE2	7	0.23
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB2	10	0.23
(1,160)	1:145:A:TYR:HE1	1:184:A:LEU:HB3	10	0.23
(1,152)	1:176:A:TYR:HE1	1:181:A:ILE:HB	20	0.23
(1,120)	1:199:A:TYR:HE1	1:137:A:ILE:HG12	13	0.23
(1,120)	1:199:A:TYR:HE1	1:137:A:ILE:HG13	13	0.23
(1,5786)	1:115:A:ASP:HA	1:117:A:GLU:H	4	0.22
(1,5786)	1:115:A:ASP:HA	1:117:A:GLU:H	6	0.22
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD21	18	0.22
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD22	18	0.22
(1,5679)	1:139:A:LYS:HB2	1:138:A:ASN:HD21	8	0.22
(1,5679)	1:139:A:LYS:HB2	1:138:A:ASN:HD22	8	0.22
(1,5679)	1:139:A:LYS:HB3	1:138:A:ASN:HD21	8	0.22
(1,5679)	1:139:A:LYS:HB3	1:138:A:ASN:HD22	8	0.22
(1,5578)	1:153:A:LEU:HA	1:157:A:VAL:H	1	0.22
(1,5554)	1:128:A:LYS:HB2	1:129:A:PHE:H	9	0.22
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	6	0.22
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	6	0.22
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE2	8	0.22
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE3	8	0.22
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	15	0.22
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	15	0.22
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE2	9	0.22
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE3	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	3	0.22
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD2	1	0.22
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD3	1	0.22
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD2	18	0.22
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD3	18	0.22
(1,5428)	1:23:A:ALA:H	1:20:A:TRP:HZ3	8	0.22
(1,5417)	1:10:A:SER:H	1:3:A:GLU:HB2	3	0.22
(1,5417)	1:10:A:SER:H	1:3:A:GLU:HB3	3	0.22
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE1	7	0.22
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE2	7	0.22
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	4	0.22
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	4	0.22
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	10	0.22
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	10	0.22
(1,5382)	1:74:A:THR:H	1:71:A:GLU:HG2	10	0.22
(1,5382)	1:74:A:THR:H	1:71:A:GLU:HG3	10	0.22
(1,5311)	1:87:A:THR:H	1:65:A:LEU:HD11	16	0.22
(1,5311)	1:87:A:THR:H	1:65:A:LEU:HD12	16	0.22
(1,5311)	1:87:A:THR:H	1:65:A:LEU:HD13	16	0.22
(1,5311)	1:87:A:THR:H	1:65:A:LEU:HD21	16	0.22
(1,5311)	1:87:A:THR:H	1:65:A:LEU:HD22	16	0.22
(1,5311)	1:87:A:THR:H	1:65:A:LEU:HD23	16	0.22
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	18	0.22
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	18	0.22
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	18	0.22
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	7	0.22
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	7	0.22
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	7	0.22
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	9	0.22
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	9	0.22
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	9	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG21	3	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG22	3	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG23	3	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	4	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	4	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	4	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG21	15	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG22	15	0.22
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG23	15	0.22
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	17	0.22
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	17	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD11	16	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD12	16	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD13	16	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD21	16	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD22	16	0.22
(1,5125)	1:196:A:TYR:H	1:153:A:LEU:HD23	16	0.22
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD11	14	0.22
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD12	14	0.22
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD13	14	0.22
(1,4994)	1:222:A:LEU:H	1:222:A:LEU:HG	6	0.22
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	16	0.22
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	17	0.22
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	17	0.22
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD2	18	0.22
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD3	18	0.22
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	3	0.22
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	3	0.22
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	19	0.22
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	19	0.22
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	5	0.22
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	11	0.22
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	5	0.22
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	5	0.22
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	5	0.22
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	5	0.22
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	5	0.22
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	5	0.22
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	5	0.22
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	5	0.22
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	5	0.22
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	5	0.22
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	5	0.22
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	5	0.22
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	13	0.22
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	13	0.22
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	13	0.22
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	13	0.22
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	13	0.22
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	13	0.22
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	13	0.22
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	13	0.22
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	13	0.22
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	13	0.22
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	13	0.22
(1,3398)	1:15:A:THR:HG21	1:16:A:GLU:HG2	10	0.22
(1,3398)	1:15:A:THR:HG21	1:16:A:GLU:HG3	10	0.22
(1,3398)	1:15:A:THR:HG22	1:16:A:GLU:HG2	10	0.22
(1,3398)	1:15:A:THR:HG22	1:16:A:GLU:HG3	10	0.22
(1,3398)	1:15:A:THR:HG23	1:16:A:GLU:HG2	10	0.22
(1,3398)	1:15:A:THR:HG23	1:16:A:GLU:HG3	10	0.22
(1,3381)	1:72:A:LEU:HB2	1:79:A:GLN:HG2	11	0.22
(1,3381)	1:72:A:LEU:HB2	1:79:A:GLN:HG3	11	0.22
(1,3381)	1:72:A:LEU:HB3	1:79:A:GLN:HG2	11	0.22
(1,3381)	1:72:A:LEU:HB3	1:79:A:GLN:HG3	11	0.22
(1,3351)	1:61:A:GLU:HB2	1:60:A:LYS:HB2	1	0.22
(1,3351)	1:61:A:GLU:HB2	1:60:A:LYS:HB3	1	0.22
(1,3351)	1:61:A:GLU:HB3	1:60:A:LYS:HB2	1	0.22
(1,3351)	1:61:A:GLU:HB3	1:60:A:LYS:HB3	1	0.22
(1,3351)	1:61:A:GLU:HB2	1:60:A:LYS:HB2	15	0.22
(1,3351)	1:61:A:GLU:HB2	1:60:A:LYS:HB3	15	0.22
(1,3351)	1:61:A:GLU:HB3	1:60:A:LYS:HB2	15	0.22
(1,3351)	1:61:A:GLU:HB3	1:60:A:LYS:HB3	15	0.22
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	3	0.22
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	3	0.22
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	3	0.22
(1,3303)	1:191:A:ASN:HB2	1:143:A:LEU:HG	7	0.22
(1,3287)	1:140:A:PRO:HD3	1:139:A:LYS:HD2	12	0.22
(1,3287)	1:140:A:PRO:HD3	1:139:A:LYS:HD3	12	0.22
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	3	0.22
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	3	0.22
(1,3221)	1:38:A:LYS:HA	1:38:A:LYS:HD2	4	0.22
(1,3221)	1:38:A:LYS:HA	1:38:A:LYS:HD3	4	0.22
(1,3217)	1:128:A:LYS:HA	1:96:A:MET:HG2	2	0.22
(1,3217)	1:128:A:LYS:HA	1:96:A:MET:HG3	2	0.22
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG21	19	0.22
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG22	19	0.22
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG23	19	0.22
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	7	0.22
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	7	0.22
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	7	0.22
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	9	0.22
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	9	0.22
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG2	7	0.22
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG3	7	0.22
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	18	0.22
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	18	0.22
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	18	0.22
(1,3097)	1:82:A:SER:H	1:79:A:GLN:HG2	17	0.22
(1,3097)	1:82:A:SER:H	1:79:A:GLN:HG3	17	0.22
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG2	2	0.22
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG3	2	0.22
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG21	14	0.22
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG22	14	0.22
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG23	14	0.22
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	8	0.22
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	8	0.22
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	8	0.22
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	8	0.22
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	8	0.22
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	8	0.22
(1,3012)	1:173:A:LYS:HB3	1:174:A:GLN:HA	15	0.22
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	1	0.22
(1,2988)	1:86:A:LYS:HG3	1:86:A:LYS:HA	17	0.22
(1,2975)	1:179:A:LEU:HD22	1:176:A:TYR:HA	20	0.22
(1,2946)	1:190:A:TYR:HB2	1:189:A:SER:HB2	9	0.22
(1,2946)	1:190:A:TYR:HB2	1:189:A:SER:HB3	9	0.22
(1,2917)	1:196:A:TYR:HA	1:195:A:ALA:H	14	0.22
(1,2887)	1:101:A:ILE:HB	1:99:A:SER:H	18	0.22
(1,2872)	1:100:A:GLU:HB3	1:101:A:ILE:HD11	2	0.22
(1,2872)	1:100:A:GLU:HB3	1:101:A:ILE:HD12	2	0.22
(1,2872)	1:100:A:GLU:HB3	1:101:A:ILE:HD13	2	0.22
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	5	0.22
(1,2840)	1:22:A:PRO:HA	1:81:A:ALA:HB1	11	0.22
(1,2840)	1:22:A:PRO:HA	1:81:A:ALA:HB2	11	0.22
(1,2840)	1:22:A:PRO:HA	1:81:A:ALA:HB3	11	0.22
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG21	2	0.22
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG22	2	0.22
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG23	2	0.22
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG11	4	0.22
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG12	4	0.22
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG13	4	0.22
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG21	4	0.22
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG22	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2744)	1:195:A:ALA:HB3	1:192:A:VAL:HG23	4	0.22
(1,2717)	1:130:A:MET:HE3	1:198:A:LYS:HB2	16	0.22
(1,2717)	1:130:A:MET:HE3	1:198:A:LYS:HB3	16	0.22
(1,2699)	1:8:A:VAL:HG12	1:85:A:LEU:HB2	14	0.22
(1,2699)	1:8:A:VAL:HG12	1:85:A:LEU:HB3	14	0.22
(1,2699)	1:8:A:VAL:HG13	1:85:A:LEU:HB2	18	0.22
(1,2699)	1:8:A:VAL:HG13	1:85:A:LEU:HB3	18	0.22
(1,2692)	1:195:A:ALA:HB3	1:150:A:LEU:HB2	11	0.22
(1,2692)	1:195:A:ALA:HB3	1:150:A:LEU:HB3	11	0.22
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG2	6	0.22
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG3	6	0.22
(1,2607)	1:137:A:ILE:HD13	1:127:A:TYR:HA	9	0.22
(1,2577)	1:166:A:ILE:HD12	1:160:A:GLN:HA	14	0.22
(1,2562)	1:72:A:LEU:HG	1:69:A:GLU:HA	11	0.22
(1,2552)	1:101:A:ILE:HG23	1:102:A:LEU:HA	4	0.22
(1,2551)	1:98:A:ILE:HG22	1:98:A:ILE:HA	7	0.22
(1,2538)	1:183:A:ILE:HD11	1:184:A:LEU:HA	16	0.22
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	1	0.22
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	9	0.22
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	14	0.22
(1,2496)	1:46:A:PHE:HD1	1:44:A:ARG:HG2	8	0.22
(1,2496)	1:46:A:PHE:HD1	1:44:A:ARG:HG3	8	0.22
(1,2411)	1:88:A:ARG:HD2	1:88:A:ARG:H	7	0.22
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	12	0.22
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	7	0.22
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	5	0.22
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD11	4	0.22
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD12	4	0.22
(1,1679)	1:54:A:ILE:HG21	1:54:A:ILE:HD13	4	0.22
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD11	4	0.22
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD12	4	0.22
(1,1679)	1:54:A:ILE:HG22	1:54:A:ILE:HD13	4	0.22
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD11	4	0.22
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD12	4	0.22
(1,1679)	1:54:A:ILE:HG23	1:54:A:ILE:HD13	4	0.22
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD11	14	0.22
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD12	14	0.22
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD13	14	0.22
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD21	14	0.22
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD22	14	0.22
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD23	14	0.22
(1,5870)	1:110:A:LYS:HE2	1:111:A:GLU:H	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5870)	1:110:A:LYS:HE3	1:111:A:GLU:H	7	0.21
(1,5850)	1:113:A:GLU:HG3	1:113:A:GLU:H	7	0.21
(1,5843)	1:111:A:GLU:H	1:110:A:LYS:HE2	7	0.21
(1,5843)	1:111:A:GLU:H	1:110:A:LYS:HE3	7	0.21
(1,5813)	1:108:A:LYS:HG2	1:106:A:SER:HB2	15	0.21
(1,5813)	1:108:A:LYS:HG2	1:106:A:SER:HB3	15	0.21
(1,5813)	1:108:A:LYS:HG3	1:106:A:SER:HB2	15	0.21
(1,5813)	1:108:A:LYS:HG3	1:106:A:SER:HB3	15	0.21
(1,5792)	1:76:A:PRO:HD2	1:75:A:LYS:HB2	5	0.21
(1,5792)	1:76:A:PRO:HD2	1:75:A:LYS:HB3	5	0.21
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD21	4	0.21
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD22	4	0.21
(1,5689)	1:137:A:ILE:HA	1:138:A:ASN:HD21	16	0.21
(1,5689)	1:137:A:ILE:HA	1:138:A:ASN:HD22	16	0.21
(1,5681)	1:94:A:TRP:HZ3	1:94:A:TRP:H	18	0.21
(1,5642)	1:187:A:ALA:HB2	1:191:A:ASN:HD21	16	0.21
(1,5642)	1:187:A:ALA:HB2	1:191:A:ASN:HD22	16	0.21
(1,5602)	1:34:A:ILE:HG21	1:53:A:SER:H	17	0.21
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	12	0.21
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	12	0.21
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE2	10	0.21
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE3	10	0.21
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	2	0.21
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	2	0.21
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	12	0.21
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	12	0.21
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD11	5	0.21
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD12	5	0.21
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD13	5	0.21
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD21	5	0.21
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD22	5	0.21
(1,5463)	1:178:A:ASP:H	1:153:A:LEU:HD23	5	0.21
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE1	2	0.21
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE2	2	0.21
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	11	0.21
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	11	0.21
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB2	2	0.21
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB3	2	0.21
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD1	14	0.21
(1,5386)	1:200:A:LEU:H	1:201:A:TYR:HD2	14	0.21
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	11	0.21
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	17	0.21
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	17	0.21
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	8	0.21
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	8	0.21
(1,5313)	1:20:A:TRP:HE1	1:71:A:GLU:HG2	11	0.21
(1,5313)	1:20:A:TRP:HE1	1:71:A:GLU:HG3	11	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	5	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	5	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	5	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	5	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	5	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	5	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	12	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	12	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	12	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	12	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	12	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	12	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	14	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	14	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	14	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	14	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	14	0.21
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	14	0.21
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB2	10	0.21
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB3	10	0.21
(1,5267)	1:160:A:GLN:HE21	1:175:A:ILE:HD11	12	0.21
(1,5267)	1:160:A:GLN:HE21	1:175:A:ILE:HD12	12	0.21
(1,5267)	1:160:A:GLN:HE21	1:175:A:ILE:HD13	12	0.21
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD21	20	0.21
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD22	20	0.21
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG2	5	0.21
(1,5237)	1:145:A:TYR:H	1:146:A:LYS:HG3	5	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	8	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	8	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	8	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	10	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	10	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	10	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	12	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	12	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	13	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	13	0.21
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	13	0.21
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	18	0.21
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	18	0.21
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB2	2	0.21
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB3	2	0.21
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG21	17	0.21
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG22	17	0.21
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HG23	17	0.21
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	1	0.21
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	1	0.21
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	1	0.21
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG11	20	0.21
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG12	20	0.21
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG13	20	0.21
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG21	20	0.21
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG22	20	0.21
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG23	20	0.21
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG11	15	0.21
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG12	15	0.21
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG13	15	0.21
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG21	15	0.21
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG22	15	0.21
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG23	15	0.21
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD11	3	0.21
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD12	3	0.21
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD13	3	0.21
(1,5054)	1:78:A:LEU:H	1:47:A:ILE:HG12	14	0.21
(1,5054)	1:78:A:LEU:H	1:47:A:ILE:HG13	14	0.21
(1,5052)	1:78:A:LEU:H	1:75:A:LYS:HB2	8	0.21
(1,5052)	1:78:A:LEU:H	1:75:A:LYS:HB3	8	0.21
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	11	0.21
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	11	0.21
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG2	14	0.21
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG3	14	0.21
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	4	0.21
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD11	12	0.21
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD12	12	0.21
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD13	12	0.21
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD21	12	0.21
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD22	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD23	12	0.21
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB2	4	0.21
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB3	4	0.21
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB2	4	0.21
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB3	4	0.21
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	15	0.21
(1,3492)	1:148:A:LEU:HG	1:148:A:LEU:HA	16	0.21
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	3	0.21
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	3	0.21
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB2	10	0.21
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB3	10	0.21
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	8	0.21
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	8	0.21
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	8	0.21
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	8	0.21
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	8	0.21
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	8	0.21
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	8	0.21
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	8	0.21
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	8	0.21
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	8	0.21
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	8	0.21
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	8	0.21
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	20	0.21
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	20	0.21
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	20	0.21
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	20	0.21
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	20	0.21
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	20	0.21
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	20	0.21
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	20	0.21
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	20	0.21
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	20	0.21
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	20	0.21
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	20	0.21
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	20	0.21
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	20	0.21
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	20	0.21
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	20	0.21
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	20	0.21
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	20	0.21
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	20	0.21
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	20	0.21
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	20	0.21
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	20	0.21
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	20	0.21
(1,3428)	1:72:A:LEU:HD13	1:69:A:GLU:HB2	13	0.21
(1,3428)	1:72:A:LEU:HD13	1:69:A:GLU:HB3	13	0.21
(1,3379)	1:75:A:LYS:HG3	1:19:A:GLU:HG2	7	0.21
(1,3379)	1:75:A:LYS:HG3	1:19:A:GLU:HG3	7	0.21
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	18	0.21
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	18	0.21
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	18	0.21
(1,3340)	1:19:A:GLU:HB2	1:75:A:LYS:HG2	20	0.21
(1,3340)	1:19:A:GLU:HB2	1:75:A:LYS:HG3	20	0.21
(1,3340)	1:19:A:GLU:HB3	1:75:A:LYS:HG2	20	0.21
(1,3340)	1:19:A:GLU:HB3	1:75:A:LYS:HG3	20	0.21
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB2	18	0.21
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB3	18	0.21
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	2	0.21
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	2	0.21
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	20	0.21
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	20	0.21
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG2	13	0.21
(1,3144)	1:20:A:TRP:HD1	1:19:A:GLU:HG3	13	0.21
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG21	7	0.21
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG22	7	0.21
(1,3120)	1:212:A:ILE:H	1:212:A:ILE:HG23	7	0.21
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG2	5	0.21
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG3	5	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	8	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	8	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	8	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	10	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	10	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	10	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	12	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	12	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	12	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	13	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	13	0.21
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	13	0.21
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG2	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3096)	1:104:A:SER:H	1:103:A:GLU:HG3	1	0.21
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	15	0.21
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	15	0.21
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	15	0.21
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	15	0.21
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	15	0.21
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	15	0.21
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	3	0.21
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	3	0.21
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	3	0.21
(1,3051)	1:34:A:ILE:HG22	1:53:A:SER:HA	3	0.21
(1,2975)	1:179:A:LEU:HD12	1:176:A:TYR:HA	6	0.21
(1,2975)	1:179:A:LEU:HD22	1:176:A:TYR:HA	7	0.21
(1,2973)	1:166:A:ILE:HB	1:166:A:ILE:HA	11	0.21
(1,2973)	1:166:A:ILE:HB	1:166:A:ILE:HA	14	0.21
(1,2973)	1:166:A:ILE:HB	1:166:A:ILE:HA	16	0.21
(1,2973)	1:166:A:ILE:HB	1:166:A:ILE:HA	20	0.21
(1,2887)	1:101:A:ILE:HB	1:99:A:SER:H	2	0.21
(1,2841)	1:166:A:ILE:HD13	1:157:A:VAL:H	20	0.21
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD11	12	0.21
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD12	12	0.21
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD13	12	0.21
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD21	12	0.21
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD22	12	0.21
(1,2770)	1:101:A:ILE:HD13	1:123:A:LEU:HD23	12	0.21
(1,2708)	1:137:A:ILE:HD11	1:139:A:LYS:HB2	8	0.21
(1,2708)	1:137:A:ILE:HD11	1:139:A:LYS:HB3	8	0.21
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG2	3	0.21
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG3	3	0.21
(1,2665)	1:47:A:ILE:HD11	1:76:A:PRO:HB2	3	0.21
(1,2665)	1:47:A:ILE:HD11	1:76:A:PRO:HB3	3	0.21
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB2	7	0.21
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB3	7	0.21
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB2	10	0.21
(1,2643)	1:187:A:ALA:HB2	1:190:A:TYR:HB3	10	0.21
(1,2561)	1:65:A:LEU:HG	1:86:A:LYS:HA	20	0.21
(1,2551)	1:98:A:ILE:HG23	1:98:A:ILE:HA	15	0.21
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	12	0.21
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	16	0.21
(1,2479)	1:194:A:THR:HG23	1:190:A:TYR:HD1	19	0.21
(1,2479)	1:194:A:THR:HG23	1:190:A:TYR:HD2	19	0.21
(1,2443)	1:83:A:ILE:HD11	1:83:A:ILE:H	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2426)	1:101:A:ILE:HG22	1:103:A:GLU:H	3	0.21
(1,2425)	1:54:A:ILE:HG21	1:57:A:LYS:H	9	0.21
(1,2418)	1:200:A:LEU:HD22	1:199:A:TYR:H	20	0.21
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG2	14	0.21
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG3	14	0.21
(1,2400)	1:34:A:ILE:HD13	1:52:A:TYR:H	8	0.21
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	13	0.21
(1,2212)	1:138:A:ASN:HD21	1:137:A:ILE:HA	16	0.21
(1,2212)	1:138:A:ASN:HD22	1:137:A:ILE:HA	16	0.21
(1,1919)	1:81:A:ALA:H	1:85:A:LEU:HG	17	0.21
(1,362)	1:150:A:LEU:HG	1:119:A:ARG:HA	16	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD11	14	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD12	14	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD13	14	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD21	14	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD22	14	0.21
(1,150)	1:127:A:TYR:HE1	1:123:A:LEU:HD23	14	0.21
(1,150)	1:127:A:TYR:HE2	1:141:A:PRO:HG2	20	0.21
(1,150)	1:127:A:TYR:HE2	1:141:A:PRO:HG3	20	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD11	4	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD12	4	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD13	4	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD21	4	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD22	4	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD23	4	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD11	16	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD12	16	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD13	16	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD21	16	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD22	16	0.21
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD23	16	0.21
(1,5856)	1:115:A:ASP:HA	1:114:A:LEU:HA	12	0.2
(1,5848)	1:113:A:GLU:HB2	1:114:A:LEU:HG	17	0.2
(1,5832)	1:109:A:ASP:H	1:108:A:LYS:HB2	9	0.2
(1,5832)	1:109:A:ASP:H	1:108:A:LYS:HB3	9	0.2
(1,5828)	1:108:A:LYS:H	1:108:A:LYS:HB2	10	0.2
(1,5828)	1:108:A:LYS:H	1:108:A:LYS:HB3	10	0.2
(1,5807)	1:99:A:SER:H	1:97:A:ASP:HB2	10	0.2
(1,5807)	1:99:A:SER:H	1:97:A:ASP:HB3	10	0.2
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD21	6	0.2
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD22	6	0.2
(1,5690)	1:65:A:LEU:HA	1:66:A:ASN:HD21	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5690)	1:65:A:LEU:HA	1:66:A:ASN:HD22	9	0.2
(1,5623)	1:61:A:GLU:HG2	1:1:A:ASN:HD21	6	0.2
(1,5623)	1:61:A:GLU:HG2	1:1:A:ASN:HD22	6	0.2
(1,5623)	1:61:A:GLU:HG3	1:1:A:ASN:HD21	6	0.2
(1,5623)	1:61:A:GLU:HG3	1:1:A:ASN:HD22	6	0.2
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	15	0.2
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	5	0.2
(1,5534)	1:78:A:LEU:HB3	1:81:A:ALA:H	6	0.2
(1,5534)	1:78:A:LEU:HB2	1:81:A:ALA:H	9	0.2
(1,5522)	1:64:A:ILE:HD12	1:23:A:ALA:H	15	0.2
(1,5500)	1:154:A:PHE:H	1:153:A:LEU:HG	14	0.2
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	8	0.2
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	8	0.2
(1,5496)	1:20:A:TRP:HE1	1:62:A:VAL:HB	9	0.2
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD21	15	0.2
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD22	15	0.2
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	1	0.2
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	2	0.2
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	6	0.2
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	8	0.2
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	12	0.2
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	12	0.2
(1,5387)	1:200:A:LEU:H	1:197:A:ARG:HA	5	0.2
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	4	0.2
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	4	0.2
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	10	0.2
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	10	0.2
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	1	0.2
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	8	0.2
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	13	0.2
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	13	0.2
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	13	0.2
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	13	0.2
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	13	0.2
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	13	0.2
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB2	3	0.2
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB3	3	0.2
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	17	0.2
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	17	0.2
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	17	0.2
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB1	14	0.2
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB2	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB3	14	0.2
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	1	0.2
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	1	0.2
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	1	0.2
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	5	0.2
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	5	0.2
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	5	0.2
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	7	0.2
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	7	0.2
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	7	0.2
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	11	0.2
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	11	0.2
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	11	0.2
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD11	12	0.2
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD12	12	0.2
(1,5139)	1:80:A:LYS:H	1:83:A:ILE:HD13	12	0.2
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG11	8	0.2
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG12	8	0.2
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG13	8	0.2
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG21	8	0.2
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG22	8	0.2
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG23	8	0.2
(1,5103)	1:123:A:LEU:H	1:119:A:ARG:HB2	6	0.2
(1,5103)	1:123:A:LEU:H	1:119:A:ARG:HB3	6	0.2
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB2	19	0.2
(1,4996)	1:75:A:LYS:H	1:71:A:GLU:HB3	19	0.2
(1,4994)	1:222:A:LEU:H	1:222:A:LEU:HG	11	0.2
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD1	13	0.2
(1,4965)	1:84:A:PHE:H	1:46:A:PHE:HD2	13	0.2
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD11	7	0.2
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD12	7	0.2
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD13	7	0.2
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD21	7	0.2
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD22	7	0.2
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD23	7	0.2
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD2	8	0.2
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD3	8	0.2
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD2	12	0.2
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD3	12	0.2
(1,3721)	1:18:A:THR:HB	1:19:A:GLU:H	8	0.2
(1,3681)	1:212:A:ILE:HD11	1:213:A:GLN:H	13	0.2
(1,3681)	1:212:A:ILE:HD12	1:213:A:GLN:H	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3681)	1:212:A:ILE:HD13	1:213:A:GLN:H	13	0.2
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB2	1	0.2
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB3	1	0.2
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB2	1	0.2
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB3	1	0.2
(1,3505)	1:197:A:ARG:HG2	1:197:A:ARG:HA	4	0.2
(1,3505)	1:197:A:ARG:HG2	1:197:A:ARG:HA	19	0.2
(1,3431)	1:83:A:ILE:HG21	1:87:A:THR:HG21	1	0.2
(1,3431)	1:83:A:ILE:HG21	1:87:A:THR:HG22	1	0.2
(1,3431)	1:83:A:ILE:HG21	1:87:A:THR:HG23	1	0.2
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	7	0.2
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	7	0.2
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	7	0.2
(1,3289)	1:68:A:PRO:HD2	1:72:A:LEU:HG	19	0.2
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD2	3	0.2
(1,3259)	1:56:A:ARG:HA	1:56:A:ARG:HD3	3	0.2
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	17	0.2
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	17	0.2
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	17	0.2
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG2	4	0.2
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG3	4	0.2
(1,3053)	1:55:A:ALA:HB2	1:40:A:GLN:HA	4	0.2
(1,3051)	1:34:A:ILE:HG22	1:53:A:SER:HA	7	0.2
(1,2988)	1:86:A:LYS:HG2	1:86:A:LYS:HA	11	0.2
(1,2975)	1:179:A:LEU:HD22	1:176:A:TYR:HA	15	0.2
(1,2973)	1:166:A:ILE:HB	1:166:A:ILE:HA	4	0.2
(1,2958)	1:72:A:LEU:H	1:70:A:SER:HB2	14	0.2
(1,2958)	1:72:A:LEU:H	1:70:A:SER:HB3	14	0.2
(1,2922)	1:64:A:ILE:HD12	1:62:A:VAL:HB	2	0.2
(1,2871)	1:175:A:ILE:HG13	1:175:A:ILE:HA	1	0.2
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	15	0.2
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG21	13	0.2
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG22	13	0.2
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG23	13	0.2
(1,2841)	1:166:A:ILE:HD13	1:157:A:VAL:H	16	0.2
(1,2804)	1:171:A:VAL:HG11	1:175:A:ILE:HD11	11	0.2
(1,2804)	1:171:A:VAL:HG11	1:175:A:ILE:HD12	11	0.2
(1,2804)	1:171:A:VAL:HG11	1:175:A:ILE:HD13	11	0.2
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG11	15	0.2
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG12	15	0.2
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG13	15	0.2
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG21	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG22	15	0.2
(1,2776)	1:54:A:ILE:HB	1:43:A:VAL:HG23	15	0.2
(1,2685)	1:67:A:LEU:HD21	1:71:A:GLU:HB2	19	0.2
(1,2685)	1:67:A:LEU:HD21	1:71:A:GLU:HB3	19	0.2
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB2	6	0.2
(1,2643)	1:187:A:ALA:HB3	1:190:A:TYR:HB3	6	0.2
(1,2639)	1:11:A:VAL:HG12	1:20:A:TRP:HB2	18	0.2
(1,2639)	1:11:A:VAL:HG12	1:20:A:TRP:HB3	18	0.2
(1,2562)	1:72:A:LEU:HG	1:69:A:GLU:HA	20	0.2
(1,2533)	1:9:A:VAL:HG22	1:25:A:VAL:HA	20	0.2
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	11	0.2
(1,2502)	1:42:A:LEU:HG	1:27:A:SER:HA	4	0.2
(1,2462)	1:197:A:ARG:HD2	1:201:A:TYR:HD1	1	0.2
(1,2462)	1:197:A:ARG:HD2	1:201:A:TYR:HD2	1	0.2
(1,2428)	1:64:A:ILE:HD13	1:65:A:LEU:H	19	0.2
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	3	0.2
(1,2373)	1:26:A:ILE:HD13	1:43:A:VAL:H	19	0.2
(1,2289)	1:119:A:ARG:HA	1:117:A:GLU:H	11	0.2
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB2	3	0.2
(1,2260)	1:101:A:ILE:HA	1:140:A:PRO:HB3	3	0.2
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	18	0.2
(1,624)	1:221:A:GLU:H	1:221:A:GLU:HG2	20	0.2
(1,624)	1:221:A:GLU:H	1:221:A:GLU:HG3	20	0.2
(1,152)	1:176:A:TYR:HE1	1:181:A:ILE:HB	16	0.2
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD11	18	0.2
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD12	18	0.2
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD13	18	0.2
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD21	18	0.2
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD22	18	0.2
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD23	18	0.2
(1,5842)	1:111:A:GLU:H	1:111:A:GLU:HG2	1	0.19
(1,5842)	1:111:A:GLU:H	1:111:A:GLU:HG3	1	0.19
(1,5832)	1:108:A:LYS:H	1:108:A:LYS:HB2	15	0.19
(1,5832)	1:108:A:LYS:H	1:108:A:LYS:HB3	15	0.19
(1,5828)	1:108:A:LYS:H	1:108:A:LYS:HB2	15	0.19
(1,5828)	1:108:A:LYS:H	1:108:A:LYS:HB3	15	0.19
(1,5812)	1:64:A:ILE:HD11	1:8:A:VAL:HB	9	0.19
(1,5792)	1:76:A:PRO:HD2	1:75:A:LYS:HB2	11	0.19
(1,5792)	1:76:A:PRO:HD2	1:75:A:LYS:HB3	11	0.19
(1,5785)	1:111:A:GLU:H	1:111:A:GLU:HG2	1	0.19
(1,5785)	1:111:A:GLU:H	1:111:A:GLU:HG3	1	0.19
(1,5690)	1:65:A:LEU:HA	1:66:A:ASN:HD21	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5690)	1:65:A:LEU:HA	1:66:A:ASN:HD22	11	0.19
(1,5689)	1:137:A:ILE:HA	1:138:A:ASN:HD21	3	0.19
(1,5689)	1:137:A:ILE:HA	1:138:A:ASN:HD22	3	0.19
(1,5681)	1:94:A:TRP:HZ3	1:94:A:TRP:H	1	0.19
(1,5642)	1:143:A:LEU:HG	1:191:A:ASN:HD21	10	0.19
(1,5642)	1:143:A:LEU:HG	1:191:A:ASN:HD22	10	0.19
(1,5602)	1:34:A:ILE:HG22	1:53:A:SER:H	1	0.19
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	2	0.19
(1,5534)	1:47:A:ILE:HB	1:81:A:ALA:H	16	0.19
(1,5534)	1:78:A:LEU:HB3	1:81:A:ALA:H	18	0.19
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	1	0.19
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	1	0.19
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE2	7	0.19
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE3	7	0.19
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	20	0.19
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	20	0.19
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE1	20	0.19
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE2	20	0.19
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB2	10	0.19
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB3	10	0.19
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	12	0.19
(1,5359)	1:6:A:GLY:H	1:25:A:VAL:H	7	0.19
(1,5331)	1:75:A:LYS:H	1:71:A:GLU:HG2	11	0.19
(1,5331)	1:75:A:LYS:H	1:71:A:GLU:HG3	11	0.19
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	4	0.19
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	4	0.19
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	3	0.19
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	6	0.19
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	6	0.19
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	6	0.19
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	6	0.19
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	6	0.19
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	6	0.19
(1,5290)	1:73:A:SER:H	1:79:A:GLN:HG2	7	0.19
(1,5290)	1:73:A:SER:H	1:79:A:GLN:HG3	7	0.19
(1,5233)	1:1:A:ASN:HD22	1:9:A:VAL:HB	20	0.19
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	5	0.19
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	5	0.19
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	5	0.19
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB2	5	0.19
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB3	5	0.19
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB2	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB3	9	0.19
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	13	0.19
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	13	0.19
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	13	0.19
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD11	8	0.19
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD12	8	0.19
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD13	8	0.19
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD21	8	0.19
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD22	8	0.19
(1,5128)	1:197:A:ARG:H	1:153:A:LEU:HD23	8	0.19
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG11	10	0.19
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG12	10	0.19
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG13	10	0.19
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG21	10	0.19
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG22	10	0.19
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG23	10	0.19
(1,5118)	1:7:A:LYS:H	1:5:A:LEU:HG	16	0.19
(1,5070)	1:40:A:GLN:H	1:56:A:ARG:H	16	0.19
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD11	6	0.19
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD12	6	0.19
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD13	6	0.19
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB2	17	0.19
(1,5053)	1:78:A:LEU:H	1:72:A:LEU:HB3	17	0.19
(1,5052)	1:78:A:LEU:H	1:78:A:LEU:HB2	9	0.19
(1,5052)	1:78:A:LEU:H	1:78:A:LEU:HB3	9	0.19
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	20	0.19
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	20	0.19
(1,4975)	1:75:A:LYS:H	1:74:A:THR:HB	13	0.19
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	3	0.19
(1,4933)	1:46:A:PHE:H	1:24:A:LEU:HD11	15	0.19
(1,4933)	1:46:A:PHE:H	1:24:A:LEU:HD12	15	0.19
(1,4933)	1:46:A:PHE:H	1:24:A:LEU:HD13	15	0.19
(1,4933)	1:46:A:PHE:H	1:24:A:LEU:HD21	15	0.19
(1,4933)	1:46:A:PHE:H	1:24:A:LEU:HD22	15	0.19
(1,4933)	1:46:A:PHE:H	1:24:A:LEU:HD23	15	0.19
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	13	0.19
(1,3721)	1:18:A:THR:HB	1:19:A:GLU:H	6	0.19
(1,3604)	1:149:A:ASN:HB2	1:150:A:LEU:H	13	0.19
(1,3604)	1:149:A:ASN:HB3	1:150:A:LEU:H	13	0.19
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB2	15	0.19
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB3	15	0.19
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB2	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB3	15	0.19
(1,3505)	1:197:A:ARG:HG2	1:197:A:ARG:HA	10	0.19
(1,3505)	1:197:A:ARG:HG3	1:197:A:ARG:HA	20	0.19
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	4	0.19
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	18	0.19
(1,3431)	1:83:A:ILE:HG22	1:87:A:THR:HG21	4	0.19
(1,3431)	1:83:A:ILE:HG22	1:87:A:THR:HG22	4	0.19
(1,3431)	1:83:A:ILE:HG22	1:87:A:THR:HG23	4	0.19
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE2	9	0.19
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE3	9	0.19
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE2	9	0.19
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE3	9	0.19
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE2	10	0.19
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE3	10	0.19
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE2	10	0.19
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE3	10	0.19
(1,3385)	1:7:A:LYS:HG3	1:9:A:VAL:HG11	14	0.19
(1,3385)	1:7:A:LYS:HG3	1:9:A:VAL:HG12	14	0.19
(1,3385)	1:7:A:LYS:HG3	1:9:A:VAL:HG13	14	0.19
(1,3385)	1:7:A:LYS:HG3	1:9:A:VAL:HG21	14	0.19
(1,3385)	1:7:A:LYS:HG3	1:9:A:VAL:HG22	14	0.19
(1,3385)	1:7:A:LYS:HG3	1:9:A:VAL:HG23	14	0.19
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG2	4	0.19
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG3	4	0.19
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG2	4	0.19
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG3	4	0.19
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG2	19	0.19
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG3	19	0.19
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG2	19	0.19
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG3	19	0.19
(1,3346)	1:177:A:MET:HE1	1:183:A:ILE:HD11	14	0.19
(1,3346)	1:177:A:MET:HE1	1:183:A:ILE:HD12	14	0.19
(1,3346)	1:177:A:MET:HE1	1:183:A:ILE:HD13	14	0.19
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD11	13	0.19
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD12	13	0.19
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD13	13	0.19
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD21	13	0.19
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD22	13	0.19
(1,3253)	1:86:A:LYS:HA	1:65:A:LEU:HD23	13	0.19
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	11	0.19
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	11	0.19
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	12	0.19
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG21	3	0.19
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG22	3	0.19
(1,3161)	1:181:A:ILE:H	1:181:A:ILE:HG23	3	0.19
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	13	0.19
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	13	0.19
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	13	0.19
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG2	9	0.19
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG3	9	0.19
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	5	0.19
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	5	0.19
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	5	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD11	4	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD12	4	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD13	4	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD21	4	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD22	4	0.19
(1,3102)	1:90:A:VAL:H	1:85:A:LEU:HD23	4	0.19
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG21	17	0.19
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG22	17	0.19
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG23	17	0.19
(1,3053)	1:55:A:ALA:HB1	1:40:A:GLN:HA	2	0.19
(1,2948)	1:63:A:ASP:HB3	1:64:A:ILE:HA	10	0.19
(1,2946)	1:190:A:TYR:HB2	1:189:A:SER:HB2	20	0.19
(1,2946)	1:190:A:TYR:HB2	1:189:A:SER:HB3	20	0.19
(1,2920)	1:54:A:ILE:HD13	1:52:A:TYR:HA	6	0.19
(1,2826)	1:59:A:ILE:HB	1:61:A:GLU:HG2	20	0.19
(1,2826)	1:59:A:ILE:HB	1:61:A:GLU:HG3	20	0.19
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD11	17	0.19
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD12	17	0.19
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD13	17	0.19
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD21	17	0.19
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD22	17	0.19
(1,2759)	1:71:A:GLU:HB3	1:67:A:LEU:HD23	17	0.19
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB2	6	0.19
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB3	6	0.19
(1,2682)	1:62:A:VAL:HB	1:9:A:VAL:HB	5	0.19
(1,2643)	1:187:A:ALA:HB1	1:190:A:TYR:HB2	19	0.19
(1,2643)	1:187:A:ALA:HB1	1:190:A:TYR:HB3	19	0.19
(1,2587)	1:137:A:ILE:HG13	1:127:A:TYR:HA	4	0.19
(1,2577)	1:166:A:ILE:HD13	1:160:A:GLN:HA	8	0.19
(1,2548)	1:150:A:LEU:HD22	1:141:A:PRO:HA	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2471)	1:12:A:VAL:HG11	1:17:A:ARG:HE	16	0.19
(1,2425)	1:54:A:ILE:HG23	1:12:A:VAL:H	4	0.19
(1,2400)	1:34:A:ILE:HD13	1:52:A:TYR:H	2	0.19
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	18	0.19
(1,2257)	1:101:A:ILE:HA	1:100:A:GLU:H	11	0.19
(1,2212)	1:138:A:ASN:HD21	1:137:A:ILE:HA	3	0.19
(1,2212)	1:138:A:ASN:HD22	1:137:A:ILE:HA	3	0.19
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD11	3	0.19
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD12	3	0.19
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD13	3	0.19
(1,732)	1:142:A:VAL:H	1:142:A:VAL:HB	6	0.19
(1,732)	1:142:A:VAL:H	1:142:A:VAL:HB	13	0.19
(1,283)	1:88:A:ARG:HE	1:84:A:PHE:HA	17	0.19
(1,249)	1:133:A:ARG:H	1:136:A:PRO:HA	16	0.19
(1,5835)	1:110:A:LYS:HA	1:110:A:LYS:H	11	0.18
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD11	3	0.18
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD12	3	0.18
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD13	3	0.18
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD11	3	0.18
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD12	3	0.18
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD13	3	0.18
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD11	15	0.18
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD12	15	0.18
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD13	15	0.18
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD11	15	0.18
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD12	15	0.18
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD13	15	0.18
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG21	7	0.18
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG22	7	0.18
(1,5810)	1:61:A:GLU:HB3	1:59:A:ILE:HG23	7	0.18
(1,5807)	1:2:A:ASP:H	1:2:A:ASP:HB2	14	0.18
(1,5807)	1:2:A:ASP:H	1:2:A:ASP:HB3	14	0.18
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD21	7	0.18
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD22	7	0.18
(1,5690)	1:65:A:LEU:HA	1:66:A:ASN:HD21	10	0.18
(1,5690)	1:65:A:LEU:HA	1:66:A:ASN:HD22	10	0.18
(1,5679)	1:139:A:LYS:HD2	1:138:A:ASN:HD21	9	0.18
(1,5679)	1:139:A:LYS:HD2	1:138:A:ASN:HD22	9	0.18
(1,5679)	1:139:A:LYS:HD3	1:138:A:ASN:HD21	9	0.18
(1,5679)	1:139:A:LYS:HD3	1:138:A:ASN:HD22	9	0.18
(1,5642)	1:143:A:LEU:HG	1:191:A:ASN:HD21	18	0.18
(1,5642)	1:143:A:LEU:HG	1:191:A:ASN:HD22	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	18	0.18
(1,5578)	1:38:A:LYS:HA	1:40:A:GLN:H	17	0.18
(1,5522)	1:9:A:VAL:HG23	1:23:A:ALA:H	7	0.18
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	18	0.18
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	18	0.18
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE2	18	0.18
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE3	18	0.18
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	10	0.18
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	10	0.18
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	20	0.18
(1,5453)	1:172:A:TRP:H	1:174:A:GLN:HB2	15	0.18
(1,5453)	1:172:A:TRP:H	1:174:A:GLN:HB3	15	0.18
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE1	15	0.18
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE2	15	0.18
(1,5428)	1:23:A:ALA:H	1:46:A:PHE:HD1	16	0.18
(1,5428)	1:23:A:ALA:H	1:46:A:PHE:HD2	16	0.18
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE1	19	0.18
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE2	19	0.18
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE1	20	0.18
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE2	20	0.18
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	18	0.18
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	18	0.18
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB2	6	0.18
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB3	6	0.18
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	1	0.18
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	1	0.18
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	19	0.18
(1,5290)	1:73:A:SER:H	1:79:A:GLN:HG2	11	0.18
(1,5290)	1:73:A:SER:H	1:79:A:GLN:HG3	11	0.18
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	15	0.18
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	15	0.18
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	15	0.18
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB2	10	0.18
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB3	10	0.18
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB2	15	0.18
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB3	15	0.18
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB2	18	0.18
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB3	18	0.18
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	2	0.18
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	2	0.18
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	2	0.18
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG11	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG12	5	0.18
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG13	5	0.18
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG21	5	0.18
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG22	5	0.18
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG23	5	0.18
(1,5118)	1:7:A:LYS:H	1:5:A:LEU:HG	12	0.18
(1,5070)	1:40:A:GLN:H	1:56:A:ARG:H	19	0.18
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	2	0.18
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	2	0.18
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	15	0.18
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	15	0.18
(1,5041)	1:20:A:TRP:H	1:19:A:GLU:HG2	20	0.18
(1,5041)	1:20:A:TRP:H	1:19:A:GLU:HG3	20	0.18
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG21	9	0.18
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG22	9	0.18
(1,5008)	1:64:A:ILE:H	1:64:A:ILE:HG23	9	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD11	4	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD12	4	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD13	4	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD21	4	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD22	4	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD23	4	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD11	8	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD12	8	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD13	8	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD21	8	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD22	8	0.18
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD23	8	0.18
(1,3871)	1:198:A:LYS:HB2	1:201:A:TYR:H	8	0.18
(1,3871)	1:198:A:LYS:HB3	1:201:A:TYR:H	8	0.18
(1,3869)	1:153:A:LEU:HG	1:179:A:LEU:H	1	0.18
(1,3848)	1:223:A:GLU:HG2	1:223:A:GLU:H	19	0.18
(1,3848)	1:223:A:GLU:HG3	1:223:A:GLU:H	19	0.18
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	17	0.18
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	20	0.18
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	7	0.18
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	7	0.18
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	18	0.18
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	18	0.18
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	18	0.18
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	18	0.18
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	18	0.18
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	18	0.18
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	18	0.18
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	18	0.18
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	18	0.18
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	18	0.18
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	18	0.18
(1,3429)	1:184:A:LEU:HD11	1:182:A:PRO:HG2	5	0.18
(1,3429)	1:184:A:LEU:HD11	1:182:A:PRO:HG3	5	0.18
(1,3429)	1:184:A:LEU:HD12	1:182:A:PRO:HG2	5	0.18
(1,3429)	1:184:A:LEU:HD12	1:182:A:PRO:HG3	5	0.18
(1,3429)	1:184:A:LEU:HD13	1:182:A:PRO:HG2	5	0.18
(1,3429)	1:184:A:LEU:HD13	1:182:A:PRO:HG3	5	0.18
(1,3429)	1:184:A:LEU:HD21	1:182:A:PRO:HG2	5	0.18
(1,3429)	1:184:A:LEU:HD21	1:182:A:PRO:HG3	5	0.18
(1,3429)	1:184:A:LEU:HD22	1:182:A:PRO:HG2	5	0.18
(1,3429)	1:184:A:LEU:HD22	1:182:A:PRO:HG3	5	0.18
(1,3429)	1:184:A:LEU:HD23	1:182:A:PRO:HG2	5	0.18
(1,3429)	1:184:A:LEU:HD23	1:182:A:PRO:HG3	5	0.18
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE2	4	0.18
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE3	4	0.18
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE2	4	0.18
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE3	4	0.18
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE2	4	0.18
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE3	4	0.18
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE2	7	0.18
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE3	7	0.18
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE2	7	0.18
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE3	7	0.18
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG2	10	0.18
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG3	10	0.18
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG2	10	0.18
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG3	10	0.18
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG2	18	0.18
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG3	18	0.18
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG2	18	0.18
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG3	18	0.18
(1,3379)	1:75:A:LYS:HG2	1:19:A:GLU:HG2	2	0.18
(1,3379)	1:75:A:LYS:HG2	1:19:A:GLU:HG3	2	0.18
(1,3351)	1:17:A:ARG:HB2	1:60:A:LYS:HB2	8	0.18
(1,3351)	1:17:A:ARG:HB2	1:60:A:LYS:HB3	8	0.18
(1,3351)	1:17:A:ARG:HB3	1:60:A:LYS:HB2	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3351)	1:17:A:ARG:HB3	1:60:A:LYS:HB3	8	0.18
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	12	0.18
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	12	0.18
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	12	0.18
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	16	0.18
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	16	0.18
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	16	0.18
(1,3289)	1:68:A:PRO:HD2	1:72:A:LEU:HG	20	0.18
(1,3236)	1:17:A:ARG:HA	1:17:A:ARG:HD2	11	0.18
(1,3236)	1:17:A:ARG:HA	1:17:A:ARG:HD3	11	0.18
(1,3221)	1:170:A:ALA:HA	1:173:A:LYS:HD2	14	0.18
(1,3221)	1:170:A:ALA:HA	1:173:A:LYS:HD3	14	0.18
(1,3197)	1:18:A:THR:HB	1:75:A:LYS:HD2	5	0.18
(1,3197)	1:18:A:THR:HB	1:75:A:LYS:HD3	5	0.18
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	7	0.18
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	7	0.18
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	14	0.18
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	14	0.18
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	17	0.18
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	17	0.18
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	18	0.18
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	18	0.18
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	15	0.18
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	15	0.18
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	15	0.18
(1,3089)	1:57:A:LYS:H	1:57:A:LYS:HE2	20	0.18
(1,3089)	1:57:A:LYS:H	1:57:A:LYS:HE3	20	0.18
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG2	18	0.18
(1,3082)	1:38:A:LYS:H	1:37:A:LYS:HG3	18	0.18
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	12	0.18
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	12	0.18
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	12	0.18
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	12	0.18
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	12	0.18
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	12	0.18
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG21	5	0.18
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG22	5	0.18
(1,3063)	1:207:A:CYS:H	1:212:A:ILE:HG23	5	0.18
(1,2975)	1:179:A:LEU:HD12	1:176:A:TYR:HA	2	0.18
(1,2973)	1:85:A:LEU:HB2	1:82:A:SER:HA	3	0.18
(1,2973)	1:85:A:LEU:HB2	1:82:A:SER:HA	6	0.18
(1,2973)	1:85:A:LEU:HB2	1:82:A:SER:HA	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2973)	1:85:A:LEU:HB2	1:82:A:SER:HA	10	0.18
(1,2948)	1:63:A:ASP:HB3	1:64:A:ILE:HA	2	0.18
(1,2948)	1:96:A:MET:HG2	1:101:A:ILE:HA	9	0.18
(1,2903)	1:11:A:VAL:HG11	1:54:A:ILE:HB	17	0.18
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	3	0.18
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	4	0.18
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	6	0.18
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	7	0.18
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	10	0.18
(1,2869)	1:194:A:THR:HB	1:190:A:TYR:HD1	11	0.18
(1,2869)	1:194:A:THR:HB	1:190:A:TYR:HD2	11	0.18
(1,2869)	1:194:A:THR:HB	1:190:A:TYR:HD1	12	0.18
(1,2869)	1:194:A:THR:HB	1:190:A:TYR:HD2	12	0.18
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG12	13	0.18
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG13	13	0.18
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG21	18	0.18
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG22	18	0.18
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG23	18	0.18
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG11	19	0.18
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG12	19	0.18
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG13	19	0.18
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG21	19	0.18
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG22	19	0.18
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG23	19	0.18
(1,2578)	1:64:A:ILE:HD13	1:62:A:VAL:HA	17	0.18
(1,2571)	1:130:A:MET:HE3	1:136:A:PRO:HA	8	0.18
(1,2552)	1:101:A:ILE:HG23	1:102:A:LEU:HA	2	0.18
(1,2549)	1:36:A:VAL:HG11	1:37:A:LYS:HA	11	0.18
(1,2549)	1:36:A:VAL:HG11	1:37:A:LYS:HA	18	0.18
(1,2530)	1:36:A:VAL:HG11	1:37:A:LYS:HA	11	0.18
(1,2530)	1:36:A:VAL:HG11	1:37:A:LYS:HA	18	0.18
(1,2496)	1:46:A:PHE:HD2	1:23:A:ALA:HB1	4	0.18
(1,2496)	1:46:A:PHE:HD2	1:23:A:ALA:HB2	4	0.18
(1,2496)	1:46:A:PHE:HD2	1:23:A:ALA:HB3	4	0.18
(1,2496)	1:46:A:PHE:HD2	1:23:A:ALA:HB1	15	0.18
(1,2496)	1:46:A:PHE:HD2	1:23:A:ALA:HB2	15	0.18
(1,2496)	1:46:A:PHE:HD2	1:23:A:ALA:HB3	15	0.18
(1,2485)	1:34:A:ILE:HG12	1:51:A:PHE:HD1	1	0.18
(1,2485)	1:34:A:ILE:HG12	1:51:A:PHE:HD2	1	0.18
(1,2454)	1:78:A:LEU:HD21	1:78:A:LEU:H	13	0.18
(1,2435)	1:153:A:LEU:HG	1:179:A:LEU:H	1	0.18
(1,2400)	1:34:A:ILE:HD11	1:52:A:TYR:H	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2390)	1:8:A:VAL:HG11	1:24:A:LEU:H	4	0.18
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	6	0.18
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	6	0.18
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	6	0.18
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	6	0.18
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	6	0.18
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	6	0.18
(1,2205)	1:40:A:GLN:HB2	1:54:A:ILE:HG21	12	0.18
(1,2205)	1:40:A:GLN:HB2	1:54:A:ILE:HG22	12	0.18
(1,2205)	1:40:A:GLN:HB2	1:54:A:ILE:HG23	12	0.18
(1,2205)	1:40:A:GLN:HB3	1:54:A:ILE:HG21	12	0.18
(1,2205)	1:40:A:GLN:HB3	1:54:A:ILE:HG22	12	0.18
(1,2205)	1:40:A:GLN:HB3	1:54:A:ILE:HG23	12	0.18
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	11	0.18
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	11	0.18
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD21	2	0.18
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD22	2	0.18
(1,152)	1:176:A:TYR:HE2	1:181:A:ILE:HB	13	0.18
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG2	13	0.18
(1,128)	1:51:A:PHE:HD1	1:44:A:ARG:HG3	13	0.18
(2,92)	1:50:A:LYS:CB	1:130:A:MET:N	13	0.17
(1,5782)	1:153:A:LEU:HD13	1:179:A:LEU:HD11	6	0.17
(1,5782)	1:153:A:LEU:HD13	1:179:A:LEU:HD12	6	0.17
(1,5782)	1:153:A:LEU:HD13	1:179:A:LEU:HD13	6	0.17
(1,5782)	1:153:A:LEU:HD13	1:179:A:LEU:HD21	6	0.17
(1,5782)	1:153:A:LEU:HD13	1:179:A:LEU:HD22	6	0.17
(1,5782)	1:153:A:LEU:HD13	1:179:A:LEU:HD23	6	0.17
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	6	0.17
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	11	0.17
(1,5554)	1:128:A:LYS:HB2	1:129:A:PHE:H	13	0.17
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	13	0.17
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	13	0.17
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	18	0.17
(1,5446)	1:64:A:ILE:H	1:82:A:SER:HA	4	0.17
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB2	12	0.17
(1,5416)	1:10:A:SER:H	1:61:A:GLU:HB3	12	0.17
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE1	16	0.17
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE2	16	0.17
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD11	1	0.17
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD12	1	0.17
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD13	1	0.17
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD21	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD22	1	0.17
(1,5397)	1:127:A:TYR:H	1:123:A:LEU:HD23	1	0.17
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	3	0.17
(1,5361)	1:199:A:TYR:H	1:197:A:ARG:HB2	8	0.17
(1,5361)	1:199:A:TYR:H	1:197:A:ARG:HB3	8	0.17
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB1	2	0.17
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB2	2	0.17
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB3	2	0.17
(1,5314)	1:20:A:TRP:HE1	1:18:A:THR:HG21	9	0.17
(1,5314)	1:20:A:TRP:HE1	1:18:A:THR:HG22	9	0.17
(1,5314)	1:20:A:TRP:HE1	1:18:A:THR:HG23	9	0.17
(1,5313)	1:20:A:TRP:HE1	1:71:A:GLU:HG2	20	0.17
(1,5313)	1:20:A:TRP:HE1	1:71:A:GLU:HG3	20	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	3	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	3	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	3	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	3	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	3	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	3	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD11	11	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD12	11	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD13	11	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD21	11	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD22	11	0.17
(1,5299)	1:73:A:SER:H	1:72:A:LEU:HD23	11	0.17
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG2	14	0.17
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG3	14	0.17
(1,5279)	1:29:A:SER:H	1:42:A:LEU:HD11	19	0.17
(1,5279)	1:29:A:SER:H	1:42:A:LEU:HD12	19	0.17
(1,5279)	1:29:A:SER:H	1:42:A:LEU:HD13	19	0.17
(1,5279)	1:29:A:SER:H	1:42:A:LEU:HD21	19	0.17
(1,5279)	1:29:A:SER:H	1:42:A:LEU:HD22	19	0.17
(1,5279)	1:29:A:SER:H	1:42:A:LEU:HD23	19	0.17
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD21	13	0.17
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD22	13	0.17
(1,5233)	1:1:A:ASN:HD21	1:61:A:GLU:HG2	19	0.17
(1,5233)	1:1:A:ASN:HD21	1:61:A:GLU:HG3	19	0.17
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD11	17	0.17
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD12	17	0.17
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD13	17	0.17
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD21	17	0.17
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD22	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD23	17	0.17
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG11	7	0.17
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG12	7	0.17
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG13	7	0.17
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG21	7	0.17
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG22	7	0.17
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG23	7	0.17
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	1	0.17
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	18	0.17
(1,3502)	1:22:A:PRO:HB2	1:21:A:TYR:HA	5	0.17
(1,3502)	1:22:A:PRO:HB2	1:21:A:TYR:HA	10	0.17
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB2	14	0.17
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB3	14	0.17
(1,3448)	1:43:A:VAL:HG11	1:41:A:CYS:HB2	10	0.17
(1,3448)	1:43:A:VAL:HG11	1:41:A:CYS:HB3	10	0.17
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	12	0.17
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	12	0.17
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	12	0.17
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	12	0.17
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	12	0.17
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	12	0.17
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	12	0.17
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	12	0.17
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	12	0.17
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	12	0.17
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	12	0.17
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	12	0.17
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG11	4	0.17
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG12	4	0.17
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG13	4	0.17
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG21	4	0.17
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG22	4	0.17
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG23	4	0.17
(1,3399)	1:64:A:ILE:HG13	1:62:A:VAL:HB	15	0.17
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	6	0.17
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	6	0.17
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	6	0.17
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD11	9	0.17
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD12	9	0.17
(1,3346)	1:79:A:GLN:HB3	1:83:A:ILE:HD13	9	0.17
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD11	2	0.17
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD12	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD13	2	0.17
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD21	2	0.17
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD22	2	0.17
(1,3341)	1:153:A:LEU:HB2	1:179:A:LEU:HD23	2	0.17
(1,3270)	1:144:A:GLY:HA3	1:146:A:LYS:HD2	9	0.17
(1,3270)	1:144:A:GLY:HA3	1:146:A:LYS:HD3	9	0.17
(1,3256)	1:13:A:SER:HB2	1:15:A:THR:HG21	19	0.17
(1,3256)	1:13:A:SER:HB2	1:15:A:THR:HG22	19	0.17
(1,3256)	1:13:A:SER:HB2	1:15:A:THR:HG23	19	0.17
(1,3201)	1:2:A:ASP:HA	1:5:A:LEU:HG	18	0.17
(1,3145)	1:127:A:TYR:HD1	1:96:A:MET:HG2	10	0.17
(1,3145)	1:127:A:TYR:HD1	1:96:A:MET:HG3	10	0.17
(1,3145)	1:127:A:TYR:HD2	1:96:A:MET:HG2	10	0.17
(1,3145)	1:127:A:TYR:HD2	1:96:A:MET:HG3	10	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	4	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	4	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	4	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	4	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	4	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	4	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	19	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	19	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	19	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	19	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	19	0.17
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	19	0.17
(1,2978)	1:98:A:ILE:HG13	1:98:A:ILE:HA	11	0.17
(1,2977)	1:62:A:VAL:HB	1:62:A:VAL:HA	7	0.17
(1,2975)	1:179:A:LEU:HD21	1:176:A:TYR:HA	12	0.17
(1,2975)	1:179:A:LEU:HD12	1:176:A:TYR:HA	18	0.17
(1,2973)	1:85:A:LEU:HB2	1:82:A:SER:HA	2	0.17
(1,2947)	1:30:A:CYS:HB2	1:29:A:SER:HB2	12	0.17
(1,2947)	1:30:A:CYS:HB2	1:29:A:SER:HB3	12	0.17
(1,2887)	1:101:A:ILE:HB	1:99:A:SER:H	13	0.17
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	12	0.17
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	13	0.17
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	16	0.17
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	17	0.17
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG21	16	0.17
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG22	16	0.17
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG23	16	0.17
(1,2841)	1:166:A:ILE:HD13	1:157:A:VAL:H	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	10	0.17
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG21	1	0.17
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG22	1	0.17
(1,2766)	1:55:A:ALA:HB1	1:54:A:ILE:HG23	1	0.17
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG2	15	0.17
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG3	15	0.17
(1,2639)	1:11:A:VAL:HG11	1:20:A:TRP:HB2	4	0.17
(1,2639)	1:11:A:VAL:HG11	1:20:A:TRP:HB3	4	0.17
(1,2639)	1:11:A:VAL:HG12	1:20:A:TRP:HB2	15	0.17
(1,2639)	1:11:A:VAL:HG12	1:20:A:TRP:HB3	15	0.17
(1,2587)	1:137:A:ILE:HG13	1:127:A:TYR:HA	2	0.17
(1,2578)	1:64:A:ILE:HD12	1:62:A:VAL:HA	9	0.17
(1,2562)	1:72:A:LEU:HG	1:69:A:GLU:HA	9	0.17
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	14	0.17
(1,2551)	1:98:A:ILE:HG23	1:98:A:ILE:HA	5	0.17
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	5	0.17
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD1	3	0.17
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD2	3	0.17
(1,2458)	1:171:A:VAL:HG12	1:174:A:GLN:H	4	0.17
(1,2443)	1:83:A:ILE:HD12	1:83:A:ILE:H	16	0.17
(1,2428)	1:64:A:ILE:HD13	1:65:A:LEU:H	12	0.17
(1,2411)	1:88:A:ARG:HD2	1:88:A:ARG:H	8	0.17
(1,2400)	1:34:A:ILE:HD11	1:52:A:TYR:H	3	0.17
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	20	0.17
(1,1218)	1:62:A:VAL:HA	1:62:A:VAL:HB	7	0.17
(1,1218)	1:62:A:VAL:HA	1:62:A:VAL:HB	20	0.17
(1,750)	1:114:A:LEU:H	1:114:A:LEU:HG	2	0.17
(1,693)	1:85:A:LEU:H	1:85:A:LEU:HG	17	0.17
(1,625)	1:143:A:LEU:H	1:142:A:VAL:HB	7	0.17
(1,625)	1:143:A:LEU:H	1:142:A:VAL:HB	12	0.17
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	6	0.17
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	6	0.17
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	13	0.17
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	13	0.17
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	20	0.17
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	20	0.17
(1,263)	1:137:A:ILE:HG12	1:136:A:PRO:HA	16	0.17
(1,263)	1:137:A:ILE:HG13	1:136:A:PRO:HA	16	0.17
(1,132)	1:154:A:PHE:HD1	1:158:A:TYR:HB2	12	0.17
(1,132)	1:154:A:PHE:HD1	1:158:A:TYR:HB3	12	0.17
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD11	20	0.17
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD12	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD13	20	0.17
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD21	20	0.17
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD22	20	0.17
(1,120)	1:199:A:TYR:HE2	1:143:A:LEU:HD23	20	0.17
(1,16)	1:212:A:ILE:HD11	1:203:A:PHE:HD1	12	0.17
(1,16)	1:212:A:ILE:HD11	1:203:A:PHE:HD2	12	0.17
(1,16)	1:212:A:ILE:HD12	1:203:A:PHE:HD1	12	0.17
(1,16)	1:212:A:ILE:HD12	1:203:A:PHE:HD2	12	0.17
(1,16)	1:212:A:ILE:HD13	1:203:A:PHE:HD1	12	0.17
(1,16)	1:212:A:ILE:HD13	1:203:A:PHE:HD2	12	0.17
(1,5848)	1:113:A:GLU:HB3	1:114:A:LEU:HG	4	0.16
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD11	7	0.16
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD12	7	0.16
(1,5815)	1:211:A:ASN:HB2	1:212:A:ILE:HD13	7	0.16
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD11	7	0.16
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD12	7	0.16
(1,5815)	1:211:A:ASN:HB3	1:212:A:ILE:HD13	7	0.16
(1,5813)	1:108:A:LYS:HG2	1:106:A:SER:HB2	11	0.16
(1,5813)	1:108:A:LYS:HG2	1:106:A:SER:HB3	11	0.16
(1,5813)	1:108:A:LYS:HG3	1:106:A:SER:HB2	11	0.16
(1,5813)	1:108:A:LYS:HG3	1:106:A:SER:HB3	11	0.16
(1,5791)	1:102:A:LEU:HB2	1:105:A:SER:HB2	11	0.16
(1,5791)	1:102:A:LEU:HB2	1:105:A:SER:HB3	11	0.16
(1,5714)	1:3:A:GLU:HB2	1:9:A:VAL:HG11	10	0.16
(1,5714)	1:3:A:GLU:HB2	1:9:A:VAL:HG12	10	0.16
(1,5714)	1:3:A:GLU:HB2	1:9:A:VAL:HG13	10	0.16
(1,5714)	1:3:A:GLU:HB2	1:9:A:VAL:HG21	10	0.16
(1,5714)	1:3:A:GLU:HB2	1:9:A:VAL:HG22	10	0.16
(1,5714)	1:3:A:GLU:HB2	1:9:A:VAL:HG23	10	0.16
(1,5691)	1:22:A:PRO:HG3	1:23:A:ALA:H	5	0.16
(1,5691)	1:22:A:PRO:HG3	1:23:A:ALA:H	11	0.16
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD21	16	0.16
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD22	16	0.16
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	5	0.16
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	20	0.16
(1,5554)	1:128:A:LYS:HB2	1:129:A:PHE:H	15	0.16
(1,5547)	1:100:A:GLU:HG3	1:100:A:GLU:H	17	0.16
(1,5546)	1:8:A:VAL:HB	1:8:A:VAL:H	4	0.16
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	17	0.16
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	17	0.16
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	20	0.16
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD21	5	0.16
(1,5488)	1:195:A:ALA:H	1:191:A:ASN:HD22	5	0.16
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	9	0.16
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	10	0.16
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	15	0.16
(1,5428)	1:23:A:ALA:H	1:20:A:TRP:HZ3	1	0.16
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE1	17	0.16
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE2	17	0.16
(1,5397)	1:127:A:TYR:H	1:137:A:ILE:HG12	2	0.16
(1,5397)	1:127:A:TYR:H	1:137:A:ILE:HG13	2	0.16
(1,5373)	1:134:A:GLY:H	1:44:A:ARG:HD2	20	0.16
(1,5373)	1:134:A:GLY:H	1:44:A:ARG:HD3	20	0.16
(1,5313)	1:20:A:TRP:HE1	1:71:A:GLU:HG2	14	0.16
(1,5313)	1:20:A:TRP:HE1	1:71:A:GLU:HG3	14	0.16
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG2	15	0.16
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG3	15	0.16
(1,5247)	1:40:A:GLN:HE21	1:55:A:ALA:HA	20	0.16
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB2	16	0.16
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB3	16	0.16
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB1	5	0.16
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB2	5	0.16
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB3	5	0.16
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG21	16	0.16
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG22	16	0.16
(1,5181)	1:59:A:ILE:H	1:59:A:ILE:HG23	16	0.16
(1,5168)	1:5:A:LEU:H	1:3:A:GLU:HB2	12	0.16
(1,5168)	1:5:A:LEU:H	1:3:A:GLU:HB3	12	0.16
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG11	10	0.16
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG12	10	0.16
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG13	10	0.16
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG21	10	0.16
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG22	10	0.16
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG23	10	0.16
(1,5118)	1:7:A:LYS:H	1:5:A:LEU:HG	9	0.16
(1,5118)	1:7:A:LYS:H	1:5:A:LEU:HG	18	0.16
(1,5062)	1:58:A:ASP:H	1:11:A:VAL:HG11	16	0.16
(1,5062)	1:58:A:ASP:H	1:11:A:VAL:HG12	16	0.16
(1,5062)	1:58:A:ASP:H	1:11:A:VAL:HG13	16	0.16
(1,5062)	1:58:A:ASP:H	1:11:A:VAL:HG21	16	0.16
(1,5062)	1:58:A:ASP:H	1:11:A:VAL:HG22	16	0.16
(1,5062)	1:58:A:ASP:H	1:11:A:VAL:HG23	16	0.16
(1,5020)	1:85:A:LEU:H	1:88:A:ARG:HE	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	1	0.16
(1,4855)	1:67:A:LEU:HG	1:67:A:LEU:H	14	0.16
(1,4502)	1:133:A:ARG:HE	1:202:A:GLY:H	15	0.16
(1,4267)	1:198:A:LYS:HB2	1:199:A:TYR:H	13	0.16
(1,4267)	1:198:A:LYS:HB3	1:199:A:TYR:H	13	0.16
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	15	0.16
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	15	0.16
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	15	0.16
(1,3849)	1:109:A:ASP:HB2	1:109:A:ASP:H	1	0.16
(1,3849)	1:109:A:ASP:HB3	1:109:A:ASP:H	1	0.16
(1,3846)	1:111:A:GLU:HG2	1:111:A:GLU:H	10	0.16
(1,3846)	1:111:A:GLU:HG3	1:111:A:GLU:H	10	0.16
(1,3784)	1:101:A:ILE:HG21	1:102:A:LEU:H	10	0.16
(1,3784)	1:101:A:ILE:HG22	1:102:A:LEU:H	10	0.16
(1,3784)	1:101:A:ILE:HG23	1:102:A:LEU:H	10	0.16
(1,3721)	1:18:A:THR:HB	1:19:A:GLU:H	11	0.16
(1,3544)	1:97:A:ASP:HB3	1:99:A:SER:HA	8	0.16
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB2	6	0.16
(1,3516)	1:44:A:ARG:HB2	1:46:A:PHE:HB3	6	0.16
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB2	6	0.16
(1,3516)	1:44:A:ARG:HB3	1:46:A:PHE:HB3	6	0.16
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	6	0.16
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	6	0.16
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB2	1	0.16
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB3	1	0.16
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	1	0.16
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	1	0.16
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	1	0.16
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	1	0.16
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	1	0.16
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	1	0.16
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	1	0.16
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	1	0.16
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	1	0.16
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	1	0.16
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	1	0.16
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	1	0.16
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	14	0.16
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	14	0.16
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	14	0.16
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	14	0.16
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	14	0.16
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	14	0.16
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	14	0.16
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	14	0.16
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	14	0.16
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	14	0.16
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	14	0.16
(1,3330)	1:100:A:GLU:HG3	1:101:A:ILE:HG12	11	0.16
(1,3330)	1:100:A:GLU:HG3	1:101:A:ILE:HG13	11	0.16
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG21	6	0.16
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG22	6	0.16
(1,3320)	1:51:A:PHE:HB3	1:34:A:ILE:HG23	6	0.16
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	1	0.16
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	1	0.16
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	10	0.16
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	10	0.16
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD11	10	0.16
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD12	10	0.16
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD13	10	0.16
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD21	10	0.16
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD22	10	0.16
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD23	10	0.16
(1,3236)	1:17:A:ARG:HA	1:17:A:ARG:HD2	20	0.16
(1,3236)	1:17:A:ARG:HA	1:17:A:ARG:HD3	20	0.16
(1,3235)	1:17:A:ARG:HA	1:17:A:ARG:HD2	20	0.16
(1,3235)	1:17:A:ARG:HA	1:17:A:ARG:HD3	20	0.16
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD11	7	0.16
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD12	7	0.16
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD13	7	0.16
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD21	7	0.16
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD22	7	0.16
(1,3224)	1:65:A:LEU:HA	1:85:A:LEU:HD23	7	0.16
(1,3221)	1:170:A:ALA:HA	1:173:A:LYS:HD2	20	0.16
(1,3221)	1:170:A:ALA:HA	1:173:A:LYS:HD3	20	0.16
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	3	0.16
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	3	0.16
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	16	0.16
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	16	0.16
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	19	0.16
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	19	0.16
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG21	16	0.16
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG22	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3154)	1:59:A:ILE:H	1:59:A:ILE:HG23	16	0.16
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG2	15	0.16
(1,3115)	1:80:A:LYS:H	1:22:A:PRO:HG3	15	0.16
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG21	8	0.16
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG22	8	0.16
(1,3087)	1:85:A:LEU:H	1:83:A:ILE:HG23	8	0.16
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG2	14	0.16
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG3	14	0.16
(1,2978)	1:98:A:ILE:HG13	1:98:A:ILE:HA	10	0.16
(1,2977)	1:62:A:VAL:HB	1:62:A:VAL:HA	4	0.16
(1,2973)	1:85:A:LEU:HB2	1:82:A:SER:HA	19	0.16
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB2	5	0.16
(1,2970)	1:71:A:GLU:HB2	1:70:A:SER:HB3	5	0.16
(1,2948)	1:63:A:ASP:HB2	1:64:A:ILE:HA	11	0.16
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD11	3	0.16
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD12	3	0.16
(1,2872)	1:100:A:GLU:HB2	1:101:A:ILE:HD13	3	0.16
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	2	0.16
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	5	0.16
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	8	0.16
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	18	0.16
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG21	10	0.16
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG22	10	0.16
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG23	10	0.16
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG21	17	0.16
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG22	17	0.16
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG23	17	0.16
(1,2848)	1:11:A:VAL:HG23	1:44:A:ARG:H	14	0.16
(1,2842)	1:181:A:ILE:HD11	1:176:A:TYR:HB2	7	0.16
(1,2842)	1:181:A:ILE:HD11	1:176:A:TYR:HB3	7	0.16
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	5	0.16
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	5	0.16
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	15	0.16
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	15	0.16
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG11	7	0.16
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG12	7	0.16
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG13	7	0.16
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG21	7	0.16
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG22	7	0.16
(1,2783)	1:61:A:GLU:HG2	1:9:A:VAL:HG23	7	0.16
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG11	5	0.16
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG12	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG13	5	0.16
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG21	5	0.16
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG22	5	0.16
(1,2776)	1:54:A:ILE:HB	1:11:A:VAL:HG23	5	0.16
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG21	11	0.16
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG22	11	0.16
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG23	11	0.16
(1,2745)	1:137:A:ILE:HD13	1:126:A:LEU:HB2	18	0.16
(1,2745)	1:137:A:ILE:HD13	1:126:A:LEU:HB3	18	0.16
(1,2717)	1:130:A:MET:HE1	1:133:A:ARG:HG2	20	0.16
(1,2717)	1:130:A:MET:HE1	1:133:A:ARG:HG3	20	0.16
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB2	5	0.16
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB3	5	0.16
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB2	18	0.16
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB3	18	0.16
(1,2682)	1:62:A:VAL:HB	1:9:A:VAL:HB	11	0.16
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG2	8	0.16
(1,2680)	1:181:A:ILE:HB	1:182:A:PRO:HG3	8	0.16
(1,2643)	1:187:A:ALA:HB1	1:190:A:TYR:HB2	5	0.16
(1,2643)	1:187:A:ALA:HB1	1:190:A:TYR:HB3	5	0.16
(1,2639)	1:11:A:VAL:HG11	1:20:A:TRP:HB2	2	0.16
(1,2639)	1:11:A:VAL:HG11	1:20:A:TRP:HB3	2	0.16
(1,2575)	1:64:A:ILE:HG23	1:78:A:LEU:HA	1	0.16
(1,2562)	1:72:A:LEU:HG	1:69:A:GLU:HA	12	0.16
(1,2552)	1:101:A:ILE:HG23	1:102:A:LEU:HA	9	0.16
(1,2541)	1:142:A:VAL:HB	1:141:A:PRO:HA	12	0.16
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	2	0.16
(1,2489)	1:87:A:THR:HG23	1:84:A:PHE:HD1	6	0.16
(1,2489)	1:87:A:THR:HG23	1:84:A:PHE:HD2	6	0.16
(1,2373)	1:26:A:ILE:HD13	1:43:A:VAL:H	14	0.16
(1,2372)	1:96:A:MET:HE3	1:127:A:TYR:H	10	0.16
(1,2334)	1:22:A:PRO:HA	1:46:A:PHE:HE1	13	0.16
(1,2334)	1:22:A:PRO:HA	1:46:A:PHE:HE2	13	0.16
(1,2306)	1:81:A:ALA:HA	1:78:A:LEU:HA	1	0.16
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG21	16	0.16
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG22	16	0.16
(1,2255)	1:105:A:SER:HB3	1:101:A:ILE:HG23	16	0.16
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	5	0.16
(1,1518)	1:8:A:VAL:HB	1:24:A:LEU:HD11	15	0.16
(1,1518)	1:8:A:VAL:HB	1:24:A:LEU:HD12	15	0.16
(1,1518)	1:8:A:VAL:HB	1:24:A:LEU:HD13	15	0.16
(1,1518)	1:8:A:VAL:HB	1:24:A:LEU:HD21	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:8:A:VAL:HB	1:24:A:LEU:HD22	15	0.16
(1,1518)	1:8:A:VAL:HB	1:24:A:LEU:HD23	15	0.16
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD11	2	0.16
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD12	2	0.16
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD13	2	0.16
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD11	2	0.16
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD12	2	0.16
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD13	2	0.16
(1,1218)	1:62:A:VAL:HA	1:62:A:VAL:HB	3	0.16
(1,1218)	1:62:A:VAL:HA	1:62:A:VAL:HB	4	0.16
(1,1184)	1:184:A:LEU:HA	1:184:A:LEU:HD11	16	0.16
(1,1184)	1:184:A:LEU:HA	1:184:A:LEU:HD12	16	0.16
(1,1184)	1:184:A:LEU:HA	1:184:A:LEU:HD13	16	0.16
(1,1184)	1:184:A:LEU:HA	1:184:A:LEU:HD21	16	0.16
(1,1184)	1:184:A:LEU:HA	1:184:A:LEU:HD22	16	0.16
(1,1184)	1:184:A:LEU:HA	1:184:A:LEU:HD23	16	0.16
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	14	0.16
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	14	0.16
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	14	0.16
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	14	0.16
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	14	0.16
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	14	0.16
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	14	0.16
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	14	0.16
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	14	0.16
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	14	0.16
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	14	0.16
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	14	0.16
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG21	9	0.16
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG22	9	0.16
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG23	9	0.16
(1,625)	1:143:A:LEU:H	1:142:A:VAL:HB	4	0.16
(1,625)	1:143:A:LEU:H	1:142:A:VAL:HB	19	0.16
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	4	0.16
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	4	0.16
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	19	0.16
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	19	0.16
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE1	12	0.16
(1,183)	1:145:A:TYR:H	1:145:A:TYR:HE2	12	0.16
(1,58)	1:96:A:MET:HB2	1:127:A:TYR:HD1	15	0.16
(1,58)	1:96:A:MET:HB2	1:127:A:TYR:HD2	15	0.16
(1,58)	1:96:A:MET:HB3	1:127:A:TYR:HD1	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:96:A:MET:HB3	1:127:A:TYR:HD2	15	0.16
(2,320)	1:118:A:GLU:CB	1:114:A:LEU:N	5	0.15
(2,320)	1:118:A:GLU:CB	1:114:A:LEU:N	15	0.15
(2,36)	1:4:A:LEU:CB	1:210:A:ALA:N	18	0.15
(1,5861)	1:116:A:PRO:HG2	1:117:A:GLU:H	13	0.15
(1,5853)	1:114:A:LEU:HG	1:114:A:LEU:HA	2	0.15
(1,5845)	1:111:A:GLU:H	1:111:A:GLU:HA	8	0.15
(1,5835)	1:110:A:LYS:HA	1:110:A:LYS:H	4	0.15
(1,5813)	1:108:A:LYS:HG2	1:106:A:SER:HB2	13	0.15
(1,5813)	1:108:A:LYS:HG2	1:106:A:SER:HB3	13	0.15
(1,5813)	1:108:A:LYS:HG3	1:106:A:SER:HB2	13	0.15
(1,5813)	1:108:A:LYS:HG3	1:106:A:SER:HB3	13	0.15
(1,5786)	1:115:A:ASP:HA	1:117:A:GLU:H	7	0.15
(1,5786)	1:115:A:ASP:HA	1:117:A:GLU:H	20	0.15
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD21	1	0.15
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD22	1	0.15
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD21	3	0.15
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD22	3	0.15
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD21	14	0.15
(1,5690)	1:62:A:VAL:HA	1:66:A:ASN:HD22	14	0.15
(1,5689)	1:137:A:ILE:HA	1:138:A:ASN:HD21	20	0.15
(1,5689)	1:137:A:ILE:HA	1:138:A:ASN:HD22	20	0.15
(1,5626)	1:142:A:VAL:HG11	1:145:A:TYR:H	10	0.15
(1,5623)	1:61:A:GLU:HG2	1:1:A:ASN:HD21	13	0.15
(1,5623)	1:61:A:GLU:HG2	1:1:A:ASN:HD22	13	0.15
(1,5623)	1:61:A:GLU:HG3	1:1:A:ASN:HD21	13	0.15
(1,5623)	1:61:A:GLU:HG3	1:1:A:ASN:HD22	13	0.15
(1,5602)	1:34:A:ILE:HG23	1:53:A:SER:H	10	0.15
(1,5556)	1:96:A:MET:HB2	1:95:A:LYS:H	18	0.15
(1,5554)	1:128:A:LYS:HB2	1:129:A:PHE:H	4	0.15
(1,5549)	1:204:A:GLU:HB3	1:201:A:TYR:H	3	0.15
(1,5534)	1:47:A:ILE:HB	1:81:A:ALA:H	10	0.15
(1,5522)	1:9:A:VAL:HG21	1:23:A:ALA:H	8	0.15
(1,5507)	1:88:A:ARG:HE	1:85:A:LEU:HD11	3	0.15
(1,5507)	1:88:A:ARG:HE	1:85:A:LEU:HD12	3	0.15
(1,5507)	1:88:A:ARG:HE	1:85:A:LEU:HD13	3	0.15
(1,5507)	1:88:A:ARG:HE	1:85:A:LEU:HD21	3	0.15
(1,5507)	1:88:A:ARG:HE	1:85:A:LEU:HD22	3	0.15
(1,5507)	1:88:A:ARG:HE	1:85:A:LEU:HD23	3	0.15
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE2	7	0.15
(1,5475)	1:197:A:ARG:H	1:193:A:LYS:HE3	7	0.15
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	13	0.15
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	11	0.15
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD2	8	0.15
(1,5466)	1:47:A:ILE:H	1:22:A:PRO:HD3	8	0.15
(1,5359)	1:6:A:GLY:H	1:25:A:VAL:H	6	0.15
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	1	0.15
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	1	0.15
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	1	0.15
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	1	0.15
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	10	0.15
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	10	0.15
(1,5290)	1:73:A:SER:H	1:79:A:GLN:HG2	15	0.15
(1,5290)	1:73:A:SER:H	1:79:A:GLN:HG3	15	0.15
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB2	14	0.15
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB3	14	0.15
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD21	4	0.15
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD22	4	0.15
(1,5235)	1:70:A:SER:H	1:69:A:GLU:HB2	1	0.15
(1,5235)	1:70:A:SER:H	1:69:A:GLU:HB3	1	0.15
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB1	3	0.15
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB2	3	0.15
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB3	3	0.15
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	10	0.15
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	10	0.15
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	10	0.15
(1,5118)	1:7:A:LYS:H	1:5:A:LEU:HG	4	0.15
(1,5118)	1:7:A:LYS:H	1:5:A:LEU:HG	15	0.15
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD11	11	0.15
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD12	11	0.15
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD13	11	0.15
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	6	0.15
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	6	0.15
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	18	0.15
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	18	0.15
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	16	0.15
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD11	18	0.15
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD12	18	0.15
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD13	18	0.15
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD21	18	0.15
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD22	18	0.15
(1,4938)	1:148:A:LEU:H	1:148:A:LEU:HD23	18	0.15
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB1	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB2	4	0.15
(1,4928)	1:54:A:ILE:H	1:55:A:ALA:HB3	4	0.15
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	7	0.15
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD2	11	0.15
(1,4908)	1:20:A:TRP:HE1	1:75:A:LYS:HD3	11	0.15
(1,4775)	1:60:A:LYS:HG2	1:59:A:ILE:H	15	0.15
(1,4775)	1:60:A:LYS:HG3	1:59:A:ILE:H	15	0.15
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	2	0.15
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	2	0.15
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	2	0.15
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	6	0.15
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	6	0.15
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	6	0.15
(1,3869)	1:153:A:LEU:HG	1:179:A:LEU:H	11	0.15
(1,3868)	1:102:A:LEU:HB2	1:103:A:GLU:H	2	0.15
(1,3868)	1:102:A:LEU:HB3	1:103:A:GLU:H	2	0.15
(1,3868)	1:102:A:LEU:HB2	1:103:A:GLU:H	5	0.15
(1,3868)	1:102:A:LEU:HB3	1:103:A:GLU:H	5	0.15
(1,3848)	1:223:A:GLU:HG2	1:223:A:GLU:H	10	0.15
(1,3848)	1:223:A:GLU:HG3	1:223:A:GLU:H	10	0.15
(1,3846)	1:111:A:GLU:HG2	1:111:A:GLU:H	6	0.15
(1,3846)	1:111:A:GLU:HG3	1:111:A:GLU:H	6	0.15
(1,3669)	1:112:A:LYS:HB2	1:113:A:GLU:H	16	0.15
(1,3669)	1:112:A:LYS:HB3	1:113:A:GLU:H	16	0.15
(1,3604)	1:149:A:ASN:HB2	1:150:A:LEU:H	8	0.15
(1,3604)	1:149:A:ASN:HB3	1:150:A:LEU:H	8	0.15
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	5	0.15
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	5	0.15
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	10	0.15
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	10	0.15
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB2	3	0.15
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB3	3	0.15
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB2	5	0.15
(1,3477)	1:64:A:ILE:H	1:65:A:LEU:HB3	5	0.15
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB2	3	0.15
(1,3444)	1:12:A:VAL:HG11	1:60:A:LYS:HB3	3	0.15
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB2	3	0.15
(1,3444)	1:12:A:VAL:HG12	1:60:A:LYS:HB3	3	0.15
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB2	3	0.15
(1,3444)	1:12:A:VAL:HG13	1:60:A:LYS:HB3	3	0.15
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB2	3	0.15
(1,3444)	1:12:A:VAL:HG21	1:60:A:LYS:HB3	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB2	3	0.15
(1,3444)	1:12:A:VAL:HG22	1:60:A:LYS:HB3	3	0.15
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB2	3	0.15
(1,3444)	1:12:A:VAL:HG23	1:60:A:LYS:HB3	3	0.15
(1,3400)	1:90:A:VAL:HG11	1:86:A:LYS:HB2	14	0.15
(1,3400)	1:90:A:VAL:HG11	1:86:A:LYS:HB3	14	0.15
(1,3400)	1:90:A:VAL:HG12	1:86:A:LYS:HB2	14	0.15
(1,3400)	1:90:A:VAL:HG12	1:86:A:LYS:HB3	14	0.15
(1,3400)	1:90:A:VAL:HG13	1:86:A:LYS:HB2	14	0.15
(1,3400)	1:90:A:VAL:HG13	1:86:A:LYS:HB3	14	0.15
(1,3400)	1:90:A:VAL:HG21	1:86:A:LYS:HB2	14	0.15
(1,3400)	1:90:A:VAL:HG21	1:86:A:LYS:HB3	14	0.15
(1,3400)	1:90:A:VAL:HG22	1:86:A:LYS:HB2	14	0.15
(1,3400)	1:90:A:VAL:HG22	1:86:A:LYS:HB3	14	0.15
(1,3400)	1:90:A:VAL:HG23	1:86:A:LYS:HB2	14	0.15
(1,3400)	1:90:A:VAL:HG23	1:86:A:LYS:HB3	14	0.15
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE2	13	0.15
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE3	13	0.15
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE2	13	0.15
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE3	13	0.15
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG2	17	0.15
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG3	17	0.15
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG2	17	0.15
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG3	17	0.15
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	5	0.15
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	5	0.15
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	15	0.15
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	15	0.15
(1,3097)	1:82:A:SER:H	1:79:A:GLN:HG2	4	0.15
(1,3097)	1:82:A:SER:H	1:79:A:GLN:HG3	4	0.15
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG21	19	0.15
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG22	19	0.15
(1,3086)	1:35:A:THR:H	1:35:A:THR:HG23	19	0.15
(1,2998)	1:178:A:ASP:HB3	1:153:A:LEU:HA	13	0.15
(1,2975)	1:179:A:LEU:HD21	1:176:A:TYR:HA	4	0.15
(1,2922)	1:64:A:ILE:HD13	1:85:A:LEU:HB2	6	0.15
(1,2922)	1:64:A:ILE:HD13	1:85:A:LEU:HB3	6	0.15
(1,2917)	1:196:A:TYR:HA	1:201:A:TYR:H	2	0.15
(1,2884)	1:61:A:GLU:HG3	1:3:A:GLU:HA	19	0.15
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	9	0.15
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	14	0.15
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2869)	1:194:A:THR:HB	1:190:A:TYR:HD1	14	0.15
(1,2869)	1:194:A:THR:HB	1:190:A:TYR:HD2	14	0.15
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	14	0.15
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	17	0.15
(1,2835)	1:126:A:LEU:HD11	1:130:A:MET:H	7	0.15
(1,2717)	1:130:A:MET:HE3	1:198:A:LYS:HB2	11	0.15
(1,2717)	1:130:A:MET:HE3	1:198:A:LYS:HB3	11	0.15
(1,2685)	1:67:A:LEU:HD11	1:71:A:GLU:HB2	13	0.15
(1,2685)	1:67:A:LEU:HD11	1:71:A:GLU:HB3	13	0.15
(1,2682)	1:62:A:VAL:HB	1:9:A:VAL:HB	13	0.15
(1,2645)	1:54:A:ILE:HG21	1:41:A:CYS:HB2	14	0.15
(1,2645)	1:54:A:ILE:HG21	1:41:A:CYS:HB3	14	0.15
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB2	3	0.15
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB3	3	0.15
(1,2636)	1:65:A:LEU:HD11	1:66:A:ASN:HB2	16	0.15
(1,2636)	1:65:A:LEU:HD11	1:66:A:ASN:HB3	16	0.15
(1,2606)	1:64:A:ILE:HD11	1:78:A:LEU:HA	3	0.15
(1,2577)	1:166:A:ILE:HD13	1:160:A:GLN:HA	19	0.15
(1,2552)	1:101:A:ILE:HG22	1:102:A:LEU:HA	1	0.15
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	20	0.15
(1,2527)	1:142:A:VAL:HB	1:143:A:LEU:HA	3	0.15
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD1	4	0.15
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD2	4	0.15
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD1	19	0.15
(1,2474)	1:101:A:ILE:HD12	1:127:A:TYR:HD2	19	0.15
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD11	9	0.15
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD12	9	0.15
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD13	9	0.15
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD21	9	0.15
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD22	9	0.15
(1,2469)	1:84:A:PHE:HE2	1:24:A:LEU:HD23	9	0.15
(1,2458)	1:171:A:VAL:HG13	1:174:A:GLN:H	15	0.15
(1,2448)	1:130:A:MET:HE2	1:200:A:LEU:H	2	0.15
(1,2443)	1:83:A:ILE:HD11	1:83:A:ILE:H	4	0.15
(1,2443)	1:83:A:ILE:HD12	1:83:A:ILE:H	5	0.15
(1,2443)	1:83:A:ILE:HD11	1:83:A:ILE:H	12	0.15
(1,2428)	1:64:A:ILE:HD13	1:65:A:LEU:H	14	0.15
(1,2422)	1:126:A:LEU:HD11	1:130:A:MET:H	7	0.15
(1,2398)	1:9:A:VAL:HG22	1:25:A:VAL:H	11	0.15
(1,2398)	1:9:A:VAL:HG23	1:10:A:SER:H	14	0.15
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	19	0.15
(1,2372)	1:96:A:MET:HE2	1:127:A:TYR:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2352)	1:21:A:TYR:HA	1:78:A:LEU:HD11	15	0.15
(1,2352)	1:21:A:TYR:HA	1:78:A:LEU:HD12	15	0.15
(1,2352)	1:21:A:TYR:HA	1:78:A:LEU:HD13	15	0.15
(1,2352)	1:21:A:TYR:HA	1:78:A:LEU:HD21	15	0.15
(1,2352)	1:21:A:TYR:HA	1:78:A:LEU:HD22	15	0.15
(1,2352)	1:21:A:TYR:HA	1:78:A:LEU:HD23	15	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	1	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	1	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	1	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	1	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	1	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	1	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	11	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	11	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	11	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	11	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	11	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	11	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	17	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	17	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	17	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	17	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	17	0.15
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	17	0.15
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	14	0.15
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	17	0.15
(1,2212)	1:138:A:ASN:HD21	1:137:A:ILE:HA	20	0.15
(1,2212)	1:138:A:ASN:HD22	1:137:A:ILE:HA	20	0.15
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	17	0.15
(1,1465)	1:204:A:GLU:HB2	1:157:A:VAL:HG11	6	0.15
(1,1465)	1:204:A:GLU:HB2	1:157:A:VAL:HG12	6	0.15
(1,1465)	1:204:A:GLU:HB2	1:157:A:VAL:HG13	6	0.15
(1,1465)	1:204:A:GLU:HB2	1:157:A:VAL:HG21	6	0.15
(1,1465)	1:204:A:GLU:HB2	1:157:A:VAL:HG22	6	0.15
(1,1465)	1:204:A:GLU:HB2	1:157:A:VAL:HG23	6	0.15
(1,1465)	1:204:A:GLU:HB3	1:157:A:VAL:HG11	6	0.15
(1,1465)	1:204:A:GLU:HB3	1:157:A:VAL:HG12	6	0.15
(1,1465)	1:204:A:GLU:HB3	1:157:A:VAL:HG13	6	0.15
(1,1465)	1:204:A:GLU:HB3	1:157:A:VAL:HG21	6	0.15
(1,1465)	1:204:A:GLU:HB3	1:157:A:VAL:HG22	6	0.15
(1,1465)	1:204:A:GLU:HB3	1:157:A:VAL:HG23	6	0.15
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD2	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD3	20	0.15
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD2	20	0.15
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD3	20	0.15
(1,1218)	1:62:A:VAL:HA	1:62:A:VAL:HB	10	0.15
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE1	5	0.15
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE2	5	0.15
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE3	5	0.15
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE1	19	0.15
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE2	19	0.15
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE3	19	0.15
(1,732)	1:142:A:VAL:H	1:142:A:VAL:HB	20	0.15
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB2	4	0.15
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB3	4	0.15
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB2	17	0.15
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB3	17	0.15
(1,627)	1:10:A:SER:H	1:62:A:VAL:HB	1	0.15
(1,362)	1:150:A:LEU:HG	1:119:A:ARG:HA	4	0.15
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	1	0.15
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	1	0.15
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	2	0.15
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	2	0.15
(1,43)	1:50:A:LYS:HE2	1:51:A:PHE:HD1	17	0.15
(1,43)	1:50:A:LYS:HE2	1:51:A:PHE:HD2	17	0.15
(1,43)	1:50:A:LYS:HE3	1:51:A:PHE:HD1	17	0.15
(1,43)	1:50:A:LYS:HE3	1:51:A:PHE:HD2	17	0.15
(1,34)	1:146:A:LYS:HB2	1:145:A:TYR:HD1	16	0.15
(1,34)	1:146:A:LYS:HB2	1:145:A:TYR:HD2	16	0.15
(1,34)	1:146:A:LYS:HB3	1:145:A:TYR:HD1	16	0.15
(1,34)	1:146:A:LYS:HB3	1:145:A:TYR:HD2	16	0.15
(2,165)	1:121:A:ASN:CB	1:95:A:LYS:N	18	0.14
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	3	0.14
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	12	0.14
(1,5845)	1:111:A:GLU:H	1:111:A:GLU:HA	14	0.14
(1,5602)	1:34:A:ILE:HG23	1:53:A:SER:H	9	0.14
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	7	0.14
(1,5572)	1:94:A:TRP:HD1	1:94:A:TRP:H	9	0.14
(1,5554)	1:128:A:LYS:HB2	1:129:A:PHE:H	11	0.14
(1,5536)	1:183:A:ILE:HG13	1:188:A:ALA:H	19	0.14
(1,5522)	1:64:A:ILE:HD11	1:23:A:ALA:H	17	0.14
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	7	0.14
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	5	0.14
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	17	0.14
(1,5471)	1:79:A:GLN:HE21	1:72:A:LEU:HB2	7	0.14
(1,5471)	1:79:A:GLN:HE21	1:72:A:LEU:HB3	7	0.14
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB2	14	0.14
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB3	14	0.14
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	14	0.14
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	14	0.14
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE1	4	0.14
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE2	4	0.14
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE1	8	0.14
(1,5430)	1:24:A:LEU:H	1:46:A:PHE:HE2	8	0.14
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE1	6	0.14
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE2	6	0.14
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG12	5	0.14
(1,5398)	1:127:A:TYR:H	1:101:A:ILE:HG13	5	0.14
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB2	18	0.14
(1,5396)	1:124:A:GLN:H	1:126:A:LEU:HB3	18	0.14
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	14	0.14
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	14	0.14
(1,5359)	1:6:A:GLY:H	1:25:A:VAL:H	17	0.14
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB1	17	0.14
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB2	17	0.14
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB3	17	0.14
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	13	0.14
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	13	0.14
(1,5332)	1:16:A:GLU:H	1:16:A:GLU:HG2	11	0.14
(1,5332)	1:16:A:GLU:H	1:16:A:GLU:HG3	11	0.14
(1,5318)	1:36:A:VAL:H	1:37:A:LYS:HG2	11	0.14
(1,5318)	1:36:A:VAL:H	1:37:A:LYS:HG3	11	0.14
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	10	0.14
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	16	0.14
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB2	20	0.14
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB3	20	0.14
(1,5230)	1:82:A:SER:H	1:79:A:GLN:HB2	10	0.14
(1,5230)	1:82:A:SER:H	1:79:A:GLN:HB3	10	0.14
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB1	18	0.14
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB2	18	0.14
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB3	18	0.14
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	9	0.14
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	9	0.14
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	9	0.14
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB2	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5212)	1:66:A:ASN:H	1:65:A:LEU:HB3	11	0.14
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG11	3	0.14
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG12	3	0.14
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG13	3	0.14
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG21	3	0.14
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG22	3	0.14
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG23	3	0.14
(1,5118)	1:7:A:LYS:H	1:5:A:LEU:HG	11	0.14
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD11	5	0.14
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD12	5	0.14
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD13	5	0.14
(1,5053)	1:78:A:LEU:H	1:75:A:LYS:HD2	10	0.14
(1,5053)	1:78:A:LEU:H	1:75:A:LYS:HD3	10	0.14
(1,5050)	1:223:A:GLU:H	1:222:A:LEU:HB2	6	0.14
(1,5050)	1:223:A:GLU:H	1:222:A:LEU:HB3	6	0.14
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	8	0.14
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	8	0.14
(1,4994)	1:222:A:LEU:H	1:222:A:LEU:HG	9	0.14
(1,4993)	1:19:A:GLU:H	1:17:A:ARG:HB2	2	0.14
(1,4993)	1:19:A:GLU:H	1:17:A:ARG:HB3	2	0.14
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	12	0.14
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD2	3	0.14
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD3	3	0.14
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD2	9	0.14
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD3	9	0.14
(1,4848)	1:17:A:ARG:HG2	1:17:A:ARG:H	9	0.14
(1,4848)	1:17:A:ARG:HG3	1:17:A:ARG:H	9	0.14
(1,4745)	1:177:A:MET:HA	1:174:A:GLN:HE21	2	0.14
(1,4745)	1:177:A:MET:HA	1:174:A:GLN:HE22	2	0.14
(1,4502)	1:133:A:ARG:HE	1:202:A:GLY:H	5	0.14
(1,4267)	1:198:A:LYS:HB2	1:199:A:TYR:H	19	0.14
(1,4267)	1:198:A:LYS:HB3	1:199:A:TYR:H	19	0.14
(1,4252)	1:163:A:CYS:HB2	1:213:A:GLN:HE21	20	0.14
(1,4252)	1:163:A:CYS:HB2	1:213:A:GLN:HE22	20	0.14
(1,4252)	1:163:A:CYS:HB3	1:213:A:GLN:HE21	20	0.14
(1,4252)	1:163:A:CYS:HB3	1:213:A:GLN:HE22	20	0.14
(1,3869)	1:153:A:LEU:HG	1:179:A:LEU:H	20	0.14
(1,3774)	1:43:A:VAL:HG11	1:24:A:LEU:H	9	0.14
(1,3774)	1:43:A:VAL:HG12	1:24:A:LEU:H	9	0.14
(1,3774)	1:43:A:VAL:HG13	1:24:A:LEU:H	9	0.14
(1,3774)	1:43:A:VAL:HG21	1:24:A:LEU:H	9	0.14
(1,3774)	1:43:A:VAL:HG22	1:24:A:LEU:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3774)	1:43:A:VAL:HG23	1:24:A:LEU:H	9	0.14
(1,3507)	1:67:A:LEU:H	1:65:A:LEU:HB2	7	0.14
(1,3507)	1:67:A:LEU:H	1:65:A:LEU:HB3	7	0.14
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	13	0.14
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	8	0.14
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	8	0.14
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	12	0.14
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	12	0.14
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	13	0.14
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	13	0.14
(1,3477)	1:83:A:ILE:H	1:65:A:LEU:HB2	20	0.14
(1,3477)	1:83:A:ILE:H	1:65:A:LEU:HB3	20	0.14
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE2	19	0.14
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE3	19	0.14
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE2	19	0.14
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE3	19	0.14
(1,3381)	1:72:A:LEU:HB2	1:79:A:GLN:HG2	15	0.14
(1,3381)	1:72:A:LEU:HB2	1:79:A:GLN:HG3	15	0.14
(1,3381)	1:72:A:LEU:HB3	1:79:A:GLN:HG2	15	0.14
(1,3381)	1:72:A:LEU:HB3	1:79:A:GLN:HG3	15	0.14
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	11	0.14
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	11	0.14
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	19	0.14
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	19	0.14
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	20	0.14
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	20	0.14
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB2	6	0.14
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB3	6	0.14
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB2	7	0.14
(1,3273)	1:151:A:PHE:HA	1:119:A:ARG:HB3	7	0.14
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	1	0.14
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	1	0.14
(1,3161)	1:133:A:ARG:HE	1:135:A:THR:HG21	13	0.14
(1,3161)	1:133:A:ARG:HE	1:135:A:THR:HG22	13	0.14
(1,3161)	1:133:A:ARG:HE	1:135:A:THR:HG23	13	0.14
(1,3123)	1:16:A:GLU:H	1:16:A:GLU:HG2	11	0.14
(1,3123)	1:16:A:GLU:H	1:16:A:GLU:HG3	11	0.14
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	9	0.14
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	9	0.14
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	9	0.14
(1,2978)	1:98:A:ILE:HG13	1:98:A:ILE:HA	7	0.14
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG21	5	0.14
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG22	5	0.14
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG23	5	0.14
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG21	6	0.14
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG22	6	0.14
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG23	6	0.14
(1,2839)	1:11:A:VAL:HG21	1:23:A:ALA:HA	18	0.14
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	14	0.14
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB2	11	0.14
(1,2685)	1:67:A:LEU:HD13	1:71:A:GLU:HB3	11	0.14
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB2	1	0.14
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB3	1	0.14
(1,2630)	1:47:A:ILE:HD11	1:21:A:TYR:HB2	4	0.14
(1,2630)	1:47:A:ILE:HD11	1:21:A:TYR:HB3	4	0.14
(1,2575)	1:64:A:ILE:HG23	1:78:A:LEU:HA	12	0.14
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	17	0.14
(1,2552)	1:101:A:ILE:HG22	1:102:A:LEU:HA	20	0.14
(1,2548)	1:150:A:LEU:HD11	1:141:A:PRO:HA	15	0.14
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	2	0.14
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	10	0.14
(1,2443)	1:83:A:ILE:HD12	1:83:A:ILE:H	8	0.14
(1,2435)	1:153:A:LEU:HG	1:179:A:LEU:H	20	0.14
(1,2434)	1:85:A:LEU:HG	1:64:A:ILE:H	17	0.14
(1,2400)	1:34:A:ILE:HD11	1:52:A:TYR:H	13	0.14
(1,2389)	1:42:A:LEU:HG	1:36:A:VAL:H	15	0.14
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	2	0.14
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	2	0.14
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	2	0.14
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	2	0.14
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	2	0.14
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	2	0.14
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD11	1	0.14
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD12	1	0.14
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD13	1	0.14
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD11	13	0.14
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD12	13	0.14
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD13	13	0.14
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	16	0.14
(1,1570)	1:88:A:ARG:HG2	1:87:A:THR:HG21	3	0.14
(1,1570)	1:88:A:ARG:HG2	1:87:A:THR:HG22	3	0.14
(1,1570)	1:88:A:ARG:HG2	1:87:A:THR:HG23	3	0.14
(1,1570)	1:88:A:ARG:HG3	1:87:A:THR:HG21	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1570)	1:88:A:ARG:HG3	1:87:A:THR:HG22	3	0.14
(1,1570)	1:88:A:ARG:HG3	1:87:A:THR:HG23	3	0.14
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD11	16	0.14
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD12	16	0.14
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD13	16	0.14
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD11	16	0.14
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD12	16	0.14
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD13	16	0.14
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB1	2	0.14
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB2	2	0.14
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB3	2	0.14
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB1	6	0.14
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB2	6	0.14
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB3	6	0.14
(1,695)	1:17:A:ARG:H	1:17:A:ARG:HG2	9	0.14
(1,695)	1:17:A:ARG:H	1:17:A:ARG:HG3	9	0.14
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB2	1	0.14
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB3	1	0.14
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB2	12	0.14
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB3	12	0.14
(1,627)	1:10:A:SER:H	1:62:A:VAL:HB	6	0.14
(1,625)	1:143:A:LEU:H	1:142:A:VAL:HB	18	0.14
(1,549)	1:42:A:LEU:H	1:59:A:ILE:HD11	7	0.14
(1,549)	1:42:A:LEU:H	1:59:A:ILE:HD12	7	0.14
(1,549)	1:42:A:LEU:H	1:59:A:ILE:HD13	7	0.14
(1,362)	1:150:A:LEU:HG	1:119:A:ARG:HA	8	0.14
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	3	0.14
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	3	0.14
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	12	0.14
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	12	0.14
(1,335)	1:120:A:ASP:HB2	1:117:A:GLU:HA	12	0.14
(1,335)	1:120:A:ASP:HB3	1:117:A:GLU:HA	12	0.14
(1,175)	1:190:A:TYR:HA	1:190:A:TYR:HD1	16	0.14
(1,175)	1:190:A:TYR:HA	1:190:A:TYR:HD2	16	0.14
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD21	9	0.14
(1,168)	1:190:A:TYR:HE2	1:191:A:ASN:HD22	9	0.14
(1,160)	1:145:A:TYR:HE2	1:184:A:LEU:HB2	8	0.14
(1,160)	1:145:A:TYR:HE2	1:184:A:LEU:HB3	8	0.14
(1,152)	1:176:A:TYR:HE2	1:181:A:ILE:HB	6	0.14
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD11	11	0.14
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD12	11	0.14
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD13	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD21	11	0.14
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD22	11	0.14
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD23	11	0.14
(1,114)	1:176:A:TYR:HD1	1:192:A:VAL:HB	12	0.14
(1,113)	1:176:A:TYR:HD2	1:182:A:PRO:HA	3	0.14
(1,113)	1:176:A:TYR:HD1	1:182:A:PRO:HA	17	0.14
(1,34)	1:146:A:LYS:HB2	1:145:A:TYR:HD1	8	0.14
(1,34)	1:146:A:LYS:HB2	1:145:A:TYR:HD2	8	0.14
(1,34)	1:146:A:LYS:HB3	1:145:A:TYR:HD1	8	0.14
(1,34)	1:146:A:LYS:HB3	1:145:A:TYR:HD2	8	0.14
(2,210)	1:134:A:GLY:HA2	1:205:A:GLU:N	6	0.13
(2,210)	1:134:A:GLY:HA3	1:205:A:GLU:N	6	0.13
(2,141)	1:93:A:ASN:CB	1:84:A:PHE:N	9	0.13
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	14	0.13
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	20	0.13
(1,5835)	1:110:A:LYS:HA	1:110:A:LYS:H	1	0.13
(1,5835)	1:110:A:LYS:HA	1:110:A:LYS:H	20	0.13
(1,5807)	1:99:A:SER:H	1:97:A:ASP:HB2	1	0.13
(1,5807)	1:99:A:SER:H	1:97:A:ASP:HB3	1	0.13
(1,5807)	1:2:A:ASP:H	1:2:A:ASP:HB2	13	0.13
(1,5807)	1:2:A:ASP:H	1:2:A:ASP:HB3	13	0.13
(1,5792)	1:76:A:PRO:HD2	1:75:A:LYS:HB2	2	0.13
(1,5792)	1:76:A:PRO:HD2	1:75:A:LYS:HB3	2	0.13
(1,5642)	1:143:A:LEU:HG	1:191:A:ASN:HD21	1	0.13
(1,5642)	1:143:A:LEU:HG	1:191:A:ASN:HD22	1	0.13
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	3	0.13
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	4	0.13
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	10	0.13
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	13	0.13
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	17	0.13
(1,5522)	1:9:A:VAL:HG21	1:23:A:ALA:H	19	0.13
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	14	0.13
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	14	0.13
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	1	0.13
(1,5453)	1:172:A:TRP:H	1:174:A:GLN:HB2	2	0.13
(1,5453)	1:172:A:TRP:H	1:174:A:GLN:HB3	2	0.13
(1,5430)	1:24:A:LEU:H	1:52:A:TYR:HE1	2	0.13
(1,5430)	1:24:A:LEU:H	1:52:A:TYR:HE2	2	0.13
(1,5428)	1:23:A:ALA:H	1:46:A:PHE:HD1	9	0.13
(1,5428)	1:23:A:ALA:H	1:46:A:PHE:HD2	9	0.13
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE1	8	0.13
(1,5402)	1:127:A:TYR:H	1:127:A:TYR:HE2	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5382)	1:74:A:THR:H	1:79:A:GLN:HB2	17	0.13
(1,5382)	1:74:A:THR:H	1:79:A:GLN:HB3	17	0.13
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	11	0.13
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	11	0.13
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB2	19	0.13
(1,5322)	1:149:A:ASN:H	1:141:A:PRO:HB3	19	0.13
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG2	5	0.13
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG3	5	0.13
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG2	6	0.13
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG3	6	0.13
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG2	19	0.13
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG3	19	0.13
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	1	0.13
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	6	0.13
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	8	0.13
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	9	0.13
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	20	0.13
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD21	19	0.13
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD22	19	0.13
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB1	1	0.13
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB2	1	0.13
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB3	1	0.13
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB1	11	0.13
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB2	11	0.13
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB3	11	0.13
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD11	4	0.13
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD12	4	0.13
(1,5219)	1:57:A:LYS:H	1:59:A:ILE:HD13	4	0.13
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB2	20	0.13
(1,5203)	1:200:A:LEU:H	1:198:A:LYS:HB3	20	0.13
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	11	0.13
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	11	0.13
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	11	0.13
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD11	16	0.13
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD12	16	0.13
(1,5141)	1:101:A:ILE:H	1:101:A:ILE:HD13	16	0.13
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD11	11	0.13
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD12	11	0.13
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD13	11	0.13
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD11	17	0.13
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD12	17	0.13
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD13	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5131)	1:45:A:SER:H	1:43:A:VAL:HG11	8	0.13
(1,5131)	1:45:A:SER:H	1:43:A:VAL:HG12	8	0.13
(1,5131)	1:45:A:SER:H	1:43:A:VAL:HG13	8	0.13
(1,5131)	1:45:A:SER:H	1:43:A:VAL:HG21	8	0.13
(1,5131)	1:45:A:SER:H	1:43:A:VAL:HG22	8	0.13
(1,5131)	1:45:A:SER:H	1:43:A:VAL:HG23	8	0.13
(1,5103)	1:123:A:LEU:H	1:119:A:ARG:HB2	17	0.13
(1,5103)	1:123:A:LEU:H	1:119:A:ARG:HB3	17	0.13
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD11	18	0.13
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD12	18	0.13
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD13	18	0.13
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD21	18	0.13
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD22	18	0.13
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD23	18	0.13
(1,5052)	1:78:A:LEU:H	1:75:A:LYS:HB2	20	0.13
(1,5052)	1:78:A:LEU:H	1:75:A:LYS:HB3	20	0.13
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	9	0.13
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	9	0.13
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	13	0.13
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	13	0.13
(1,5041)	1:20:A:TRP:H	1:19:A:GLU:HG2	11	0.13
(1,5041)	1:20:A:TRP:H	1:19:A:GLU:HG3	11	0.13
(1,5011)	1:62:A:VAL:H	1:62:A:VAL:HG11	9	0.13
(1,5011)	1:62:A:VAL:H	1:62:A:VAL:HG12	9	0.13
(1,5011)	1:62:A:VAL:H	1:62:A:VAL:HG13	9	0.13
(1,5011)	1:62:A:VAL:H	1:62:A:VAL:HG21	9	0.13
(1,5011)	1:62:A:VAL:H	1:62:A:VAL:HG22	9	0.13
(1,5011)	1:62:A:VAL:H	1:62:A:VAL:HG23	9	0.13
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD11	15	0.13
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD12	15	0.13
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD13	15	0.13
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD21	15	0.13
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD22	15	0.13
(1,5008)	1:64:A:ILE:H	1:65:A:LEU:HD23	15	0.13
(1,4956)	1:178:A:ASP:H	1:175:A:ILE:HG12	20	0.13
(1,4956)	1:178:A:ASP:H	1:175:A:ILE:HG13	20	0.13
(1,4922)	1:11:A:VAL:H	1:20:A:TRP:HD1	16	0.13
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	4	0.13
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	6	0.13
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	11	0.13
(1,4289)	1:150:A:LEU:HD11	1:199:A:TYR:H	8	0.13
(1,4289)	1:150:A:LEU:HD12	1:199:A:TYR:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4289)	1:150:A:LEU:HD13	1:199:A:TYR:H	8	0.13
(1,4289)	1:150:A:LEU:HD21	1:199:A:TYR:H	8	0.13
(1,4289)	1:150:A:LEU:HD22	1:199:A:TYR:H	8	0.13
(1,4289)	1:150:A:LEU:HD23	1:199:A:TYR:H	8	0.13
(1,4267)	1:198:A:LYS:HB2	1:199:A:TYR:H	3	0.13
(1,4267)	1:198:A:LYS:HB3	1:199:A:TYR:H	3	0.13
(1,4153)	1:38:A:LYS:HG2	1:39:A:ASP:H	13	0.13
(1,4153)	1:38:A:LYS:HG3	1:39:A:ASP:H	13	0.13
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	3	0.13
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	3	0.13
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	3	0.13
(1,3982)	1:50:A:LYS:HD2	1:50:A:LYS:H	11	0.13
(1,3982)	1:50:A:LYS:HD3	1:50:A:LYS:H	11	0.13
(1,3927)	1:46:A:PHE:HE1	1:80:A:LYS:H	6	0.13
(1,3927)	1:46:A:PHE:HE2	1:80:A:LYS:H	6	0.13
(1,3869)	1:153:A:LEU:HG	1:179:A:LEU:H	13	0.13
(1,3849)	1:109:A:ASP:HB2	1:109:A:ASP:H	19	0.13
(1,3849)	1:109:A:ASP:HB3	1:109:A:ASP:H	19	0.13
(1,3848)	1:223:A:GLU:HG2	1:223:A:GLU:H	1	0.13
(1,3848)	1:223:A:GLU:HG3	1:223:A:GLU:H	1	0.13
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	14	0.13
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	16	0.13
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	16	0.13
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE2	8	0.13
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE3	8	0.13
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE2	9	0.13
(1,3434)	1:181:A:ILE:HG12	1:146:A:LYS:HE3	9	0.13
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE2	1	0.13
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE3	1	0.13
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE2	1	0.13
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE3	1	0.13
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE2	1	0.13
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE3	1	0.13
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE2	11	0.13
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE3	11	0.13
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE2	11	0.13
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE3	11	0.13
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE2	11	0.13
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE3	11	0.13
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	12	0.13
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	12	0.13
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	4	0.13
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG2	12	0.13
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG3	12	0.13
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG2	20	0.13
(1,3112)	1:80:A:LYS:H	1:79:A:GLN:HG3	20	0.13
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD11	4	0.13
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD12	4	0.13
(1,3109)	1:57:A:LYS:H	1:59:A:ILE:HD13	4	0.13
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG2	3	0.13
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG3	3	0.13
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG11	18	0.13
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG12	18	0.13
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG13	18	0.13
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG21	18	0.13
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG22	18	0.13
(1,3070)	1:10:A:SER:H	1:9:A:VAL:HG23	18	0.13
(1,2978)	1:98:A:ILE:HG13	1:98:A:ILE:HA	17	0.13
(1,2973)	1:85:A:LEU:HB2	1:82:A:SER:HA	8	0.13
(1,2871)	1:175:A:ILE:HG12	1:175:A:ILE:HA	19	0.13
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	10	0.13
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG12	20	0.13
(1,2866)	1:210:A:ALA:HA	1:212:A:ILE:HG13	20	0.13
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG21	11	0.13
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG22	11	0.13
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG23	11	0.13
(1,2842)	1:181:A:ILE:HD11	1:176:A:TYR:HB2	20	0.13
(1,2842)	1:181:A:ILE:HD11	1:176:A:TYR:HB3	20	0.13
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD2	20	0.13
(1,2828)	1:137:A:ILE:HB	1:141:A:PRO:HD3	20	0.13
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	9	0.13
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG21	17	0.13
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG22	17	0.13
(1,2766)	1:55:A:ALA:HB2	1:54:A:ILE:HG23	17	0.13
(1,2666)	1:72:A:LEU:HB2	1:79:A:GLN:HG2	17	0.13
(1,2666)	1:72:A:LEU:HB2	1:79:A:GLN:HG3	17	0.13
(1,2666)	1:72:A:LEU:HB3	1:79:A:GLN:HG2	17	0.13
(1,2666)	1:72:A:LEU:HB3	1:79:A:GLN:HG3	17	0.13
(1,2645)	1:54:A:ILE:HG21	1:41:A:CYS:HB2	11	0.13
(1,2645)	1:54:A:ILE:HG21	1:41:A:CYS:HB3	11	0.13
(1,2639)	1:11:A:VAL:HG22	1:10:A:SER:HB2	5	0.13
(1,2639)	1:11:A:VAL:HG22	1:10:A:SER:HB3	5	0.13
(1,2639)	1:11:A:VAL:HG12	1:20:A:TRP:HB2	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2639)	1:11:A:VAL:HG12	1:20:A:TRP:HB3	14	0.13
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB2	14	0.13
(1,2636)	1:65:A:LEU:HD13	1:66:A:ASN:HB3	14	0.13
(1,2590)	1:85:A:LEU:HA	1:88:A:ARG:HB2	3	0.13
(1,2590)	1:85:A:LEU:HA	1:88:A:ARG:HB3	3	0.13
(1,2562)	1:72:A:LEU:HG	1:69:A:GLU:HA	13	0.13
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	2	0.13
(1,2529)	1:5:A:LEU:HD12	1:2:A:ASP:HA	1	0.13
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD11	7	0.13
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD12	7	0.13
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD13	7	0.13
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD21	7	0.13
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD22	7	0.13
(1,2498)	1:46:A:PHE:HD1	1:24:A:LEU:HD23	7	0.13
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD11	7	0.13
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD12	7	0.13
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD13	7	0.13
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD21	7	0.13
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD22	7	0.13
(1,2497)	1:46:A:PHE:HD1	1:24:A:LEU:HD23	7	0.13
(1,2466)	1:60:A:LYS:HD3	1:20:A:TRP:HD1	12	0.13
(1,2411)	1:88:A:ARG:HD2	1:88:A:ARG:H	6	0.13
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	4	0.13
(1,2385)	1:34:A:ILE:HB	1:52:A:TYR:H	5	0.13
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD11	2	0.13
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD12	2	0.13
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD13	2	0.13
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD21	2	0.13
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD22	2	0.13
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD23	2	0.13
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	3	0.13
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	3	0.13
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	3	0.13
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	3	0.13
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	3	0.13
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	3	0.13
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	10	0.13
(1,2277)	1:131:A:GLU:HA	1:134:A:GLY:H	17	0.13
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD11	1	0.13
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD12	1	0.13
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD13	1	0.13
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD11	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD12	10	0.13
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD13	10	0.13
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD11	12	0.13
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD12	12	0.13
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD13	12	0.13
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD11	18	0.13
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD12	18	0.13
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD13	18	0.13
(1,1930)	1:42:A:LEU:H	1:26:A:ILE:HD11	19	0.13
(1,1930)	1:42:A:LEU:H	1:26:A:ILE:HD12	19	0.13
(1,1930)	1:42:A:LEU:H	1:26:A:ILE:HD13	19	0.13
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	10	0.13
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	13	0.13
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	15	0.13
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD11	17	0.13
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD12	17	0.13
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD13	17	0.13
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD21	17	0.13
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD22	17	0.13
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD23	17	0.13
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD11	17	0.13
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD12	17	0.13
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD13	17	0.13
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD21	17	0.13
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD22	17	0.13
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD23	17	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD11	1	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD12	1	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD13	1	0.13
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD11	1	0.13
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD12	1	0.13
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD13	1	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD11	7	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD12	7	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD13	7	0.13
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD11	7	0.13
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD12	7	0.13
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD13	7	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD11	11	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD12	11	0.13
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD13	11	0.13
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD11	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD12	11	0.13
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD13	11	0.13
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG11	19	0.13
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG12	19	0.13
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG13	19	0.13
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG21	19	0.13
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG22	19	0.13
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG23	19	0.13
(1,1218)	1:62:A:VAL:HA	1:62:A:VAL:HB	17	0.13
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB1	13	0.13
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB2	13	0.13
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB3	13	0.13
(1,1171)	1:143:A:LEU:HA	1:143:A:LEU:HG	5	0.13
(1,1092)	1:151:A:PHE:HE1	1:123:A:LEU:HD11	6	0.13
(1,1092)	1:151:A:PHE:HE1	1:123:A:LEU:HD12	6	0.13
(1,1092)	1:151:A:PHE:HE1	1:123:A:LEU:HD13	6	0.13
(1,1092)	1:151:A:PHE:HE1	1:123:A:LEU:HD21	6	0.13
(1,1092)	1:151:A:PHE:HE1	1:123:A:LEU:HD22	6	0.13
(1,1092)	1:151:A:PHE:HE1	1:123:A:LEU:HD23	6	0.13
(1,1092)	1:151:A:PHE:HE2	1:123:A:LEU:HD11	6	0.13
(1,1092)	1:151:A:PHE:HE2	1:123:A:LEU:HD12	6	0.13
(1,1092)	1:151:A:PHE:HE2	1:123:A:LEU:HD13	6	0.13
(1,1092)	1:151:A:PHE:HE2	1:123:A:LEU:HD21	6	0.13
(1,1092)	1:151:A:PHE:HE2	1:123:A:LEU:HD22	6	0.13
(1,1092)	1:151:A:PHE:HE2	1:123:A:LEU:HD23	6	0.13
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG11	11	0.13
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG12	11	0.13
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG13	11	0.13
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG21	11	0.13
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG22	11	0.13
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG23	11	0.13
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG11	11	0.13
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG12	11	0.13
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG13	11	0.13
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG21	11	0.13
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG22	11	0.13
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG23	11	0.13
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD11	15	0.13
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD12	15	0.13
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD13	15	0.13
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD21	15	0.13
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD22	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD23	15	0.13
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD11	15	0.13
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD12	15	0.13
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD13	15	0.13
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD21	15	0.13
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD22	15	0.13
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD23	15	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	17	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	17	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	17	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	17	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	17	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	17	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	20	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	20	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	20	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	20	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	20	0.13
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	20	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	17	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	17	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	17	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	17	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	17	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	17	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	20	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	20	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	20	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	20	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	20	0.13
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	20	0.13
(1,965)	1:20:A:TRP:HD1	1:10:A:SER:HB2	11	0.13
(1,965)	1:20:A:TRP:HD1	1:10:A:SER:HB3	11	0.13
(1,857)	1:185:A:ASN:H	1:184:A:LEU:HD11	2	0.13
(1,857)	1:185:A:ASN:H	1:184:A:LEU:HD12	2	0.13
(1,857)	1:185:A:ASN:H	1:184:A:LEU:HD13	2	0.13
(1,857)	1:185:A:ASN:H	1:184:A:LEU:HD21	2	0.13
(1,857)	1:185:A:ASN:H	1:184:A:LEU:HD22	2	0.13
(1,857)	1:185:A:ASN:H	1:184:A:LEU:HD23	2	0.13
(1,855)	1:185:A:ASN:H	1:184:A:LEU:HD11	2	0.13
(1,855)	1:185:A:ASN:H	1:184:A:LEU:HD12	2	0.13
(1,855)	1:185:A:ASN:H	1:184:A:LEU:HD13	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,855)	1:185:A:ASN:H	1:184:A:LEU:HD21	2	0.13
(1,855)	1:185:A:ASN:H	1:184:A:LEU:HD22	2	0.13
(1,855)	1:185:A:ASN:H	1:184:A:LEU:HD23	2	0.13
(1,725)	1:210:A:ALA:H	1:212:A:ILE:HB	11	0.13
(1,687)	1:2:A:ASP:H	1:61:A:GLU:HB2	14	0.13
(1,687)	1:2:A:ASP:H	1:61:A:GLU:HB3	14	0.13
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB2	18	0.13
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB3	18	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG11	3	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG12	3	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG13	3	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG21	3	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG22	3	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG23	3	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG11	4	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG12	4	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG13	4	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG21	4	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG22	4	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG23	4	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG11	20	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG12	20	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG13	20	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG21	20	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG22	20	0.13
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG23	20	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG11	3	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG12	3	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG13	3	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG21	3	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG22	3	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG23	3	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG11	4	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG12	4	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG13	4	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG21	4	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG22	4	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG23	4	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG11	20	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG12	20	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG13	20	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG21	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG22	20	0.13
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG23	20	0.13
(1,401)	1:102:A:LEU:H	1:103:A:GLU:HA	10	0.13
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	7	0.13
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	7	0.13
(1,175)	1:190:A:TYR:HA	1:190:A:TYR:HD1	1	0.13
(1,175)	1:190:A:TYR:HA	1:190:A:TYR:HD2	1	0.13
(2,291)	1:30:A:CYS:CB	1:200:A:LEU:N	20	0.12
(2,156)	1:121:A:ASN:CB	1:84:A:PHE:N	18	0.12
(1,5871)	1:110:A:LYS:HE2	1:110:A:LYS:H	13	0.12
(1,5871)	1:110:A:LYS:HE3	1:110:A:LYS:H	13	0.12
(1,5851)	1:113:A:GLU:H	1:113:A:GLU:HA	2	0.12
(1,5851)	1:113:A:GLU:H	1:113:A:GLU:HA	9	0.12
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	9	0.12
(1,5806)	1:223:A:GLU:HB2	1:222:A:LEU:HB2	7	0.12
(1,5806)	1:223:A:GLU:HB2	1:222:A:LEU:HB3	7	0.12
(1,5689)	1:137:A:ILE:HA	1:138:A:ASN:HD21	15	0.12
(1,5689)	1:137:A:ILE:HA	1:138:A:ASN:HD22	15	0.12
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	16	0.12
(1,5528)	1:142:A:VAL:HB	1:143:A:LEU:H	8	0.12
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	4	0.12
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	4	0.12
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	10	0.12
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	10	0.12
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	19	0.12
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	19	0.12
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG12	18	0.12
(1,5489)	1:63:A:ASP:H	1:64:A:ILE:HG13	18	0.12
(1,5485)	1:62:A:VAL:H	1:8:A:VAL:HG11	7	0.12
(1,5485)	1:62:A:VAL:H	1:8:A:VAL:HG12	7	0.12
(1,5485)	1:62:A:VAL:H	1:8:A:VAL:HG13	7	0.12
(1,5485)	1:62:A:VAL:H	1:8:A:VAL:HG21	7	0.12
(1,5485)	1:62:A:VAL:H	1:8:A:VAL:HG22	7	0.12
(1,5485)	1:62:A:VAL:H	1:8:A:VAL:HG23	7	0.12
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	5	0.12
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	4	0.12
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	19	0.12
(1,5455)	1:193:A:LYS:H	1:143:A:LEU:HD11	5	0.12
(1,5455)	1:193:A:LYS:H	1:143:A:LEU:HD12	5	0.12
(1,5455)	1:193:A:LYS:H	1:143:A:LEU:HD13	5	0.12
(1,5455)	1:193:A:LYS:H	1:143:A:LEU:HD21	5	0.12
(1,5455)	1:193:A:LYS:H	1:143:A:LEU:HD22	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5455)	1:193:A:LYS:H	1:143:A:LEU:HD23	5	0.12
(1,5453)	1:172:A:TRP:H	1:174:A:GLN:HB2	8	0.12
(1,5453)	1:172:A:TRP:H	1:174:A:GLN:HB3	8	0.12
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG12	3	0.12
(1,5450)	1:124:A:GLN:H	1:98:A:ILE:HG13	3	0.12
(1,5428)	1:23:A:ALA:H	1:20:A:TRP:HZ3	20	0.12
(1,5413)	1:170:A:ALA:H	1:168:A:SER:H	8	0.12
(1,5397)	1:127:A:TYR:H	1:137:A:ILE:HG12	3	0.12
(1,5397)	1:127:A:TYR:H	1:137:A:ILE:HG13	3	0.12
(1,5396)	1:124:A:GLN:H	1:98:A:ILE:HG12	3	0.12
(1,5396)	1:124:A:GLN:H	1:98:A:ILE:HG13	3	0.12
(1,5394)	1:59:A:ILE:H	1:56:A:ARG:H	18	0.12
(1,5361)	1:199:A:TYR:H	1:150:A:LEU:HB2	18	0.12
(1,5361)	1:199:A:TYR:H	1:150:A:LEU:HB3	18	0.12
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB1	7	0.12
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB2	7	0.12
(1,5356)	1:48:A:ASP:H	1:23:A:ALA:HB3	7	0.12
(1,5314)	1:20:A:TRP:HE1	1:75:A:LYS:HG2	13	0.12
(1,5314)	1:20:A:TRP:HE1	1:75:A:LYS:HG3	13	0.12
(1,5312)	1:20:A:TRP:HE1	1:21:A:TYR:H	17	0.12
(1,5292)	1:18:A:THR:H	1:19:A:GLU:HG2	9	0.12
(1,5292)	1:18:A:THR:H	1:19:A:GLU:HG3	9	0.12
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	2	0.12
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	12	0.12
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB2	11	0.12
(1,5273)	1:135:A:THR:H	1:136:A:PRO:HB3	11	0.12
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD21	14	0.12
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD22	14	0.12
(1,5235)	1:70:A:SER:H	1:69:A:GLU:HB2	4	0.12
(1,5235)	1:70:A:SER:H	1:69:A:GLU:HB3	4	0.12
(1,5226)	1:82:A:SER:H	1:79:A:GLN:HA	17	0.12
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB1	8	0.12
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB2	8	0.12
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB3	8	0.12
(1,5220)	1:185:A:ASN:H	1:183:A:ILE:HG21	14	0.12
(1,5220)	1:185:A:ASN:H	1:183:A:ILE:HG22	14	0.12
(1,5220)	1:185:A:ASN:H	1:183:A:ILE:HG23	14	0.12
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB1	15	0.12
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB2	15	0.12
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB3	15	0.12
(1,5218)	1:57:A:LYS:H	1:54:A:ILE:HG21	16	0.12
(1,5218)	1:57:A:LYS:H	1:54:A:ILE:HG22	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5218)	1:57:A:LYS:H	1:54:A:ILE:HG23	16	0.12
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB2	19	0.12
(1,5211)	1:51:A:PHE:H	1:50:A:LYS:HB3	19	0.12
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB1	8	0.12
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB2	8	0.12
(1,5203)	1:200:A:LEU:H	1:195:A:ALA:HB3	8	0.12
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG11	12	0.12
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG12	12	0.12
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG13	12	0.12
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG21	12	0.12
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG22	12	0.12
(1,5125)	1:196:A:TYR:H	1:192:A:VAL:HG23	12	0.12
(1,5118)	1:7:A:LYS:H	1:5:A:LEU:HG	7	0.12
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD11	14	0.12
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD12	14	0.12
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD13	14	0.12
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD21	14	0.12
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD22	14	0.12
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD23	14	0.12
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD11	19	0.12
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD12	19	0.12
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD13	19	0.12
(1,5014)	1:67:A:LEU:H	1:67:A:LEU:HD11	5	0.12
(1,5014)	1:67:A:LEU:H	1:67:A:LEU:HD12	5	0.12
(1,5014)	1:67:A:LEU:H	1:67:A:LEU:HD13	5	0.12
(1,5014)	1:67:A:LEU:H	1:67:A:LEU:HD21	5	0.12
(1,5014)	1:67:A:LEU:H	1:67:A:LEU:HD22	5	0.12
(1,5014)	1:67:A:LEU:H	1:67:A:LEU:HD23	5	0.12
(1,4970)	1:64:A:ILE:H	1:65:A:LEU:HA	5	0.12
(1,4922)	1:11:A:VAL:H	1:20:A:TRP:HD1	4	0.12
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	9	0.12
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	14	0.12
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	16	0.12
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	20	0.12
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB2	4	0.12
(1,4907)	1:20:A:TRP:HE1	1:75:A:LYS:HB3	4	0.12
(1,4881)	1:213:A:GLN:HG2	1:211:A:ASN:HD21	6	0.12
(1,4881)	1:213:A:GLN:HG2	1:211:A:ASN:HD22	6	0.12
(1,4881)	1:213:A:GLN:HG3	1:211:A:ASN:HD21	6	0.12
(1,4881)	1:213:A:GLN:HG3	1:211:A:ASN:HD22	6	0.12
(1,4808)	1:92:A:ASP:H	1:93:A:ASN:HD21	10	0.12
(1,4808)	1:92:A:ASP:H	1:93:A:ASN:HD22	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4528)	1:205:A:GLU:HB2	1:29:A:SER:H	1	0.12
(1,4528)	1:205:A:GLU:HB3	1:29:A:SER:H	1	0.12
(1,4284)	1:213:A:GLN:HG2	1:211:A:ASN:HD21	6	0.12
(1,4284)	1:213:A:GLN:HG2	1:211:A:ASN:HD22	6	0.12
(1,4284)	1:213:A:GLN:HG3	1:211:A:ASN:HD21	6	0.12
(1,4284)	1:213:A:GLN:HG3	1:211:A:ASN:HD22	6	0.12
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	8	0.12
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	8	0.12
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	8	0.12
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	13	0.12
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	13	0.12
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	13	0.12
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	17	0.12
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	17	0.12
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	17	0.12
(1,3982)	1:50:A:LYS:HD2	1:50:A:LYS:H	1	0.12
(1,3982)	1:50:A:LYS:HD3	1:50:A:LYS:H	1	0.12
(1,3871)	1:198:A:LYS:HB2	1:201:A:TYR:H	1	0.12
(1,3871)	1:198:A:LYS:HB3	1:201:A:TYR:H	1	0.12
(1,3869)	1:153:A:LEU:HG	1:179:A:LEU:H	2	0.12
(1,3869)	1:153:A:LEU:HG	1:179:A:LEU:H	9	0.12
(1,3669)	1:112:A:LYS:HB2	1:113:A:GLU:H	20	0.12
(1,3669)	1:112:A:LYS:HB3	1:113:A:GLU:H	20	0.12
(1,3604)	1:149:A:ASN:HB2	1:150:A:LEU:H	11	0.12
(1,3604)	1:149:A:ASN:HB3	1:150:A:LEU:H	11	0.12
(1,3604)	1:149:A:ASN:HB2	1:150:A:LEU:H	18	0.12
(1,3604)	1:149:A:ASN:HB3	1:150:A:LEU:H	18	0.12
(1,3490)	1:16:A:GLU:H	1:14:A:ALA:HA	19	0.12
(1,3486)	1:2:A:ASP:H	1:1:A:ASN:HB2	18	0.12
(1,3486)	1:2:A:ASP:H	1:1:A:ASN:HB3	18	0.12
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	4	0.12
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	4	0.12
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	14	0.12
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	14	0.12
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG2	1	0.12
(1,3442)	1:9:A:VAL:HG11	1:61:A:GLU:HG3	1	0.12
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG2	1	0.12
(1,3442)	1:9:A:VAL:HG12	1:61:A:GLU:HG3	1	0.12
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG2	1	0.12
(1,3442)	1:9:A:VAL:HG13	1:61:A:GLU:HG3	1	0.12
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG2	1	0.12
(1,3442)	1:9:A:VAL:HG21	1:61:A:GLU:HG3	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG2	1	0.12
(1,3442)	1:9:A:VAL:HG22	1:61:A:GLU:HG3	1	0.12
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG2	1	0.12
(1,3442)	1:9:A:VAL:HG23	1:61:A:GLU:HG3	1	0.12
(1,3402)	1:35:A:THR:HG23	1:36:A:VAL:HB	3	0.12
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE2	12	0.12
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE3	12	0.12
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE2	12	0.12
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE3	12	0.12
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE2	12	0.12
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE3	12	0.12
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE2	15	0.12
(1,3390)	1:83:A:ILE:HG12	1:86:A:LYS:HE3	15	0.12
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE2	15	0.12
(1,3390)	1:83:A:ILE:HG13	1:86:A:LYS:HE3	15	0.12
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG2	14	0.12
(1,3381)	1:80:A:LYS:HG2	1:79:A:GLN:HG3	14	0.12
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG2	14	0.12
(1,3381)	1:80:A:LYS:HG3	1:79:A:GLN:HG3	14	0.12
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	8	0.12
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	8	0.12
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG2	6	0.12
(1,3192)	1:68:A:PRO:HA	1:69:A:GLU:HG3	6	0.12
(1,3177)	1:122:A:PHE:HD1	1:203:A:PHE:HB2	18	0.12
(1,3177)	1:122:A:PHE:HD1	1:203:A:PHE:HB3	18	0.12
(1,3177)	1:122:A:PHE:HD2	1:203:A:PHE:HB2	18	0.12
(1,3177)	1:122:A:PHE:HD2	1:203:A:PHE:HB3	18	0.12
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG2	12	0.12
(1,3081)	1:8:A:VAL:H	1:7:A:LYS:HG3	12	0.12
(1,2998)	1:178:A:ASP:HB3	1:153:A:LEU:HA	10	0.12
(1,2988)	1:89:A:VAL:HB	1:86:A:LYS:HA	9	0.12
(1,2922)	1:64:A:ILE:HD11	1:62:A:VAL:HB	15	0.12
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	4	0.12
(1,2841)	1:166:A:ILE:HD13	1:157:A:VAL:H	11	0.12
(1,2837)	1:34:A:ILE:HG12	1:51:A:PHE:HA	9	0.12
(1,2826)	1:59:A:ILE:HB	1:9:A:VAL:HB	16	0.12
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD11	13	0.12
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD12	13	0.12
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD13	13	0.12
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD21	13	0.12
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD22	13	0.12
(1,2770)	1:101:A:ILE:HD11	1:123:A:LEU:HD23	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG21	3	0.12
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG22	3	0.12
(1,2766)	1:55:A:ALA:HB3	1:54:A:ILE:HG23	3	0.12
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD11	13	0.12
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD12	13	0.12
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD13	13	0.12
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD21	13	0.12
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD22	13	0.12
(1,2759)	1:71:A:GLU:HB3	1:72:A:LEU:HD23	13	0.12
(1,2703)	1:170:A:ALA:HB3	1:171:A:VAL:HB	19	0.12
(1,2640)	1:210:A:ALA:HB1	1:207:A:CYS:HB2	19	0.12
(1,2640)	1:210:A:ALA:HB1	1:207:A:CYS:HB3	19	0.12
(1,2640)	1:210:A:ALA:HB2	1:207:A:CYS:HB2	19	0.12
(1,2640)	1:210:A:ALA:HB2	1:207:A:CYS:HB3	19	0.12
(1,2640)	1:210:A:ALA:HB3	1:207:A:CYS:HB2	19	0.12
(1,2640)	1:210:A:ALA:HB3	1:207:A:CYS:HB3	19	0.12
(1,2596)	1:90:A:VAL:HG23	1:85:A:LEU:HA	5	0.12
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	1	0.12
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	7	0.12
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	8	0.12
(1,2554)	1:175:A:ILE:HD12	1:192:A:VAL:HA	14	0.12
(1,2554)	1:175:A:ILE:HD13	1:153:A:LEU:HA	18	0.12
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	6	0.12
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	7	0.12
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	11	0.12
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	18	0.12
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	19	0.12
(1,2529)	1:5:A:LEU:HD12	1:2:A:ASP:HA	10	0.12
(1,2479)	1:194:A:THR:HG23	1:199:A:TYR:HD1	12	0.12
(1,2479)	1:194:A:THR:HG23	1:199:A:TYR:HD2	12	0.12
(1,2435)	1:153:A:LEU:HG	1:179:A:LEU:H	2	0.12
(1,2435)	1:153:A:LEU:HG	1:179:A:LEU:H	9	0.12
(1,2400)	1:34:A:ILE:HD13	1:52:A:TYR:H	1	0.12
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD11	15	0.12
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD12	15	0.12
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD13	15	0.12
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD21	15	0.12
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD22	15	0.12
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD23	15	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	4	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	4	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	4	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	4	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	4	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	13	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	13	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	13	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	13	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	13	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	13	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	18	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	18	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	18	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	18	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	18	0.12
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	18	0.12
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	4	0.12
(1,2257)	1:101:A:ILE:HA	1:100:A:GLU:H	14	0.12
(1,2212)	1:138:A:ASN:HD21	1:137:A:ILE:HA	15	0.12
(1,2212)	1:138:A:ASN:HD22	1:137:A:ILE:HA	15	0.12
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	4	0.12
(1,1559)	1:197:A:ARG:HB2	1:197:A:ARG:HD2	11	0.12
(1,1559)	1:197:A:ARG:HB2	1:197:A:ARG:HD3	11	0.12
(1,1559)	1:197:A:ARG:HB3	1:197:A:ARG:HD2	11	0.12
(1,1559)	1:197:A:ARG:HB3	1:197:A:ARG:HD3	11	0.12
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD2	19	0.12
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD3	19	0.12
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD2	19	0.12
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD3	19	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG11	12	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG12	12	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG13	12	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG21	12	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG22	12	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG23	12	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG11	20	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG12	20	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG13	20	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG21	20	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG22	20	0.12
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG23	20	0.12
(1,1074)	1:196:A:TYR:HD1	1:175:A:ILE:HG21	2	0.12
(1,1074)	1:196:A:TYR:HD1	1:175:A:ILE:HG22	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	1:196:A:TYR:HD1	1:175:A:ILE:HG23	2	0.12
(1,1074)	1:196:A:TYR:HD2	1:175:A:ILE:HG21	2	0.12
(1,1074)	1:196:A:TYR:HD2	1:175:A:ILE:HG22	2	0.12
(1,1074)	1:196:A:TYR:HD2	1:175:A:ILE:HG23	2	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	6	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	6	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	6	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	6	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	6	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	6	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	16	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	16	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	16	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	16	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	16	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	16	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	18	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	18	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	18	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	18	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	18	0.12
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	18	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	6	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	6	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	6	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	6	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	6	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	6	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	16	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	16	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	16	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	16	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	16	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	16	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	18	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	18	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	18	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	18	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	18	0.12
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	18	0.12
(1,955)	1:196:A:TYR:HE1	1:175:A:ILE:HG21	20	0.12
(1,955)	1:196:A:TYR:HE1	1:175:A:ILE:HG22	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,955)	1:196:A:TYR:HE1	1:175:A:ILE:HG23	20	0.12
(1,955)	1:196:A:TYR:HE2	1:175:A:ILE:HG21	20	0.12
(1,955)	1:196:A:TYR:HE2	1:175:A:ILE:HG22	20	0.12
(1,955)	1:196:A:TYR:HE2	1:175:A:ILE:HG23	20	0.12
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD11	9	0.12
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD12	9	0.12
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD13	9	0.12
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD11	9	0.12
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD12	9	0.12
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD13	9	0.12
(1,765)	1:87:A:THR:H	1:87:A:THR:HG21	19	0.12
(1,765)	1:87:A:THR:H	1:87:A:THR:HG22	19	0.12
(1,765)	1:87:A:THR:H	1:87:A:THR:HG23	19	0.12
(1,731)	1:148:A:LEU:H	1:142:A:VAL:HB	3	0.12
(1,714)	1:97:A:ASP:H	1:96:A:MET:HE1	15	0.12
(1,714)	1:97:A:ASP:H	1:96:A:MET:HE2	15	0.12
(1,714)	1:97:A:ASP:H	1:96:A:MET:HE3	15	0.12
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB2	20	0.12
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB3	20	0.12
(1,625)	1:143:A:LEU:H	1:142:A:VAL:HB	8	0.12
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG11	10	0.12
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG12	10	0.12
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG13	10	0.12
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG21	10	0.12
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG22	10	0.12
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG23	10	0.12
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG11	10	0.12
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG12	10	0.12
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG13	10	0.12
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG21	10	0.12
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG22	10	0.12
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG23	10	0.12
(1,362)	1:150:A:LEU:HG	1:119:A:ARG:HA	2	0.12
(1,335)	1:120:A:ASP:HB2	1:117:A:GLU:HA	1	0.12
(1,335)	1:120:A:ASP:HB3	1:117:A:GLU:HA	1	0.12
(1,335)	1:120:A:ASP:HB2	1:117:A:GLU:HA	8	0.12
(1,335)	1:120:A:ASP:HB3	1:117:A:GLU:HA	8	0.12
(1,335)	1:120:A:ASP:HB2	1:117:A:GLU:HA	15	0.12
(1,335)	1:120:A:ASP:HB3	1:117:A:GLU:HA	15	0.12
(1,298)	1:119:A:ARG:HB2	1:122:A:PHE:HA	17	0.12
(1,298)	1:119:A:ARG:HB3	1:122:A:PHE:HA	17	0.12
(1,248)	1:130:A:MET:H	1:136:A:PRO:HA	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:190:A:TYR:HE1	1:191:A:ASN:HD21	15	0.12
(1,168)	1:190:A:TYR:HE1	1:191:A:ASN:HD22	15	0.12
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD11	8	0.12
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD12	8	0.12
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD13	8	0.12
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD21	8	0.12
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD22	8	0.12
(1,120)	1:199:A:TYR:HE1	1:143:A:LEU:HD23	8	0.12
(1,111)	1:20:A:TRP:HZ2	1:67:A:LEU:HB2	5	0.12
(1,111)	1:20:A:TRP:HZ2	1:67:A:LEU:HB3	5	0.12
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE1	10	0.12
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE2	10	0.12
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE1	10	0.12
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE2	10	0.12
(1,58)	1:96:A:MET:HB2	1:127:A:TYR:HD1	5	0.12
(1,58)	1:96:A:MET:HB2	1:127:A:TYR:HD2	5	0.12
(1,58)	1:96:A:MET:HB3	1:127:A:TYR:HD1	5	0.12
(1,58)	1:96:A:MET:HB3	1:127:A:TYR:HD2	5	0.12
(1,42)	1:50:A:LYS:HA	1:51:A:PHE:HD1	18	0.12
(1,42)	1:50:A:LYS:HA	1:51:A:PHE:HD2	18	0.12
(4,59)	1:206:A:TYR:H	1:202:A:GLY:O	20	0.11
(2,537)	1:118:A:GLU:CB	1:111:A:GLU:N	17	0.11
(2,206)	1:134:A:GLY:HA2	1:202:A:GLY:N	13	0.11
(2,206)	1:134:A:GLY:HA3	1:202:A:GLY:N	13	0.11
(2,68)	1:32:A:ASP:CB	1:205:A:GLU:N	9	0.11
(2,60)	1:32:A:ASP:CB	1:201:A:TYR:N	19	0.11
(1,5851)	1:113:A:GLU:H	1:113:A:GLU:HA	6	0.11
(1,5850)	1:113:A:GLU:HG3	1:113:A:GLU:H	14	0.11
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	1	0.11
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	11	0.11
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	15	0.11
(1,5848)	1:71:A:GLU:HB3	1:72:A:LEU:HG	16	0.11
(1,5835)	1:110:A:LYS:HA	1:110:A:LYS:H	8	0.11
(1,5835)	1:110:A:LYS:HA	1:110:A:LYS:H	12	0.11
(1,5809)	1:5:A:LEU:HG	1:2:A:ASP:HB2	16	0.11
(1,5809)	1:5:A:LEU:HG	1:2:A:ASP:HB3	16	0.11
(1,5808)	1:4:A:LEU:HA	1:4:A:LEU:HG	3	0.11
(1,5808)	1:4:A:LEU:HA	1:4:A:LEU:HG	13	0.11
(1,5799)	1:5:A:LEU:HG	1:2:A:ASP:HB2	16	0.11
(1,5799)	1:5:A:LEU:HG	1:2:A:ASP:HB3	16	0.11
(1,5789)	1:108:A:LYS:H	1:107:A:SER:HB2	15	0.11
(1,5789)	1:108:A:LYS:H	1:107:A:SER:HB3	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5789)	1:108:A:LYS:H	1:107:A:SER:HB2	18	0.11
(1,5789)	1:108:A:LYS:H	1:107:A:SER:HB3	18	0.11
(1,5670)	1:65:A:LEU:HB2	1:93:A:ASN:HD21	3	0.11
(1,5670)	1:65:A:LEU:HB2	1:93:A:ASN:HD22	3	0.11
(1,5670)	1:65:A:LEU:HB3	1:93:A:ASN:HD21	3	0.11
(1,5670)	1:65:A:LEU:HB3	1:93:A:ASN:HD22	3	0.11
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	1	0.11
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	12	0.11
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	19	0.11
(1,5546)	1:8:A:VAL:HB	1:8:A:VAL:H	15	0.11
(1,5497)	1:3:A:GLU:H	1:3:A:GLU:HB2	1	0.11
(1,5497)	1:3:A:GLU:H	1:3:A:GLU:HB3	1	0.11
(1,5497)	1:3:A:GLU:H	1:3:A:GLU:HB2	7	0.11
(1,5497)	1:3:A:GLU:H	1:3:A:GLU:HB3	7	0.11
(1,5497)	1:3:A:GLU:H	1:3:A:GLU:HB2	18	0.11
(1,5497)	1:3:A:GLU:H	1:3:A:GLU:HB3	18	0.11
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB2	16	0.11
(1,5496)	1:20:A:TRP:HE1	1:17:A:ARG:HB3	16	0.11
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	6	0.11
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	16	0.11
(1,5474)	1:196:A:TYR:H	1:194:A:THR:HB	20	0.11
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	10	0.11
(1,5473)	1:197:A:ARG:H	1:198:A:LYS:HA	15	0.11
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB2	5	0.11
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB3	5	0.11
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB2	15	0.11
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB3	15	0.11
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB2	19	0.11
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB3	19	0.11
(1,5428)	1:23:A:ALA:H	1:20:A:TRP:HZ3	7	0.11
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	9	0.11
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	9	0.11
(1,5361)	1:199:A:TYR:H	1:197:A:ARG:HB2	11	0.11
(1,5361)	1:199:A:TYR:H	1:197:A:ARG:HB3	11	0.11
(1,5355)	1:48:A:ASP:H	1:77:A:GLY:HA2	12	0.11
(1,5355)	1:48:A:ASP:H	1:77:A:GLY:HA3	12	0.11
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB2	5	0.11
(1,5350)	1:128:A:LYS:H	1:96:A:MET:HB3	5	0.11
(1,5314)	1:20:A:TRP:HE1	1:75:A:LYS:HG2	8	0.11
(1,5314)	1:20:A:TRP:HE1	1:75:A:LYS:HG3	8	0.11
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG2	1	0.11
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5292)	1:18:A:THR:H	1:19:A:GLU:HG2	8	0.11
(1,5292)	1:18:A:THR:H	1:19:A:GLU:HG3	8	0.11
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	18	0.11
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	19	0.11
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB2	17	0.11
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB3	17	0.11
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD21	3	0.11
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD22	3	0.11
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD21	6	0.11
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD22	6	0.11
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG11	17	0.11
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG12	17	0.11
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG13	17	0.11
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG21	17	0.11
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG22	17	0.11
(1,5238)	1:10:A:SER:H	1:8:A:VAL:HG23	17	0.11
(1,5233)	1:1:A:ASN:HD21	1:61:A:GLU:HG2	16	0.11
(1,5233)	1:1:A:ASN:HD21	1:61:A:GLU:HG3	16	0.11
(1,5226)	1:82:A:SER:H	1:79:A:GLN:HA	19	0.11
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB1	6	0.11
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB2	6	0.11
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB3	6	0.11
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB1	13	0.11
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB2	13	0.11
(1,5220)	1:185:A:ASN:H	1:188:A:ALA:HB3	13	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD11	7	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD12	7	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD13	7	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD21	7	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD22	7	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD23	7	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD11	10	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD12	10	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD13	10	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD21	10	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD22	10	0.11
(1,5140)	1:72:A:LEU:H	1:72:A:LEU:HD23	10	0.11
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG11	1	0.11
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG12	1	0.11
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG13	1	0.11
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG21	1	0.11
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG22	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG23	1	0.11
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG11	6	0.11
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG12	6	0.11
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG13	6	0.11
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG21	6	0.11
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG22	6	0.11
(1,5137)	1:7:A:LYS:H	1:9:A:VAL:HG23	6	0.11
(1,5136)	1:7:A:LYS:H	1:25:A:VAL:HG11	20	0.11
(1,5136)	1:7:A:LYS:H	1:25:A:VAL:HG12	20	0.11
(1,5136)	1:7:A:LYS:H	1:25:A:VAL:HG13	20	0.11
(1,5136)	1:7:A:LYS:H	1:25:A:VAL:HG21	20	0.11
(1,5136)	1:7:A:LYS:H	1:25:A:VAL:HG22	20	0.11
(1,5136)	1:7:A:LYS:H	1:25:A:VAL:HG23	20	0.11
(1,5107)	1:139:A:LYS:H	1:138:A:ASN:HB2	6	0.11
(1,5107)	1:139:A:LYS:H	1:138:A:ASN:HB3	6	0.11
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD11	16	0.11
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD12	16	0.11
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD13	16	0.11
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD21	16	0.11
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD22	16	0.11
(1,5066)	1:179:A:LEU:H	1:179:A:LEU:HD23	16	0.11
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD11	7	0.11
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD12	7	0.11
(1,5064)	1:100:A:GLU:H	1:101:A:ILE:HD13	7	0.11
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG2	18	0.11
(1,5053)	1:78:A:LEU:H	1:80:A:LYS:HG3	18	0.11
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	1	0.11
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	1	0.11
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	3	0.11
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	3	0.11
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	10	0.11
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	10	0.11
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB2	17	0.11
(1,5049)	1:58:A:ASP:H	1:57:A:LYS:HB3	17	0.11
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG2	6	0.11
(1,4985)	1:19:A:GLU:H	1:16:A:GLU:HG3	6	0.11
(1,4970)	1:64:A:ILE:H	1:62:A:VAL:HA	9	0.11
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG11	17	0.11
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG12	17	0.11
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG13	17	0.11
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG21	17	0.11
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG22	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4938)	1:148:A:LEU:H	1:142:A:VAL:HG23	17	0.11
(1,4923)	1:14:A:ALA:H	1:14:A:ALA:HA	10	0.11
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	5	0.11
(1,4857)	1:89:A:VAL:H	1:95:A:LYS:H	13	0.11
(1,4788)	1:146:A:LYS:HG2	1:146:A:LYS:H	8	0.11
(1,4788)	1:146:A:LYS:HG3	1:146:A:LYS:H	8	0.11
(1,4775)	1:60:A:LYS:HG2	1:59:A:ILE:H	8	0.11
(1,4775)	1:60:A:LYS:HG3	1:59:A:ILE:H	8	0.11
(1,4745)	1:177:A:MET:HA	1:174:A:GLN:HE21	8	0.11
(1,4745)	1:177:A:MET:HA	1:174:A:GLN:HE22	8	0.11
(1,4659)	1:42:A:LEU:HB2	1:29:A:SER:H	7	0.11
(1,4659)	1:42:A:LEU:HB3	1:29:A:SER:H	7	0.11
(1,4583)	1:98:A:ILE:HD11	1:121:A:ASN:H	1	0.11
(1,4583)	1:98:A:ILE:HD12	1:121:A:ASN:H	1	0.11
(1,4583)	1:98:A:ILE:HD13	1:121:A:ASN:H	1	0.11
(1,4583)	1:98:A:ILE:HD11	1:121:A:ASN:H	6	0.11
(1,4583)	1:98:A:ILE:HD12	1:121:A:ASN:H	6	0.11
(1,4583)	1:98:A:ILE:HD13	1:121:A:ASN:H	6	0.11
(1,4502)	1:133:A:ARG:HE	1:202:A:GLY:H	2	0.11
(1,4480)	1:56:A:ARG:H	1:56:A:ARG:HE	12	0.11
(1,4433)	1:199:A:TYR:HB2	1:196:A:TYR:H	7	0.11
(1,4433)	1:199:A:TYR:HB3	1:196:A:TYR:H	7	0.11
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	4	0.11
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	4	0.11
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	4	0.11
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	10	0.11
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	10	0.11
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	10	0.11
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	16	0.11
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	16	0.11
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	16	0.11
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	20	0.11
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	20	0.11
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	20	0.11
(1,3979)	1:38:A:LYS:HG2	1:38:A:LYS:H	3	0.11
(1,3979)	1:38:A:LYS:HG3	1:38:A:LYS:H	3	0.11
(1,3868)	1:102:A:LEU:HB2	1:103:A:GLU:H	7	0.11
(1,3868)	1:102:A:LEU:HB3	1:103:A:GLU:H	7	0.11
(1,3868)	1:102:A:LEU:HB2	1:103:A:GLU:H	19	0.11
(1,3868)	1:102:A:LEU:HB3	1:103:A:GLU:H	19	0.11
(1,3774)	1:43:A:VAL:HG11	1:24:A:LEU:H	6	0.11
(1,3774)	1:43:A:VAL:HG12	1:24:A:LEU:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3774)	1:43:A:VAL:HG13	1:24:A:LEU:H	6	0.11
(1,3774)	1:43:A:VAL:HG21	1:24:A:LEU:H	6	0.11
(1,3774)	1:43:A:VAL:HG22	1:24:A:LEU:H	6	0.11
(1,3774)	1:43:A:VAL:HG23	1:24:A:LEU:H	6	0.11
(1,3747)	1:221:A:GLU:HG2	1:222:A:LEU:H	11	0.11
(1,3747)	1:221:A:GLU:HG3	1:222:A:LEU:H	11	0.11
(1,3676)	1:142:A:VAL:HG11	1:143:A:LEU:H	6	0.11
(1,3676)	1:142:A:VAL:HG12	1:143:A:LEU:H	6	0.11
(1,3676)	1:142:A:VAL:HG13	1:143:A:LEU:H	6	0.11
(1,3676)	1:142:A:VAL:HG21	1:143:A:LEU:H	6	0.11
(1,3676)	1:142:A:VAL:HG22	1:143:A:LEU:H	6	0.11
(1,3676)	1:142:A:VAL:HG23	1:143:A:LEU:H	6	0.11
(1,3524)	1:198:A:LYS:H	1:197:A:ARG:HD2	14	0.11
(1,3524)	1:198:A:LYS:H	1:197:A:ARG:HD3	14	0.11
(1,3507)	1:67:A:LEU:H	1:65:A:LEU:HB2	19	0.11
(1,3507)	1:67:A:LEU:H	1:65:A:LEU:HB3	19	0.11
(1,3486)	1:2:A:ASP:H	1:1:A:ASN:HB2	7	0.11
(1,3486)	1:2:A:ASP:H	1:1:A:ASN:HB3	7	0.11
(1,3310)	1:138:A:ASN:HB2	1:139:A:LYS:HB2	5	0.11
(1,3310)	1:138:A:ASN:HB2	1:139:A:LYS:HB3	5	0.11
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG12	14	0.11
(1,3274)	1:64:A:ILE:HA	1:64:A:ILE:HG13	14	0.11
(1,3270)	1:80:A:LYS:HA	1:83:A:ILE:HG12	17	0.11
(1,3270)	1:80:A:LYS:HA	1:83:A:ILE:HG13	17	0.11
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD11	5	0.11
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD12	5	0.11
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD13	5	0.11
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD21	5	0.11
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD22	5	0.11
(1,3253)	1:65:A:LEU:HA	1:72:A:LEU:HD23	5	0.11
(1,3236)	1:17:A:ARG:HA	1:17:A:ARG:HD2	17	0.11
(1,3236)	1:17:A:ARG:HA	1:17:A:ARG:HD3	17	0.11
(1,3201)	1:2:A:ASP:HA	1:5:A:LEU:HG	7	0.11
(1,3097)	1:177:A:MET:H	1:174:A:GLN:HG2	3	0.11
(1,3097)	1:177:A:MET:H	1:174:A:GLN:HG3	3	0.11
(1,3096)	1:19:A:GLU:H	1:16:A:GLU:HG2	6	0.11
(1,3096)	1:19:A:GLU:H	1:16:A:GLU:HG3	6	0.11
(1,3084)	1:38:A:LYS:H	1:38:A:LYS:HG2	3	0.11
(1,3084)	1:38:A:LYS:H	1:38:A:LYS:HG3	3	0.11
(1,3071)	1:143:A:LEU:H	1:142:A:VAL:HG11	6	0.11
(1,3071)	1:143:A:LEU:H	1:142:A:VAL:HG12	6	0.11
(1,3071)	1:143:A:LEU:H	1:142:A:VAL:HG13	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3071)	1:143:A:LEU:H	1:142:A:VAL:HG21	6	0.11
(1,3071)	1:143:A:LEU:H	1:142:A:VAL:HG22	6	0.11
(1,3071)	1:143:A:LEU:H	1:142:A:VAL:HG23	6	0.11
(1,3051)	1:34:A:ILE:HG23	1:53:A:SER:HA	9	0.11
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD2	13	0.11
(1,3037)	1:146:A:LYS:HG2	1:182:A:PRO:HD3	13	0.11
(1,2988)	1:86:A:LYS:HG2	1:86:A:LYS:HA	15	0.11
(1,2973)	1:85:A:LEU:HB2	1:82:A:SER:HA	7	0.11
(1,2973)	1:85:A:LEU:HB2	1:82:A:SER:HA	18	0.11
(1,2917)	1:196:A:TYR:HA	1:201:A:TYR:H	4	0.11
(1,2887)	1:101:A:ILE:HB	1:99:A:SER:H	7	0.11
(1,2868)	1:157:A:VAL:HA	1:160:A:GLN:HA	9	0.11
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG21	2	0.11
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG22	2	0.11
(1,2863)	1:48:A:ASP:HA	1:47:A:ILE:HG23	2	0.11
(1,2839)	1:11:A:VAL:HG22	1:23:A:ALA:HA	3	0.11
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD11	3	0.11
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD12	3	0.11
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD13	3	0.11
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD21	3	0.11
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD22	3	0.11
(1,2824)	1:6:A:GLY:HA3	1:5:A:LEU:HD23	3	0.11
(1,2726)	1:61:A:GLU:HG3	1:60:A:LYS:HB2	19	0.11
(1,2726)	1:61:A:GLU:HG3	1:60:A:LYS:HB3	19	0.11
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB2	2	0.11
(1,2685)	1:67:A:LEU:HD12	1:71:A:GLU:HB3	2	0.11
(1,2645)	1:54:A:ILE:HG23	1:41:A:CYS:HB2	19	0.11
(1,2645)	1:54:A:ILE:HG23	1:41:A:CYS:HB3	19	0.11
(1,2639)	1:11:A:VAL:HG21	1:10:A:SER:HB2	16	0.11
(1,2639)	1:11:A:VAL:HG21	1:10:A:SER:HB3	16	0.11
(1,2636)	1:65:A:LEU:HD11	1:66:A:ASN:HB2	8	0.11
(1,2636)	1:65:A:LEU:HD11	1:66:A:ASN:HB3	8	0.11
(1,2630)	1:47:A:ILE:HD11	1:21:A:TYR:HB2	1	0.11
(1,2630)	1:47:A:ILE:HD11	1:21:A:TYR:HB3	1	0.11
(1,2562)	1:72:A:LEU:HG	1:69:A:GLU:HA	7	0.11
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	3	0.11
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	4	0.11
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	9	0.11
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	13	0.11
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	19	0.11
(1,2554)	1:175:A:ILE:HD12	1:153:A:LEU:HA	17	0.11
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2502)	1:42:A:LEU:HG	1:27:A:SER:HA	16	0.11
(1,2474)	1:101:A:ILE:HD13	1:127:A:TYR:HD1	8	0.11
(1,2474)	1:101:A:ILE:HD13	1:127:A:TYR:HD2	8	0.11
(1,2443)	1:83:A:ILE:HD13	1:83:A:ILE:H	1	0.11
(1,2443)	1:83:A:ILE:HD13	1:83:A:ILE:H	2	0.11
(1,2418)	1:200:A:LEU:HD12	1:153:A:LEU:H	9	0.11
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG2	6	0.11
(1,2415)	1:19:A:GLU:H	1:16:A:GLU:HG3	6	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	9	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	9	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	9	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	9	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	9	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	9	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	10	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	10	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	10	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	10	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	10	0.11
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	10	0.11
(1,2327)	1:160:A:GLN:HA	1:157:A:VAL:HA	9	0.11
(1,2314)	1:88:A:ARG:HA	1:94:A:TRP:HD1	4	0.11
(1,2289)	1:119:A:ARG:HA	1:117:A:GLU:H	10	0.11
(1,2165)	1:126:A:LEU:HB2	1:137:A:ILE:HD11	15	0.11
(1,2165)	1:126:A:LEU:HB2	1:137:A:ILE:HD12	15	0.11
(1,2165)	1:126:A:LEU:HB2	1:137:A:ILE:HD13	15	0.11
(1,2165)	1:126:A:LEU:HB3	1:137:A:ILE:HD11	15	0.11
(1,2165)	1:126:A:LEU:HB3	1:137:A:ILE:HD12	15	0.11
(1,2165)	1:126:A:LEU:HB3	1:137:A:ILE:HD13	15	0.11
(1,2130)	1:142:A:VAL:HA	1:142:A:VAL:HB	15	0.11
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD11	12	0.11
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD12	12	0.11
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD13	12	0.11
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD11	20	0.11
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD12	20	0.11
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD13	20	0.11
(1,1931)	1:160:A:GLN:HE21	1:175:A:ILE:HD11	20	0.11
(1,1931)	1:160:A:GLN:HE21	1:175:A:ILE:HD12	20	0.11
(1,1931)	1:160:A:GLN:HE21	1:175:A:ILE:HD13	20	0.11
(1,1931)	1:160:A:GLN:HE22	1:175:A:ILE:HD11	20	0.11
(1,1931)	1:160:A:GLN:HE22	1:175:A:ILE:HD12	20	0.11
(1,1931)	1:160:A:GLN:HE22	1:175:A:ILE:HD13	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1926)	1:172:A:TRP:HD1	1:157:A:VAL:HG11	10	0.11
(1,1926)	1:172:A:TRP:HD1	1:157:A:VAL:HG12	10	0.11
(1,1926)	1:172:A:TRP:HD1	1:157:A:VAL:HG13	10	0.11
(1,1926)	1:172:A:TRP:HD1	1:157:A:VAL:HG21	10	0.11
(1,1926)	1:172:A:TRP:HD1	1:157:A:VAL:HG22	10	0.11
(1,1926)	1:172:A:TRP:HD1	1:157:A:VAL:HG23	10	0.11
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	3	0.11
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	9	0.11
(1,1868)	1:11:A:VAL:HA	1:59:A:ILE:HB	12	0.11
(1,1754)	1:101:A:ILE:HD11	1:96:A:MET:HE1	17	0.11
(1,1754)	1:101:A:ILE:HD11	1:96:A:MET:HE2	17	0.11
(1,1754)	1:101:A:ILE:HD11	1:96:A:MET:HE3	17	0.11
(1,1754)	1:101:A:ILE:HD12	1:96:A:MET:HE1	17	0.11
(1,1754)	1:101:A:ILE:HD12	1:96:A:MET:HE2	17	0.11
(1,1754)	1:101:A:ILE:HD12	1:96:A:MET:HE3	17	0.11
(1,1754)	1:101:A:ILE:HD13	1:96:A:MET:HE1	17	0.11
(1,1754)	1:101:A:ILE:HD13	1:96:A:MET:HE2	17	0.11
(1,1754)	1:101:A:ILE:HD13	1:96:A:MET:HE3	17	0.11
(1,1646)	1:166:A:ILE:HG12	1:175:A:ILE:HD11	2	0.11
(1,1646)	1:166:A:ILE:HG12	1:175:A:ILE:HD12	2	0.11
(1,1646)	1:166:A:ILE:HG12	1:175:A:ILE:HD13	2	0.11
(1,1646)	1:166:A:ILE:HG13	1:175:A:ILE:HD11	2	0.11
(1,1646)	1:166:A:ILE:HG13	1:175:A:ILE:HD12	2	0.11
(1,1646)	1:166:A:ILE:HG13	1:175:A:ILE:HD13	2	0.11
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD11	3	0.11
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD12	3	0.11
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD13	3	0.11
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD21	3	0.11
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD22	3	0.11
(1,1459)	1:147:A:ASP:HB2	1:148:A:LEU:HD23	3	0.11
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD11	3	0.11
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD12	3	0.11
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD13	3	0.11
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD21	3	0.11
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD22	3	0.11
(1,1459)	1:147:A:ASP:HB3	1:148:A:LEU:HD23	3	0.11
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD2	6	0.11
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD3	6	0.11
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD2	6	0.11
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD3	6	0.11
(1,1370)	1:6:A:GLY:HA2	1:24:A:LEU:HD11	19	0.11
(1,1370)	1:6:A:GLY:HA2	1:24:A:LEU:HD12	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1370)	1:6:A:GLY:HA2	1:24:A:LEU:HD13	19	0.11
(1,1370)	1:6:A:GLY:HA2	1:24:A:LEU:HD21	19	0.11
(1,1370)	1:6:A:GLY:HA2	1:24:A:LEU:HD22	19	0.11
(1,1370)	1:6:A:GLY:HA2	1:24:A:LEU:HD23	19	0.11
(1,1370)	1:6:A:GLY:HA3	1:24:A:LEU:HD11	19	0.11
(1,1370)	1:6:A:GLY:HA3	1:24:A:LEU:HD12	19	0.11
(1,1370)	1:6:A:GLY:HA3	1:24:A:LEU:HD13	19	0.11
(1,1370)	1:6:A:GLY:HA3	1:24:A:LEU:HD21	19	0.11
(1,1370)	1:6:A:GLY:HA3	1:24:A:LEU:HD22	19	0.11
(1,1370)	1:6:A:GLY:HA3	1:24:A:LEU:HD23	19	0.11
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG11	6	0.11
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG12	6	0.11
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG13	6	0.11
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG21	6	0.11
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG22	6	0.11
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG23	6	0.11
(1,1150)	1:91:A:PRO:HA	1:92:A:ASP:HB2	15	0.11
(1,1150)	1:91:A:PRO:HA	1:92:A:ASP:HB3	15	0.11
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG11	4	0.11
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG12	4	0.11
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG13	4	0.11
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG21	4	0.11
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG22	4	0.11
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG23	4	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG11	4	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG12	4	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG13	4	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG21	4	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG22	4	0.11
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG23	4	0.11
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD11	12	0.11
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD12	12	0.11
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD13	12	0.11
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD21	12	0.11
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD22	12	0.11
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD23	12	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD11	12	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD12	12	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD13	12	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD21	12	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD22	12	0.11
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD23	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	8	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	8	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	8	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	8	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	8	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	8	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	9	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	9	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	9	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	9	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	9	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	9	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	11	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	11	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	11	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	11	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	11	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	11	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	12	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	12	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	12	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	12	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	12	0.11
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	12	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	8	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	8	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	8	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	8	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	8	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	8	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	9	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	9	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	9	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	9	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	9	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	9	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	11	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	11	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	11	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	11	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	11	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	12	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	12	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	12	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	12	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	12	0.11
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	12	0.11
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD11	16	0.11
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD12	16	0.11
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD13	16	0.11
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD11	16	0.11
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD12	16	0.11
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD13	16	0.11
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD11	17	0.11
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD12	17	0.11
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD13	17	0.11
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD11	17	0.11
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD12	17	0.11
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD13	17	0.11
(1,909)	1:96:A:MET:H	1:96:A:MET:HE1	6	0.11
(1,909)	1:96:A:MET:H	1:96:A:MET:HE2	6	0.11
(1,909)	1:96:A:MET:H	1:96:A:MET:HE3	6	0.11
(1,896)	1:146:A:LYS:H	1:146:A:LYS:HG2	8	0.11
(1,896)	1:146:A:LYS:H	1:146:A:LYS:HG3	8	0.11
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE1	7	0.11
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE2	7	0.11
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE3	7	0.11
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE1	12	0.11
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE2	12	0.11
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE3	12	0.11
(1,829)	1:129:A:PHE:H	1:96:A:MET:HE1	15	0.11
(1,829)	1:129:A:PHE:H	1:96:A:MET:HE2	15	0.11
(1,829)	1:129:A:PHE:H	1:96:A:MET:HE3	15	0.11
(1,725)	1:210:A:ALA:H	1:212:A:ILE:HB	10	0.11
(1,725)	1:210:A:ALA:H	1:212:A:ILE:HB	17	0.11
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG21	12	0.11
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG22	12	0.11
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG23	12	0.11
(1,687)	1:2:A:ASP:H	1:61:A:GLU:HB2	3	0.11
(1,687)	1:2:A:ASP:H	1:61:A:GLU:HB3	3	0.11
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB2	3	0.11
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB3	3	0.11
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:35:A:THR:H	1:28:A:PRO:HB3	5	0.11
(1,627)	1:10:A:SER:H	1:62:A:VAL:HB	5	0.11
(1,566)	1:54:A:ILE:H	1:36:A:VAL:HG11	14	0.11
(1,566)	1:54:A:ILE:H	1:36:A:VAL:HG12	14	0.11
(1,566)	1:54:A:ILE:H	1:36:A:VAL:HG13	14	0.11
(1,566)	1:54:A:ILE:H	1:36:A:VAL:HG21	14	0.11
(1,566)	1:54:A:ILE:H	1:36:A:VAL:HG22	14	0.11
(1,566)	1:54:A:ILE:H	1:36:A:VAL:HG23	14	0.11
(1,511)	1:47:A:ILE:HG12	1:21:A:TYR:HA	13	0.11
(1,511)	1:47:A:ILE:HG13	1:21:A:TYR:HA	13	0.11
(1,362)	1:150:A:LEU:HG	1:119:A:ARG:HA	6	0.11
(1,353)	1:145:A:TYR:HD1	1:145:A:TYR:HA	16	0.11
(1,353)	1:145:A:TYR:HD2	1:145:A:TYR:HA	16	0.11
(1,279)	1:199:A:TYR:HD1	1:137:A:ILE:HA	18	0.11
(1,279)	1:199:A:TYR:HD2	1:137:A:ILE:HA	18	0.11
(1,263)	1:137:A:ILE:HG12	1:136:A:PRO:HA	4	0.11
(1,263)	1:137:A:ILE:HG13	1:136:A:PRO:HA	4	0.11
(1,249)	1:133:A:ARG:H	1:136:A:PRO:HA	8	0.11
(1,175)	1:190:A:TYR:HA	1:190:A:TYR:HD1	11	0.11
(1,175)	1:190:A:TYR:HA	1:190:A:TYR:HD2	11	0.11
(1,175)	1:190:A:TYR:HA	1:190:A:TYR:HD1	19	0.11
(1,175)	1:190:A:TYR:HA	1:190:A:TYR:HD2	19	0.11
(1,113)	1:176:A:TYR:HD2	1:182:A:PRO:HA	7	0.11
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE1	4	0.11
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE2	4	0.11
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE1	4	0.11
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE2	4	0.11
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE1	9	0.11
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE2	9	0.11
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE1	9	0.11
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE2	9	0.11
(1,32)	1:145:A:TYR:H	1:145:A:TYR:HD1	8	0.11
(1,32)	1:145:A:TYR:H	1:145:A:TYR:HD2	8	0.11
(4,65)	1:209:A:SER:H	1:205:A:GLU:O	12	0.1
(4,63)	1:208:A:ARG:H	1:204:A:GLU:O	4	0.1
(4,59)	1:206:A:TYR:H	1:202:A:GLY:O	15	0.1
(2,132)	1:93:A:ASN:CB	1:75:A:LYS:N	6	0.1
(2,122)	1:93:A:ASN:CB	1:70:A:SER:N	19	0.1
(2,118)	1:93:A:ASN:CB	1:67:A:LEU:N	6	0.1
(2,54)	1:32:A:ASP:CB	1:198:A:LYS:N	10	0.1
(2,36)	1:4:A:LEU:CB	1:210:A:ALA:N	2	0.1
(1,5813)	1:108:A:LYS:HG2	1:106:A:SER:HB2	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5813)	1:108:A:LYS:HG2	1:106:A:SER:HB3	2	0.1
(1,5813)	1:108:A:LYS:HG3	1:106:A:SER:HB2	2	0.1
(1,5813)	1:108:A:LYS:HG3	1:106:A:SER:HB3	2	0.1
(1,5808)	1:4:A:LEU:HA	1:4:A:LEU:HG	8	0.1
(1,5592)	1:43:A:VAL:HG12	1:44:A:ARG:H	6	0.1
(1,5579)	1:34:A:ILE:HA	1:33:A:ASP:H	8	0.1
(1,5573)	1:145:A:TYR:HD2	1:146:A:LYS:H	3	0.1
(1,5508)	1:61:A:GLU:H	1:10:A:SER:HB2	2	0.1
(1,5508)	1:61:A:GLU:H	1:10:A:SER:HB3	2	0.1
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE2	9	0.1
(1,5491)	1:37:A:LYS:H	1:37:A:LYS:HE3	9	0.1
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB2	13	0.1
(1,5451)	1:126:A:LEU:H	1:122:A:PHE:HB3	13	0.1
(1,5413)	1:170:A:ALA:H	1:168:A:SER:H	12	0.1
(1,5397)	1:127:A:TYR:H	1:137:A:ILE:HG12	20	0.1
(1,5397)	1:127:A:TYR:H	1:137:A:ILE:HG13	20	0.1
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG2	4	0.1
(1,5383)	1:74:A:THR:H	1:71:A:GLU:HG3	4	0.1
(1,5382)	1:74:A:THR:H	1:71:A:GLU:HG2	4	0.1
(1,5382)	1:74:A:THR:H	1:71:A:GLU:HG3	4	0.1
(1,5356)	1:48:A:ASP:H	1:44:A:ARG:HG2	4	0.1
(1,5356)	1:48:A:ASP:H	1:44:A:ARG:HG3	4	0.1
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG2	2	0.1
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG3	2	0.1
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG2	18	0.1
(1,5292)	1:18:A:THR:H	1:16:A:GLU:HG3	18	0.1
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	4	0.1
(1,5283)	1:15:A:THR:H	1:15:A:THR:HA	13	0.1
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB2	13	0.1
(1,5275)	1:74:A:THR:H	1:71:A:GLU:HB3	13	0.1
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD21	7	0.1
(1,5244)	1:189:A:SER:H	1:191:A:ASN:HD22	7	0.1
(1,5151)	1:105:A:SER:H	1:105:A:SER:HB2	11	0.1
(1,5151)	1:105:A:SER:H	1:105:A:SER:HB3	11	0.1
(1,5145)	1:52:A:TYR:HD2	1:52:A:TYR:H	17	0.1
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD11	1	0.1
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD12	1	0.1
(1,5135)	1:99:A:SER:H	1:101:A:ILE:HD13	1	0.1
(1,5070)	1:40:A:GLN:H	1:56:A:ARG:H	7	0.1
(1,4956)	1:178:A:ASP:H	1:175:A:ILE:HG12	5	0.1
(1,4956)	1:178:A:ASP:H	1:175:A:ILE:HG13	5	0.1
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4911)	1:172:A:TRP:HE1	1:166:A:ILE:HA	15	0.1
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD2	6	0.1
(1,4908)	1:20:A:TRP:HE1	1:60:A:LYS:HD3	6	0.1
(1,4904)	1:109:A:ASP:HB2	1:110:A:LYS:H	11	0.1
(1,4904)	1:109:A:ASP:HB3	1:110:A:LYS:H	11	0.1
(1,4902)	1:91:A:PRO:HD2	1:93:A:ASN:HD21	4	0.1
(1,4902)	1:91:A:PRO:HD2	1:93:A:ASN:HD22	4	0.1
(1,4902)	1:91:A:PRO:HD3	1:93:A:ASN:HD21	4	0.1
(1,4902)	1:91:A:PRO:HD3	1:93:A:ASN:HD22	4	0.1
(1,4583)	1:98:A:ILE:HD11	1:121:A:ASN:H	2	0.1
(1,4583)	1:98:A:ILE:HD12	1:121:A:ASN:H	2	0.1
(1,4583)	1:98:A:ILE:HD13	1:121:A:ASN:H	2	0.1
(1,4583)	1:98:A:ILE:HD11	1:121:A:ASN:H	15	0.1
(1,4583)	1:98:A:ILE:HD12	1:121:A:ASN:H	15	0.1
(1,4583)	1:98:A:ILE:HD13	1:121:A:ASN:H	15	0.1
(1,4528)	1:205:A:GLU:HB2	1:29:A:SER:H	10	0.1
(1,4528)	1:205:A:GLU:HB3	1:29:A:SER:H	10	0.1
(1,4502)	1:133:A:ARG:HE	1:202:A:GLY:H	13	0.1
(1,4494)	1:177:A:MET:HG2	1:180:A:GLY:H	13	0.1
(1,4494)	1:177:A:MET:HG3	1:180:A:GLY:H	13	0.1
(1,4341)	1:177:A:MET:HE1	1:180:A:GLY:H	10	0.1
(1,4341)	1:177:A:MET:HE2	1:180:A:GLY:H	10	0.1
(1,4341)	1:177:A:MET:HE3	1:180:A:GLY:H	10	0.1
(1,4277)	1:170:A:ALA:HB1	1:168:A:SER:H	5	0.1
(1,4277)	1:170:A:ALA:HB2	1:168:A:SER:H	5	0.1
(1,4277)	1:170:A:ALA:HB3	1:168:A:SER:H	5	0.1
(1,4092)	1:175:A:ILE:HG21	1:159:A:HIS:H	14	0.1
(1,4092)	1:175:A:ILE:HG22	1:159:A:HIS:H	14	0.1
(1,4092)	1:175:A:ILE:HG23	1:159:A:HIS:H	14	0.1
(1,3927)	1:46:A:PHE:HE1	1:80:A:LYS:H	15	0.1
(1,3927)	1:46:A:PHE:HE2	1:80:A:LYS:H	15	0.1
(1,3871)	1:198:A:LYS:HB2	1:201:A:TYR:H	14	0.1
(1,3871)	1:198:A:LYS:HB3	1:201:A:TYR:H	14	0.1
(1,3869)	1:153:A:LEU:HG	1:179:A:LEU:H	4	0.1
(1,3869)	1:153:A:LEU:HG	1:179:A:LEU:H	12	0.1
(1,3845)	1:109:A:ASP:HB2	1:110:A:LYS:H	11	0.1
(1,3845)	1:109:A:ASP:HB3	1:110:A:LYS:H	11	0.1
(1,3821)	1:222:A:LEU:HA	1:223:A:GLU:H	19	0.1
(1,3619)	1:15:A:THR:HG21	1:14:A:ALA:H	8	0.1
(1,3619)	1:15:A:THR:HG22	1:14:A:ALA:H	8	0.1
(1,3619)	1:15:A:THR:HG23	1:14:A:ALA:H	8	0.1
(1,3619)	1:15:A:THR:HG21	1:14:A:ALA:H	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3619)	1:15:A:THR:HG22	1:14:A:ALA:H	19	0.1
(1,3619)	1:15:A:THR:HG23	1:14:A:ALA:H	19	0.1
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB2	2	0.1
(1,3481)	1:175:A:ILE:HA	1:177:A:MET:HB3	2	0.1
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG11	3	0.1
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG12	3	0.1
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG13	3	0.1
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG21	3	0.1
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG22	3	0.1
(1,3409)	1:64:A:ILE:HG12	1:62:A:VAL:HG23	3	0.1
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE2	14	0.1
(1,3390)	1:87:A:THR:HG21	1:86:A:LYS:HE3	14	0.1
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE2	14	0.1
(1,3390)	1:87:A:THR:HG22	1:86:A:LYS:HE3	14	0.1
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE2	14	0.1
(1,3390)	1:87:A:THR:HG23	1:86:A:LYS:HE3	14	0.1
(1,3381)	1:72:A:LEU:HB2	1:79:A:GLN:HG2	1	0.1
(1,3381)	1:72:A:LEU:HB2	1:79:A:GLN:HG3	1	0.1
(1,3381)	1:72:A:LEU:HB3	1:79:A:GLN:HG2	1	0.1
(1,3381)	1:72:A:LEU:HB3	1:79:A:GLN:HG3	1	0.1
(1,3201)	1:2:A:ASP:HA	1:5:A:LEU:HG	16	0.1
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD11	16	0.1
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD12	16	0.1
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD13	16	0.1
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD21	16	0.1
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD22	16	0.1
(1,3102)	1:87:A:THR:H	1:85:A:LEU:HD23	16	0.1
(1,3069)	1:14:A:ALA:H	1:15:A:THR:HG21	19	0.1
(1,3069)	1:14:A:ALA:H	1:15:A:THR:HG22	19	0.1
(1,3069)	1:14:A:ALA:H	1:15:A:THR:HG23	19	0.1
(1,2841)	1:166:A:ILE:HD13	1:157:A:VAL:H	6	0.1
(1,2804)	1:171:A:VAL:HG13	1:175:A:ILE:HD11	9	0.1
(1,2804)	1:171:A:VAL:HG13	1:175:A:ILE:HD12	9	0.1
(1,2804)	1:171:A:VAL:HG13	1:175:A:ILE:HD13	9	0.1
(1,2718)	1:90:A:VAL:HG12	1:65:A:LEU:HG	10	0.1
(1,2645)	1:54:A:ILE:HG23	1:41:A:CYS:HB2	3	0.1
(1,2645)	1:54:A:ILE:HG23	1:41:A:CYS:HB3	3	0.1
(1,2639)	1:11:A:VAL:HG11	1:20:A:TRP:HB2	11	0.1
(1,2639)	1:11:A:VAL:HG11	1:20:A:TRP:HB3	11	0.1
(1,2564)	1:157:A:VAL:HG12	1:153:A:LEU:HA	15	0.1
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	15	0.1
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2561)	1:65:A:LEU:HG	1:65:A:LEU:HA	18	0.1
(1,2546)	1:222:A:LEU:HG	1:222:A:LEU:HA	9	0.1
(1,2435)	1:153:A:LEU:HG	1:179:A:LEU:H	4	0.1
(1,2435)	1:153:A:LEU:HG	1:179:A:LEU:H	12	0.1
(1,2428)	1:64:A:ILE:HD13	1:65:A:LEU:H	7	0.1
(1,2398)	1:9:A:VAL:HG22	1:10:A:SER:H	9	0.1
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD11	7	0.1
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD12	7	0.1
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD13	7	0.1
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD21	7	0.1
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD22	7	0.1
(1,2360)	1:66:A:ASN:HA	1:65:A:LEU:HD23	7	0.1
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG11	5	0.1
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG12	5	0.1
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG13	5	0.1
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG21	5	0.1
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG22	5	0.1
(1,2349)	1:20:A:TRP:HA	1:12:A:VAL:HG23	5	0.1
(1,2289)	1:119:A:ARG:HA	1:117:A:GLU:H	9	0.1
(1,2188)	1:119:A:ARG:HB2	1:116:A:PRO:HA	1	0.1
(1,2188)	1:119:A:ARG:HB3	1:116:A:PRO:HA	1	0.1
(1,2174)	1:151:A:PHE:HD1	1:122:A:PHE:HA	9	0.1
(1,2174)	1:151:A:PHE:HD2	1:122:A:PHE:HA	9	0.1
(1,2139)	1:223:A:GLU:H	1:222:A:LEU:HA	19	0.1
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD11	20	0.1
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD12	20	0.1
(1,2050)	1:201:A:TYR:H	1:137:A:ILE:HD13	20	0.1
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD11	6	0.1
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD12	6	0.1
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD13	6	0.1
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD11	16	0.1
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD12	16	0.1
(1,1933)	1:196:A:TYR:H	1:175:A:ILE:HD13	16	0.1
(1,1469)	1:165:A:ASN:HB2	1:171:A:VAL:HG11	2	0.1
(1,1469)	1:165:A:ASN:HB2	1:171:A:VAL:HG12	2	0.1
(1,1469)	1:165:A:ASN:HB2	1:171:A:VAL:HG13	2	0.1
(1,1469)	1:165:A:ASN:HB2	1:171:A:VAL:HG21	2	0.1
(1,1469)	1:165:A:ASN:HB2	1:171:A:VAL:HG22	2	0.1
(1,1469)	1:165:A:ASN:HB2	1:171:A:VAL:HG23	2	0.1
(1,1469)	1:165:A:ASN:HB3	1:171:A:VAL:HG11	2	0.1
(1,1469)	1:165:A:ASN:HB3	1:171:A:VAL:HG12	2	0.1
(1,1469)	1:165:A:ASN:HB3	1:171:A:VAL:HG13	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1469)	1:165:A:ASN:HB3	1:171:A:VAL:HG21	2	0.1
(1,1469)	1:165:A:ASN:HB3	1:171:A:VAL:HG22	2	0.1
(1,1469)	1:165:A:ASN:HB3	1:171:A:VAL:HG23	2	0.1
(1,1446)	1:139:A:LYS:HE2	1:137:A:ILE:HD11	15	0.1
(1,1446)	1:139:A:LYS:HE2	1:137:A:ILE:HD12	15	0.1
(1,1446)	1:139:A:LYS:HE2	1:137:A:ILE:HD13	15	0.1
(1,1446)	1:139:A:LYS:HE3	1:137:A:ILE:HD11	15	0.1
(1,1446)	1:139:A:LYS:HE3	1:137:A:ILE:HD12	15	0.1
(1,1446)	1:139:A:LYS:HE3	1:137:A:ILE:HD13	15	0.1
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD2	1	0.1
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD3	1	0.1
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD2	1	0.1
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD3	1	0.1
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD2	4	0.1
(1,1383)	1:145:A:TYR:HB2	1:146:A:LYS:HD3	4	0.1
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD2	4	0.1
(1,1383)	1:145:A:TYR:HB3	1:146:A:LYS:HD3	4	0.1
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD11	13	0.1
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD12	13	0.1
(1,1380)	1:53:A:SER:HB2	1:34:A:ILE:HD13	13	0.1
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD11	13	0.1
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD12	13	0.1
(1,1380)	1:53:A:SER:HB3	1:34:A:ILE:HD13	13	0.1
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG11	13	0.1
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG12	13	0.1
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG13	13	0.1
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG21	13	0.1
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG22	13	0.1
(1,1251)	1:141:A:PRO:HA	1:142:A:VAL:HG23	13	0.1
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB1	4	0.1
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB2	4	0.1
(1,1197)	1:143:A:LEU:HA	1:195:A:ALA:HB3	4	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG11	2	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG12	2	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG13	2	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG21	2	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG22	2	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG23	2	0.1
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG11	2	0.1
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG12	2	0.1
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG13	2	0.1
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG21	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG22	2	0.1
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG23	2	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG11	14	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG12	14	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG13	14	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG21	14	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG22	14	0.1
(1,1061)	1:46:A:PHE:HD1	1:8:A:VAL:HG23	14	0.1
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG11	14	0.1
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG12	14	0.1
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG13	14	0.1
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG21	14	0.1
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG22	14	0.1
(1,1061)	1:46:A:PHE:HD2	1:8:A:VAL:HG23	14	0.1
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD11	18	0.1
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD12	18	0.1
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD13	18	0.1
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD21	18	0.1
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD22	18	0.1
(1,1056)	1:46:A:PHE:HD1	1:85:A:LEU:HD23	18	0.1
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD11	18	0.1
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD12	18	0.1
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD13	18	0.1
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD21	18	0.1
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD22	18	0.1
(1,1056)	1:46:A:PHE:HD2	1:85:A:LEU:HD23	18	0.1
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG11	7	0.1
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG12	7	0.1
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG13	7	0.1
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG21	7	0.1
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG22	7	0.1
(1,1035)	1:172:A:TRP:H	1:157:A:VAL:HG23	7	0.1
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG11	7	0.1
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG12	7	0.1
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG13	7	0.1
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG21	7	0.1
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG22	7	0.1
(1,992)	1:172:A:TRP:H	1:157:A:VAL:HG23	7	0.1
(1,955)	1:196:A:TYR:HE1	1:175:A:ILE:HG21	3	0.1
(1,955)	1:196:A:TYR:HE1	1:175:A:ILE:HG22	3	0.1
(1,955)	1:196:A:TYR:HE1	1:175:A:ILE:HG23	3	0.1
(1,955)	1:196:A:TYR:HE2	1:175:A:ILE:HG21	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,955)	1:196:A:TYR:HE2	1:175:A:ILE:HG22	3	0.1
(1,955)	1:196:A:TYR:HE2	1:175:A:ILE:HG23	3	0.1
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD11	8	0.1
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD12	8	0.1
(1,914)	1:191:A:ASN:HD21	1:183:A:ILE:HD13	8	0.1
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD11	8	0.1
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD12	8	0.1
(1,914)	1:191:A:ASN:HD22	1:183:A:ILE:HD13	8	0.1
(1,876)	1:146:A:LYS:H	1:142:A:VAL:HB	8	0.1
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE1	9	0.1
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE2	9	0.1
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE3	9	0.1
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE1	16	0.1
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE2	16	0.1
(1,862)	1:131:A:GLU:H	1:96:A:MET:HE3	16	0.1
(1,771)	1:199:A:TYR:H	1:130:A:MET:HE1	8	0.1
(1,771)	1:199:A:TYR:H	1:130:A:MET:HE2	8	0.1
(1,771)	1:199:A:TYR:H	1:130:A:MET:HE3	8	0.1
(1,763)	1:150:A:LEU:H	1:150:A:LEU:HD11	14	0.1
(1,763)	1:150:A:LEU:H	1:150:A:LEU:HD12	14	0.1
(1,763)	1:150:A:LEU:H	1:150:A:LEU:HD13	14	0.1
(1,763)	1:150:A:LEU:H	1:150:A:LEU:HD21	14	0.1
(1,763)	1:150:A:LEU:H	1:150:A:LEU:HD22	14	0.1
(1,763)	1:150:A:LEU:H	1:150:A:LEU:HD23	14	0.1
(1,731)	1:148:A:LEU:H	1:142:A:VAL:HB	17	0.1
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG21	19	0.1
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG22	19	0.1
(1,707)	1:17:A:ARG:H	1:18:A:THR:HG23	19	0.1
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG11	7	0.1
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG12	7	0.1
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG13	7	0.1
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG21	7	0.1
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG22	7	0.1
(1,560)	1:9:A:VAL:H	1:62:A:VAL:HG23	7	0.1
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG11	7	0.1
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG12	7	0.1
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG13	7	0.1
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG21	7	0.1
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG22	7	0.1
(1,559)	1:9:A:VAL:H	1:62:A:VAL:HG23	7	0.1
(1,263)	1:137:A:ILE:HG12	1:136:A:PRO:HA	3	0.1
(1,263)	1:137:A:ILE:HG13	1:136:A:PRO:HA	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,263)	1:137:A:ILE:HG12	1:136:A:PRO:HA	5	0.1
(1,263)	1:137:A:ILE:HG13	1:136:A:PRO:HA	5	0.1
(1,263)	1:137:A:ILE:HG12	1:136:A:PRO:HA	7	0.1
(1,263)	1:137:A:ILE:HG13	1:136:A:PRO:HA	7	0.1
(1,263)	1:137:A:ILE:HG12	1:136:A:PRO:HA	19	0.1
(1,263)	1:137:A:ILE:HG13	1:136:A:PRO:HA	19	0.1
(1,249)	1:133:A:ARG:H	1:136:A:PRO:HA	5	0.1
(1,248)	1:130:A:MET:H	1:136:A:PRO:HA	4	0.1
(1,248)	1:130:A:MET:H	1:136:A:PRO:HA	17	0.1
(1,120)	1:199:A:TYR:HE1	1:137:A:ILE:HG12	2	0.1
(1,120)	1:199:A:TYR:HE1	1:137:A:ILE:HG13	2	0.1
(1,117)	1:52:A:TYR:HD2	1:52:A:TYR:H	17	0.1
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE1	11	0.1
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE2	11	0.1
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE1	11	0.1
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE2	11	0.1
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE1	17	0.1
(1,101)	1:191:A:ASN:HB2	1:190:A:TYR:HE2	17	0.1
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE1	17	0.1
(1,101)	1:191:A:ASN:HB3	1:190:A:TYR:HE2	17	0.1

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

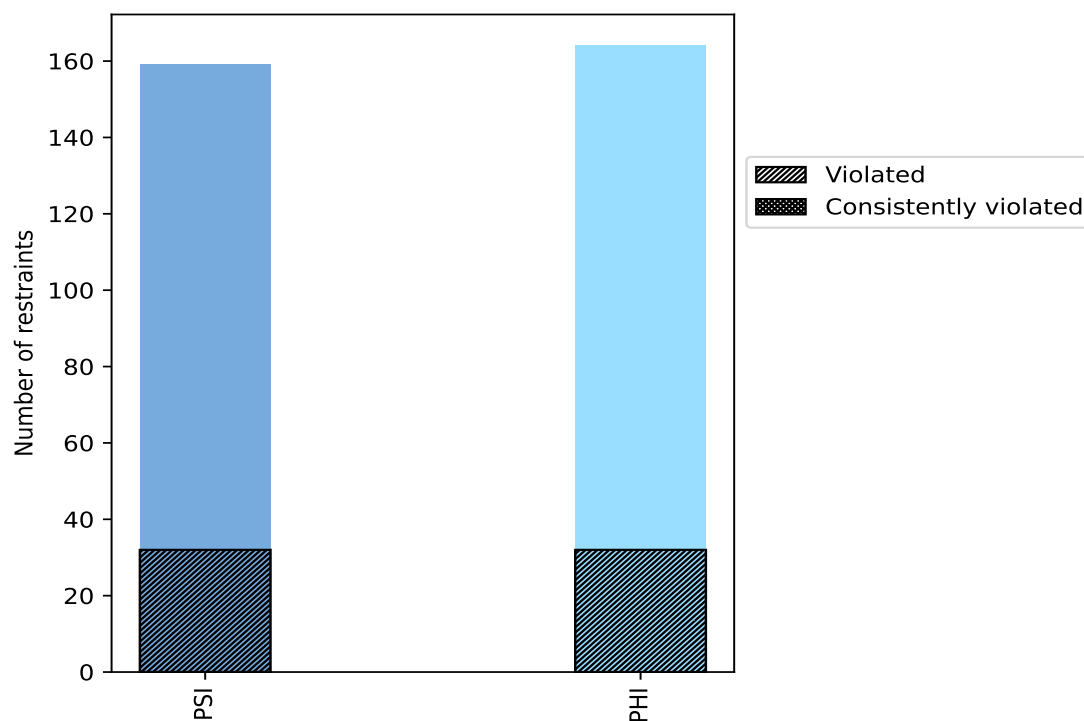
### 10.1 Summary of dihedral-angle violations [i](#)

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>
PSI	159	49.2	32	20.1	9.9	0	0.0	0.0
PHI	164	50.8	32	19.5	9.9	0	0.0	0.0
Total	323	100.0	64	19.8	19.8	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

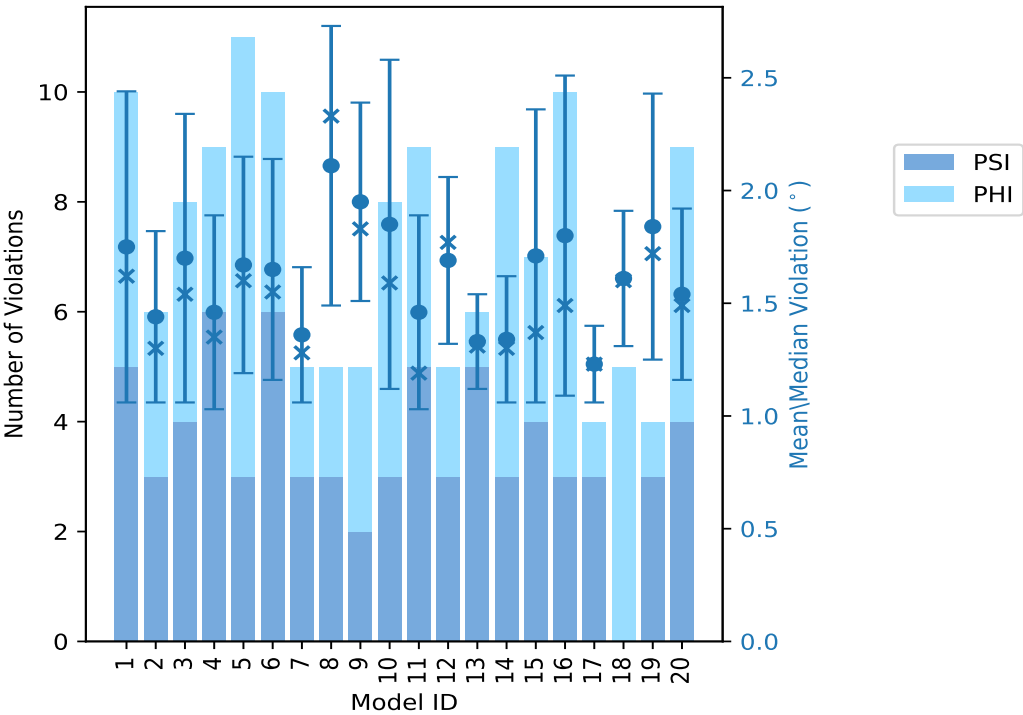


## 10.2 Dihedral-angle violation statistics for each model

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 (°)
	PSI	PHI	Total				
1	5	5	10	1.75	3.31	0.69	1.62
2	3	3	6	1.44	2.27	0.38	1.3
3	4	4	8	1.7	3.09	0.64	1.54
4	6	3	9	1.46	2.4	0.43	1.35
5	3	8	11	1.67	2.45	0.48	1.6
6	6	4	10	1.65	2.81	0.49	1.55
7	3	2	5	1.36	1.92	0.3	1.28
8	3	2	5	2.11	2.83	0.62	2.33
9	2	3	5	1.95	2.65	0.44	1.83
10	3	5	8	1.85	3.14	0.73	1.59
11	5	4	9	1.46	2.2	0.43	1.19
12	3	2	5	1.69	2.19	0.37	1.77
13	5	1	6	1.33	1.73	0.21	1.31
14	3	6	9	1.34	2.04	0.28	1.3
15	4	3	7	1.71	2.91	0.65	1.37
16	3	7	10	1.8	3.68	0.71	1.49
17	3	1	4	1.23	1.43	0.17	1.23
18	0	5	5	1.61	2.09	0.3	1.6
19	3	1	4	1.84	2.77	0.59	1.72
20	4	5	9	1.54	2.37	0.38	1.49

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
18	17	35	1	5.0
5	6	11	2	10.0
3	3	6	3	15.0
2	2	4	4	20.0
1	0	1	5	25.0
2	2	4	6	30.0
0	1	1	7	35.0
0	0	0	8	40.0
1	1	2	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

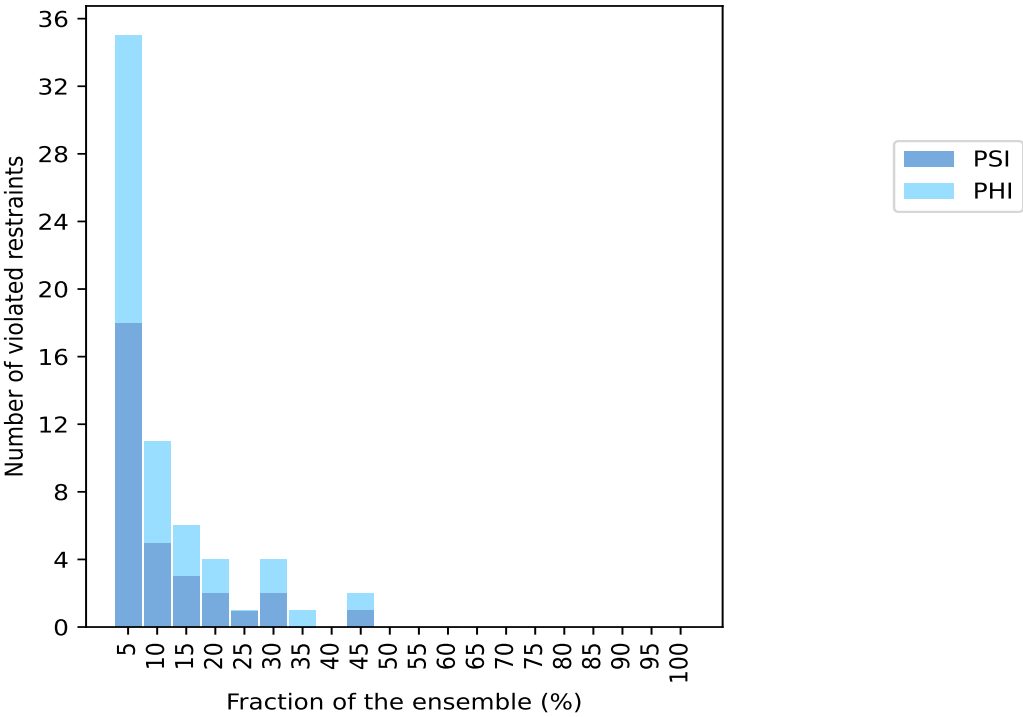
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

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

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

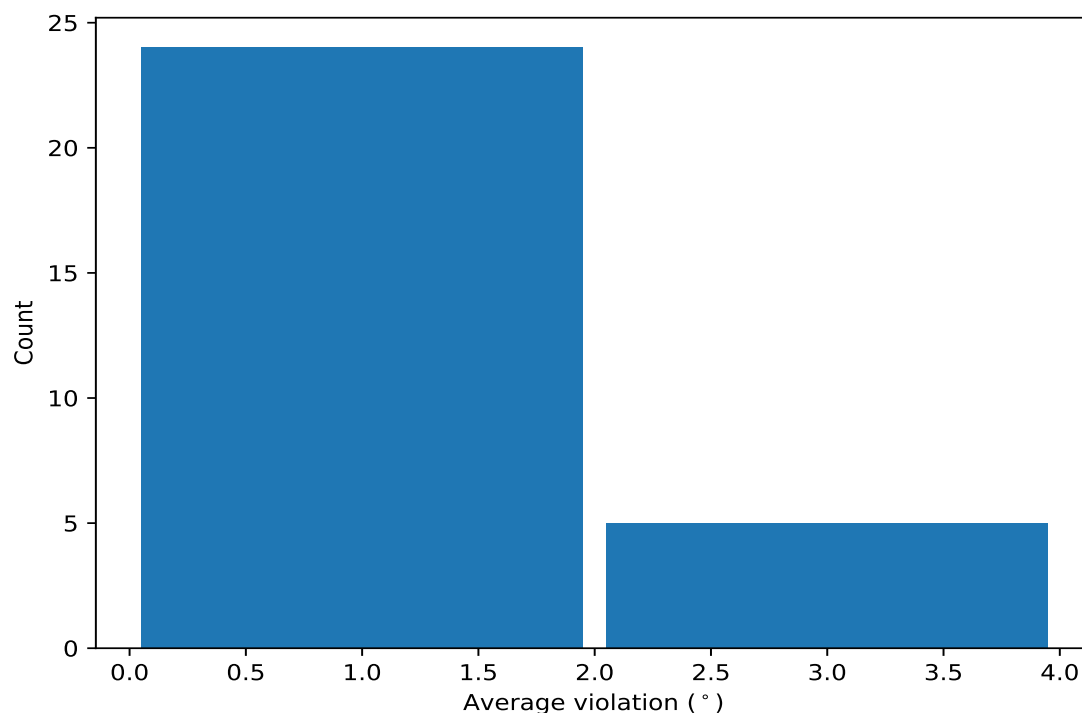


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



#### 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
(1,36)	1:31:A:ASN:C	1:32:A:ASP:N	1:32:A:ASP:CA	1:32:A:ASP:C	9	1.72	0.49	1.55
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:LYS:N	9	1.39	0.3	1.42
(1,149)	1:101:A:ILE:C	1:102:A:LEU:N	1:102:A:LEU:CA	1:102:A:LEU:C	7	1.44	0.39	1.28
(1,131)	1:91:A:PRO:C	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	6	2.64	0.63	2.5
(1,285)	1:197:A:ARG:N	1:197:A:ARG:CA	1:197:A:ARG:C	1:198:A:LYS:N	6	2.0	0.58	1.9
(1,16)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	6	1.89	0.53	1.81
(1,320)	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	1:51:A:PHE:N	6	1.46	0.5	1.21
(1,68)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:TYR:N	5	1.53	0.36	1.3
(1,315)	1:213:A:GLN:N	1:213:A:GLN:CA	1:213:A:GLN:C	1:214:A:PHE:N	4	2.0	0.44	1.91
(1,134)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:TRP:N	4	1.95	0.7	1.77
(1,234)	1:166:A:ILE:C	1:167:A:ASP:N	1:167:A:ASP:CA	1:167:A:ASP:C	4	1.47	0.14	1.47
(1,61)	1:45:A:SER:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	4	1.37	0.1	1.38
(1,175)	1:129:A:PHE:N	1:129:A:PHE:CA	1:129:A:PHE:C	1:130:A:MET:N	3	2.27	0.77	2.04
(1,286)	1:197:A:ARG:C	1:198:A:LYS:N	1:198:A:LYS:CA	1:198:A:LYS:C	3	2.09	0.2	2.14
(1,151)	1:116:A:PRO:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	3	1.95	0.36	2.04
(1,197)	1:146:A:LYS:N	1:146:A:LYS:CA	1:146:A:LYS:C	1:147:A:ASP:N	3	1.94	0.33	2.07
(1,289)	1:199:A:TYR:N	1:199:A:TYR:CA	1:199:A:TYR:C	1:200:A:LEU:N	3	1.91	0.67	1.63
(1,258)	1:178:A:ASP:C	1:179:A:LEU:N	1:179:A:LEU:CA	1:179:A:LEU:C	3	1.85	0.48	1.73
(1,102)	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	1:70:A:SER:N	2	1.94	0.84	1.94
(1,137)	1:95:A:LYS:C	1:96:A:MET:N	1:96:A:MET:CA	1:96:A:MET:C	2	1.87	0.36	1.87

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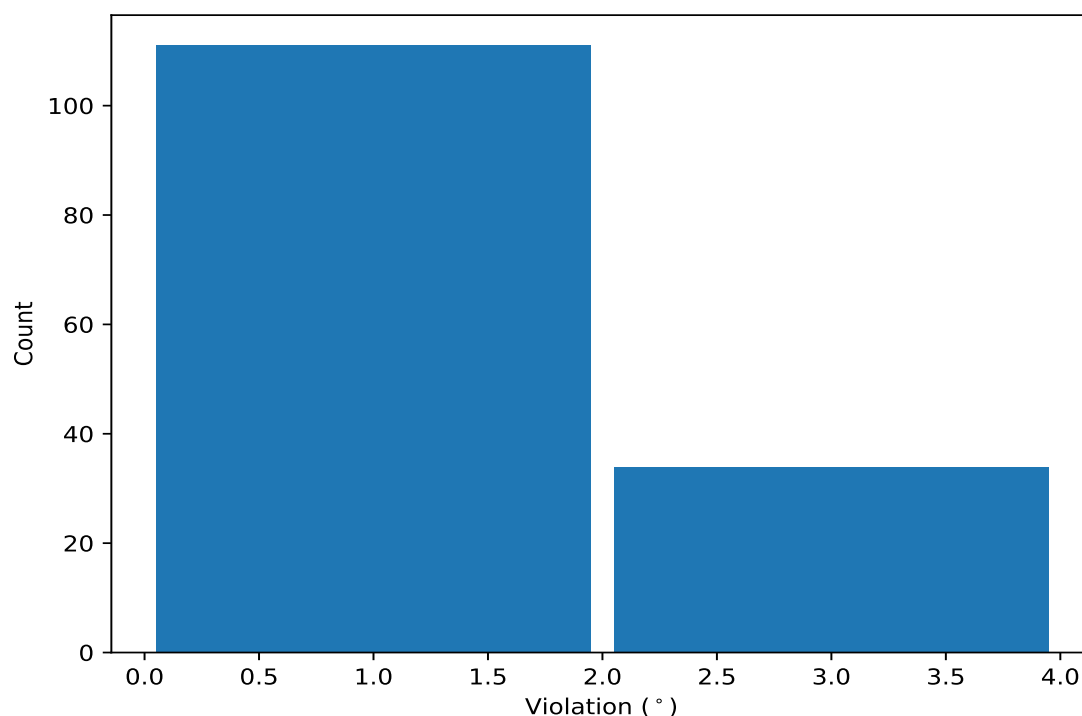
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,3)	1:5:A:LEU:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	2	1.83	0.08	1.83
(1,191)	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	1:143:A:LEU:N	2	1.71	0.57	1.71
(1,1)	1:2:A:ASP:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	2	1.6	0.54	1.6
(1,58)	1:44:A:ARG:N	1:44:A:ARG:CA	1:44:A:ARG:C	1:45:A:SER:N	2	1.54	0.05	1.54
(1,138)	1:96:A:MET:N	1:96:A:MET:CA	1:96:A:MET:C	1:97:A:ASP:N	2	1.3	0.3	1.3
(1,105)	1:70:A:SER:C	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	2	1.2	0.08	1.2
(1,69)	1:51:A:PHE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	2	1.2	0.12	1.2
(1,314)	1:212:A:ILE:C	1:213:A:GLN:N	1:213:A:GLN:CA	1:213:A:GLN:C	2	1.18	0.07	1.18
(1,181)	1:132:A:ASP:N	1:132:A:ASP:CA	1:132:A:ASP:C	1:133:A:ARG:N	2	1.15	0.01	1.15

<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 (°)
(1,131)	1:91:A:PRO:C	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	16	3.68
(1,175)	1:129:A:PHE:N	1:129:A:PHE:CA	1:129:A:PHE:C	1:130:A:MET:N	1	3.31
(1,131)	1:91:A:PRO:C	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	10	3.14
(1,134)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:TRP:N	3	3.09
(1,285)	1:197:A:ARG:N	1:197:A:ARG:CA	1:197:A:ARG:C	1:198:A:LYS:N	15	2.91
(1,289)	1:199:A:TYR:N	1:199:A:TYR:CA	1:199:A:TYR:C	1:200:A:LEU:N	8	2.83
(1,131)	1:91:A:PRO:C	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	6	2.81
(1,102)	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	1:70:A:SER:N	19	2.77
(1,315)	1:213:A:GLN:N	1:213:A:GLN:CA	1:213:A:GLN:C	1:214:A:PHE:N	10	2.7
(1,16)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	9	2.65
(1,285)	1:197:A:ARG:N	1:197:A:ARG:CA	1:197:A:ARG:C	1:198:A:LYS:N	8	2.55
(1,258)	1:178:A:ASP:C	1:179:A:LEU:N	1:179:A:LEU:CA	1:179:A:LEU:C	1	2.49
(1,36)	1:31:A:ASN:C	1:32:A:ASP:N	1:32:A:ASP:CA	1:32:A:ASP:C	15	2.47
(1,36)	1:31:A:ASN:C	1:32:A:ASP:N	1:32:A:ASP:CA	1:32:A:ASP:C	5	2.45
(1,320)	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	1:51:A:PHE:N	4	2.4
(1,16)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	20	2.37
(1,151)	1:116:A:PRO:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	8	2.33
(1,286)	1:197:A:ARG:C	1:198:A:LYS:N	1:198:A:LYS:CA	1:198:A:LYS:C	10	2.31
(1,191)	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	1:143:A:LEU:N	5	2.28
(1,197)	1:146:A:LYS:N	1:146:A:LYS:CA	1:146:A:LYS:C	1:147:A:ASP:N	2	2.27
(1,137)	1:95:A:LYS:C	1:96:A:MET:N	1:96:A:MET:CA	1:96:A:MET:C	9	2.23
(1,131)	1:91:A:PRO:C	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	11	2.2
(1,16)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	12	2.19
(1,149)	1:101:A:ILE:C	1:102:A:LEU:N	1:102:A:LEU:CA	1:102:A:LEU:C	5	2.17
(1,36)	1:31:A:ASN:C	1:32:A:ASP:N	1:32:A:ASP:CA	1:32:A:ASP:C	1	2.17
(1,68)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:TYR:N	16	2.15
(1,286)	1:197:A:ARG:C	1:198:A:LYS:N	1:198:A:LYS:CA	1:198:A:LYS:C	16	2.14
(1,1)	1:2:A:ASP:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	3	2.14
(1,131)	1:91:A:PRO:C	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	18	2.09
(1,197)	1:146:A:LYS:N	1:146:A:LYS:CA	1:146:A:LYS:C	1:147:A:ASP:N	6	2.07
(1,175)	1:129:A:PHE:N	1:129:A:PHE:CA	1:129:A:PHE:C	1:130:A:MET:N	5	2.04
(1,151)	1:116:A:PRO:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	14	2.04
(1,285)	1:197:A:ARG:N	1:197:A:ARG:CA	1:197:A:ARG:C	1:198:A:LYS:N	11	2.03
(1,40)	1:34:A:ILE:C	1:35:A:THR:N	1:35:A:THR:CA	1:35:A:THR:C	4	2.01
(1,315)	1:213:A:GLN:N	1:213:A:GLN:CA	1:213:A:GLN:C	1:214:A:PHE:N	6	1.96
(1,131)	1:91:A:PRO:C	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	7	1.92
(1,3)	1:5:A:LEU:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	16	1.91
(1,88)	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	1:62:A:VAL:N	20	1.89
(1,315)	1:213:A:GLN:N	1:213:A:GLN:CA	1:213:A:GLN:C	1:214:A:PHE:N	19	1.86
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:LYS:N	3	1.85
(1,134)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:TRP:N	12	1.84
(1,320)	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	1:51:A:PHE:N	9	1.83
(1,286)	1:197:A:ARG:C	1:198:A:LYS:N	1:198:A:LYS:CA	1:198:A:LYS:C	5	1.82
(1,285)	1:197:A:ARG:N	1:197:A:ARG:CA	1:197:A:ARG:C	1:198:A:LYS:N	1	1.77
(1,154)	1:118:A:GLU:N	1:118:A:GLU:CA	1:118:A:GLU:C	1:119:A:ARG:N	12	1.77
(1,149)	1:101:A:ILE:C	1:102:A:LEU:N	1:102:A:LEU:CA	1:102:A:LEU:C	8	1.76
(1,51)	1:40:A:GLN:C	1:41:A:CYS:N	1:41:A:CYS:CA	1:41:A:CYS:C	11	1.75
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:LYS:N	10	1.75
(1,3)	1:5:A:LEU:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	3	1.75
(1,36)	1:31:A:ASN:C	1:32:A:ASP:N	1:32:A:ASP:CA	1:32:A:ASP:C	18	1.74
(1,258)	1:178:A:ASP:C	1:179:A:LEU:N	1:179:A:LEU:CA	1:179:A:LEU:C	20	1.73
(1,68)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:TYR:N	13	1.73

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,134)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:TRP:N	11	1.7
(1,289)	1:199:A:TYR:N	1:199:A:TYR:CA	1:199:A:TYR:C	1:200:A:LEU:N	1	1.63
(1,149)	1:101:A:ILE:C	1:102:A:LEU:N	1:102:A:LEU:CA	1:102:A:LEU:C	6	1.63
(1,234)	1:166:A:ILE:C	1:167:A:ASP:N	1:167:A:ASP:CA	1:167:A:ASP:C	15	1.62
(1,32)	1:28:A:PRO:C	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1	1.61
(1,234)	1:166:A:ILE:C	1:167:A:ASP:N	1:167:A:ASP:CA	1:167:A:ASP:C	5	1.6
(1,34)	1:29:A:SER:C	1:30:A:CYS:N	1:30:A:CYS:CA	1:30:A:CYS:C	18	1.6
(1,138)	1:96:A:MET:N	1:96:A:MET:CA	1:96:A:MET:C	1:97:A:ASP:N	12	1.59
(1,58)	1:44:A:ARG:N	1:44:A:ARG:CA	1:44:A:ARG:C	1:45:A:SER:N	6	1.58
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:LYS:N	19	1.57
(1,36)	1:31:A:ASN:C	1:32:A:ASP:N	1:32:A:ASP:CA	1:32:A:ASP:C	9	1.55
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:LYS:N	6	1.52
(1,137)	1:95:A:LYS:C	1:96:A:MET:N	1:96:A:MET:CA	1:96:A:MET:C	16	1.51
(1,61)	1:45:A:SER:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	20	1.5
(1,255)	1:177:A:MET:N	1:177:A:MET:CA	1:177:A:MET:C	1:178:A:ASP:N	14	1.49
(1,197)	1:146:A:LYS:N	1:146:A:LYS:CA	1:146:A:LYS:C	1:147:A:ASP:N	20	1.49
(1,58)	1:44:A:ARG:N	1:44:A:ARG:CA	1:44:A:ARG:C	1:45:A:SER:N	9	1.49
(1,315)	1:213:A:GLN:N	1:213:A:GLN:CA	1:213:A:GLN:C	1:214:A:PHE:N	4	1.47
(1,175)	1:129:A:PHE:N	1:129:A:PHE:CA	1:129:A:PHE:C	1:130:A:MET:N	16	1.47
(1,151)	1:116:A:PRO:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	16	1.47
(1,61)	1:45:A:SER:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	17	1.43
(1,16)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	10	1.43
(1,148)	1:101:A:ILE:N	1:101:A:ILE:CA	1:101:A:ILE:C	1:102:A:LEU:N	5	1.42
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:LYS:N	2	1.42
(1,129)	1:86:A:LYS:N	1:86:A:LYS:CA	1:86:A:LYS:C	1:87:A:THR:N	13	1.39
(1,62)	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	1:47:A:ILE:N	15	1.37
(1,36)	1:31:A:ASN:C	1:32:A:ASP:N	1:32:A:ASP:CA	1:32:A:ASP:C	6	1.37
(1,16)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	18	1.37
(1,285)	1:197:A:ARG:N	1:197:A:ARG:CA	1:197:A:ARG:C	1:198:A:LYS:N	17	1.36
(1,205)	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	1:151:A:PHE:N	4	1.36
(1,132)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:ASN:N	13	1.36
(1,285)	1:197:A:ARG:N	1:197:A:ARG:CA	1:197:A:ARG:C	1:198:A:LYS:N	4	1.35
(1,16)	1:16:A:GLU:C	1:17:A:ARG:N	1:17:A:ARG:CA	1:17:A:ARG:C	1	1.35
(1,320)	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	1:51:A:PHE:N	7	1.34
(1,234)	1:166:A:ILE:C	1:167:A:ASP:N	1:167:A:ASP:CA	1:167:A:ASP:C	4	1.34
(1,85)	1:59:A:ILE:C	1:60:A:LYS:N	1:60:A:LYS:CA	1:60:A:LYS:C	2	1.33
(1,36)	1:31:A:ASN:C	1:32:A:ASP:N	1:32:A:ASP:CA	1:32:A:ASP:C	20	1.33
(1,258)	1:178:A:ASP:C	1:179:A:LEU:N	1:179:A:LEU:CA	1:179:A:LEU:C	16	1.32
(1,234)	1:166:A:ILE:C	1:167:A:ASP:N	1:167:A:ASP:CA	1:167:A:ASP:C	3	1.32
(1,61)	1:45:A:SER:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	14	1.32
(1,69)	1:51:A:PHE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	14	1.31
(1,152)	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	1:118:A:GLU:N	16	1.3
(1,68)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:TYR:N	14	1.3
(1,150)	1:102:A:LEU:N	1:102:A:LEU:CA	1:102:A:LEU:C	1:103:A:GLU:N	20	1.28
(1,149)	1:101:A:ILE:C	1:102:A:LEU:N	1:102:A:LEU:CA	1:102:A:LEU:C	7	1.28
(1,105)	1:70:A:SER:C	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	6	1.28
(1,289)	1:199:A:TYR:N	1:199:A:TYR:CA	1:199:A:TYR:C	1:200:A:LEU:N	3	1.27
(1,68)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:TYR:N	2	1.26
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:LYS:N	13	1.26
(1,314)	1:212:A:ILE:C	1:213:A:GLN:N	1:213:A:GLN:CA	1:213:A:GLN:C	15	1.25
(1,61)	1:45:A:SER:C	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	18	1.24

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	1:46:A:PHE:N	6	1.24
(1,52)	1:41:A:CYS:N	1:41:A:CYS:CA	1:41:A:CYS:C	1:42:A:LEU:N	7	1.24
(1,36)	1:31:A:ASN:C	1:32:A:ASP:N	1:32:A:ASP:CA	1:32:A:ASP:C	10	1.24
(1,319)	1:49:A:SER:C	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	5	1.23
(1,153)	1:117:A:GLU:C	1:118:A:GLU:N	1:118:A:GLU:CA	1:118:A:GLU:C	2	1.21
(1,66)	1:48:A:ASP:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	5	1.2
(1,284)	1:196:A:TYR:C	1:197:A:ARG:N	1:197:A:ARG:CA	1:197:A:ARG:C	14	1.19
(1,68)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:TYR:N	11	1.19
(1,134)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:TRP:N	15	1.18
(1,37)	1:32:A:ASP:N	1:32:A:ASP:CA	1:32:A:ASP:C	1:33:A:ASP:N	13	1.18
(1,63)	1:46:A:PHE:C	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	20	1.17
(1,36)	1:31:A:ASN:C	1:32:A:ASP:N	1:32:A:ASP:CA	1:32:A:ASP:C	19	1.17
(1,181)	1:132:A:ASP:N	1:132:A:ASP:CA	1:132:A:ASP:C	1:133:A:ARG:N	10	1.16
(1,91)	1:62:A:VAL:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	14	1.16
(1,181)	1:132:A:ASP:N	1:132:A:ASP:CA	1:132:A:ASP:C	1:133:A:ARG:N	15	1.15
(1,191)	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	1:143:A:LEU:N	14	1.14
(1,187)	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	1:139:A:LYS:N	11	1.14
(1,290)	1:199:A:TYR:C	1:200:A:LEU:N	1:200:A:LEU:CA	1:200:A:LEU:C	2	1.13
(1,105)	1:70:A:SER:C	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	3	1.13
(1,149)	1:101:A:ILE:C	1:102:A:LEU:N	1:102:A:LEU:CA	1:102:A:LEU:C	4	1.12
(1,144)	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	1:100:A:GLU:N	4	1.12
(1,314)	1:212:A:ILE:C	1:213:A:GLN:N	1:213:A:GLN:CA	1:213:A:GLN:C	5	1.1
(1,102)	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	1:70:A:SER:N	17	1.1
(1,226)	1:160:A:GLN:C	1:161:A:GLY:N	1:161:A:GLY:CA	1:161:A:GLY:C	10	1.09
(1,320)	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	1:51:A:PHE:N	8	1.08
(1,320)	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	1:51:A:PHE:N	20	1.08
(1,69)	1:51:A:PHE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	16	1.08
(1,38)	1:32:A:ASP:C	1:33:A:ASP:N	1:33:A:ASP:CA	1:33:A:ASP:C	5	1.08
(1,19)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:GLU:N	1	1.08
(1,149)	1:101:A:ILE:C	1:102:A:LEU:N	1:102:A:LEU:CA	1:102:A:LEU:C	1	1.07
(1,149)	1:101:A:ILE:C	1:102:A:LEU:N	1:102:A:LEU:CA	1:102:A:LEU:C	12	1.07
(1,139)	1:96:A:MET:C	1:97:A:ASP:N	1:97:A:ASP:CA	1:97:A:ASP:C	14	1.07
(1,1)	1:2:A:ASP:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	13	1.07
(1,174)	1:128:A:LYS:C	1:129:A:PHE:N	1:129:A:PHE:CA	1:129:A:PHE:C	11	1.06
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:LYS:N	1	1.06
(1,180)	1:131:A:GLU:C	1:132:A:ASP:N	1:132:A:ASP:CA	1:132:A:ASP:C	11	1.05
(1,112)	1:74:A:THR:N	1:74:A:THR:CA	1:74:A:THR:C	1:75:A:LYS:N	3	1.05
(1,320)	1:50:A:LYS:N	1:50:A:LYS:CA	1:50:A:LYS:C	1:51:A:PHE:N	17	1.04
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:LYS:N	11	1.03
(1,46)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:ASP:N	7	1.02
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:LYS:N	4	1.01
(1,138)	1:96:A:MET:N	1:96:A:MET:CA	1:96:A:MET:C	1:97:A:ASP:N	6	1.0