



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 12:42 AM UTC

PDB ID : 2LU2 / pdb\_00002lu2  
BMRB ID : 18506  
Title : MIC5 regulates the activity of Toxoplasma subtilisin 1 by mimicking a subtilisin prodomain  
Authors : Saouros, S.; Dou, Z.; Henry, M.; Marchant, J.; Carruthers, V.B.; Matthews, S.  
Deposited on : 2012-06-07

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

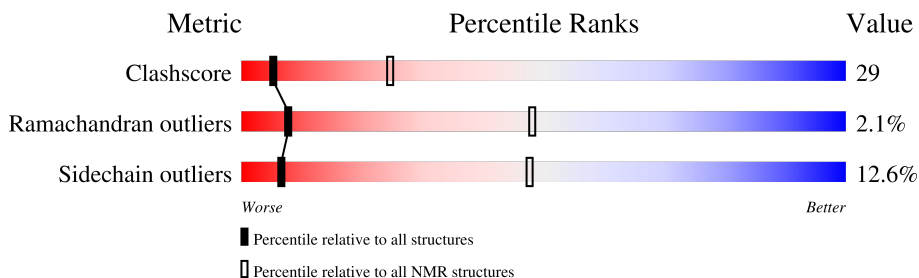
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 87%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	138	

## 2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:59-A:136 (78)	0.30	4

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

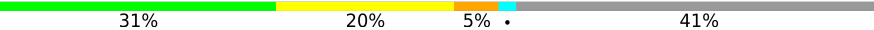
### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1246 atoms, of which 628 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Microneme TgMIC5 protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	81	1246	384	628	101	128	5	0




Chain A: 

ARG THR MET ASP THR GLN ASN ASP VAL GLU SER GLY ARG GLN SER GLU PRO MET MET GLU ALA ALA ARG GLN ALA ALA GLU HIS PRO GLY ALA THR PRO GLN SER MET LYS GLU PHE GLN GLU ILE LYS GLU VAL GLU THR LYS ASP PRO E58 M59

L62 M63 V64 K67 K71 N72 F73 F82 F85 I86 E87 L89 G90 G91 S92 S93 I93 L96 M103 I104 E105 P107 K108 T109 V110 S111 D114 M115 D116 Q117 L118 L119 H120 D121 I122 A125 V128 S133 E134 V136 K136 A138

#### 4.2.3 Score per residue for model 3

- Molecule 1: Microneme TgMIC5 protein

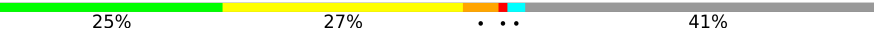
Chain A: 

ARG THR MET ASP THR GLN ASN ASP VAL GLU SER GLY ARG GLN SER SER PRO MET MET GLU ALA ALA ARG GLN ALA ALA HIS PRO GLY ALA PRO THR GLN SER MET LYS GLU PHE GLN GLU ILE LYS VAL GLU THR LYS HIS ASP PRO E58 M59 T60

R61 L62 M63 T65 E66 K67 Q68 K71 N72 S70 F73 M76 F82 R85 E87 E88 L89 G91 S92 I93 L96 M103 I104 E105 L106 P107 K108 T109 V110 S111 E112 H113 D114 M115 D116 Q117 L118 L119 H120 I122 A125 V128 S133 E134 V135 K136 L137 A138

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

- Molecule 1: Microneme TgMIC5 protein

Chain A: 


ARG THR MET ASP THR GLN ASN ASP VAL GLU SER GLY ARG GLN SER SER PRO MET MET GLU ALA ALA ARG GLN ALA ALA HIS PRO GLY ALA PRO THR GLN SER MET LYS GLU PHE GLN GLU ILE LYS VAL GLU THR LYS HIS ASP PRO E58 M59 T60

R61 L62 T65 E66 K67 Q68 K71 N72 F73 S74 M76 A77 F82 S83 T84 R85 I86 E87 E88 L89 G90 G91 S92 I93 L96 V101 T102 M103 I104 E105 L106 P107 K108 T109 S111 D114 M115 L118 M115 L119 L119 L119 I122 A125 V128 S133 E134 V135 D132 S133 E134 V135

K136 L137 A138

#### 4.2.5 Score per residue for model 5

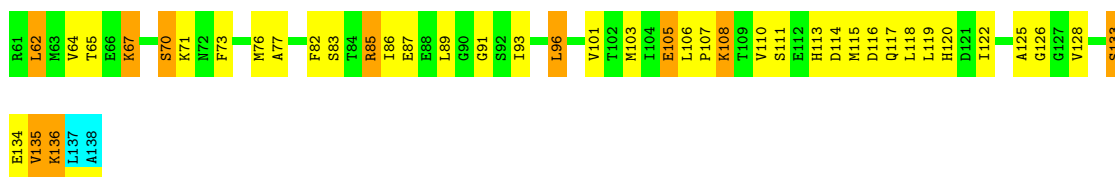
- Molecule 1: Microneme TgMIC5 protein

Chain A: 

ARG THR MET ASP THR GLN ASN ASP VAL GLU SER GLY ARG GLN SER SER PRO MET MET GLU ALA ALA ARG GLN ALA ALA HIS PRO GLY ALA PRO THR GLN SER MET LYS GLU PHE GLN GLU ILE LYS VAL GLU THR LYS HIS ASP PRO E58 M59 T60

R61 L62 M63 V64 E66 K67 S70 K71 N72 F73 M76 A77 F82 S83 T84 R85 I86 E87 E88 L89 G90 G91 S91 L96 V101 T102 M103 I104 E105 L106 P107 K108 T108 V110 S111 D114 M115 L118 L119 L119 I122 A125 V128 S133 E134 V135 K136 L137 A138

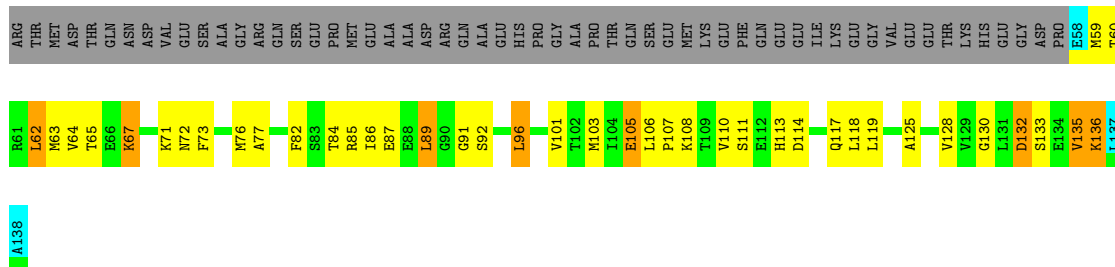




#### 4.2.10 Score per residue for model 10

- Molecule 1: Microneme TgMIC5 protein

Chain A: 27% 24% 6% 41%



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	
ARIA	refinement	
TALOS	geometry optimization	
CNS	structure solution	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	940
Number of shifts mapped to atoms	940
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

## 6 Model quality i

### 6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	595	606	604	34±3
All	All	5950	6060	6040	342

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ARG:HD3	1:A:103:MET:SD	0.79	2.18	6	3
1:A:85:ARG:NE	1:A:86:ILE:HG12	0.70	2.01	2	10
1:A:63:MET:HB3	1:A:132:ASP:OD2	0.69	1.86	6	1
1:A:76:MET:HG2	1:A:125:ALA:HB2	0.68	1.65	10	8
1:A:83:SER:O	1:A:87:GLU:HG3	0.66	1.91	9	1
1:A:114:ASP:O	1:A:118:LEU:HB2	0.65	1.90	3	10
1:A:60:THR:HG23	1:A:134:GLU:HA	0.63	1.70	8	5
1:A:87:GLU:HA	1:A:91:GLY:O	0.62	1.94	5	9
1:A:62:LEU:HD11	1:A:119:LEU:HD22	0.62	1.71	5	9
1:A:135:VAL:O	1:A:136:LYS:HD3	0.59	1.98	5	5
1:A:59:MET:SD	1:A:91:GLY:HA2	0.59	2.38	5	8
1:A:64:VAL:HA	1:A:128:VAL:O	0.58	1.98	9	5
1:A:107:PRO:O	1:A:110:VAL:HG13	0.58	1.98	3	10
1:A:86:ILE:CD1	1:A:106:LEU:HD12	0.58	2.28	6	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:ILE:HD12	1:A:106:LEU:HD12	0.58	1.74	7	10
1:A:62:LEU:HA	1:A:130:GLY:O	0.57	1.99	10	4
1:A:73:PHE:CE1	1:A:122:ILE:HG23	0.57	2.34	9	6
1:A:60:THR:HA	1:A:133:SER:O	0.57	2.00	5	3
1:A:93:ILE:HG21	1:A:95:PHE:CE2	0.56	2.36	8	1
1:A:106:LEU:HD13	1:A:119:LEU:HD21	0.56	1.78	10	6
1:A:59:MET:SD	1:A:105:GLU:HB3	0.56	2.41	5	7
1:A:85:ARG:HD3	1:A:86:ILE:H	0.55	1.62	1	10
1:A:91:GLY:HA3	1:A:105:GLU:O	0.55	2.02	7	10
1:A:135:VAL:C	1:A:136:LYS:HG3	0.54	2.26	4	1
1:A:60:THR:O	1:A:105:GLU:HA	0.54	2.01	7	4
1:A:67:LYS:O	1:A:71:LYS:HB2	0.54	2.03	5	2
1:A:107:PRO:HB2	1:A:109:THR:OG1	0.54	2.03	3	1
1:A:115:MET:O	1:A:119:LEU:HG	0.53	2.03	8	5
1:A:135:VAL:C	1:A:136:LYS:HD3	0.53	2.28	3	4
1:A:74:SER:O	1:A:78:LYS:HG3	0.53	2.04	4	1
1:A:114:ASP:OD2	1:A:118:LEU:HD12	0.53	2.04	10	1
1:A:73:PHE:CE2	1:A:122:ILE:HG23	0.53	2.39	6	3
1:A:60:THR:OG1	1:A:108:LYS:HE2	0.52	2.04	10	2
1:A:82:PHE:O	1:A:93:ILE:HD11	0.52	2.05	8	5
1:A:82:PHE:O	1:A:85:ARG:HD2	0.52	2.04	2	8
1:A:70:SER:HB3	1:A:126:GLY:O	0.51	2.05	7	2
1:A:116:ASP:O	1:A:120:HIS:HB2	0.51	2.05	2	4
1:A:60:THR:HG23	1:A:133:SER:O	0.51	2.05	10	2
1:A:65:THR:O	1:A:70:SER:HB2	0.50	2.06	5	3
1:A:62:LEU:HG	1:A:104:ILE:O	0.50	2.07	7	1
1:A:73:PHE:HA	1:A:125:ALA:HB1	0.50	1.82	10	7
1:A:87:GLU:HG2	1:A:92:SER:HA	0.50	1.83	4	4
1:A:60:THR:OG1	1:A:108:LYS:HE3	0.49	2.07	4	2
1:A:77:ALA:HA	1:A:82:PHE:CD2	0.49	2.42	9	6
1:A:96:LEU:HD22	1:A:96:LEU:N	0.49	2.23	9	5
1:A:67:LYS:O	1:A:71:LYS:N	0.49	2.45	5	7
1:A:101:VAL:HG12	1:A:103:MET:SD	0.49	2.48	4	4
1:A:113:HIS:O	1:A:117:GLN:HB3	0.49	2.06	10	1
1:A:110:VAL:HG23	1:A:111:SER:O	0.49	2.08	7	10
1:A:64:VAL:HG22	1:A:128:VAL:O	0.49	2.07	6	3
1:A:60:THR:HB	1:A:106:LEU:O	0.48	2.09	4	3
1:A:106:LEU:C	1:A:106:LEU:HD23	0.48	2.34	2	10
1:A:113:HIS:O	1:A:117:GLN:HB2	0.48	2.09	3	2
1:A:68:GLN:HE21	1:A:68:GLN:HA	0.48	1.68	6	1
1:A:106:LEU:HD13	1:A:119:LEU:CD2	0.48	2.39	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:LEU:HG	1:A:110:VAL:HB	0.47	1.86	2	2
1:A:64:VAL:O	1:A:101:VAL:HA	0.47	2.09	5	3
1:A:136:LYS:O	1:A:136:LYS:HE3	0.47	2.09	5	2
1:A:63:MET:HB3	1:A:132:ASP:OD1	0.47	2.09	7	2
1:A:107:PRO:HG2	1:A:110:VAL:HG13	0.46	1.87	3	2
1:A:85:ARG:CD	1:A:86:ILE:H	0.46	2.23	10	4
1:A:76:MET:SD	1:A:125:ALA:HB2	0.46	2.50	6	1
1:A:114:ASP:OD1	1:A:118:LEU:HD12	0.46	2.10	2	1
1:A:59:MET:HG3	1:A:105:GLU:HB3	0.45	1.88	4	1
1:A:119:LEU:O	1:A:122:ILE:HB	0.45	2.11	3	5
1:A:101:VAL:CG1	1:A:103:MET:SD	0.45	3.05	10	5
1:A:134:GLU:O	1:A:135:VAL:C	0.45	2.59	2	4
1:A:110:VAL:CG2	1:A:115:MET:HB2	0.45	2.42	3	4
1:A:64:VAL:HG11	1:A:73:PHE:CD2	0.45	2.46	5	2
1:A:72:ASN:HB2	1:A:125:ALA:O	0.44	2.12	4	2
1:A:85:ARG:NH2	1:A:93:ILE:HG13	0.44	2.27	9	1
1:A:72:ASN:HB3	1:A:125:ALA:O	0.44	2.12	2	1
1:A:107:PRO:C	1:A:109:THR:H	0.44	2.20	2	2
1:A:87:GLU:HG2	1:A:92:SER:CB	0.44	2.42	8	1
1:A:86:ILE:HG22	1:A:91:GLY:CA	0.44	2.43	5	1
1:A:59:MET:O	1:A:105:GLU:HG2	0.44	2.13	2	1
1:A:60:THR:H	1:A:106:LEU:C	0.44	2.21	9	1
1:A:96:LEU:HD23	1:A:103:MET:SD	0.43	2.53	3	4
1:A:73:PHE:CE1	1:A:122:ILE:HA	0.43	2.48	8	1
1:A:82:PHE:O	1:A:85:ARG:CD	0.43	2.65	2	5
1:A:107:PRO:HG2	1:A:110:VAL:CG1	0.43	2.44	2	1
1:A:59:MET:CG	1:A:105:GLU:HB3	0.43	2.43	4	1
1:A:67:LYS:N	1:A:67:LYS:HD3	0.43	2.29	4	1
1:A:86:ILE:HD12	1:A:114:ASP:OD2	0.42	2.13	2	1
1:A:107:PRO:C	1:A:109:THR:N	0.42	2.77	3	2
1:A:68:GLN:NE2	1:A:68:GLN:H	0.42	2.12	4	1
1:A:113:HIS:HA	1:A:117:GLN:OE1	0.42	2.15	9	1
1:A:108:LYS:HA	1:A:115:MET:HE2	0.42	1.91	5	1
1:A:67:LYS:C	1:A:69:GLU:N	0.41	2.78	3	1
1:A:85:ARG:HG3	1:A:118:LEU:HD22	0.41	1.92	8	1
1:A:61:ARG:CB	1:A:105:GLU:HG3	0.41	2.46	8	1
1:A:82:PHE:HA	1:A:85:ARG:HD2	0.41	1.92	1	2
1:A:82:PHE:CE1	1:A:85:ARG:HG3	0.40	2.51	10	1
1:A:59:MET:HB2	1:A:105:GLU:HB3	0.40	1.92	8	1
1:A:86:ILE:HD12	1:A:114:ASP:OD1	0.40	2.15	10	1
1:A:73:PHE:HE1	1:A:122:ILE:HA	0.40	1.76	8	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	78/138 (57%)	70±1 (90±2%)	6±1 (8±2%)	2±0 (2±1%)	8	48
All	All	780/1380 (57%)	704 (90%)	60 (8%)	16 (2%)	8	48

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	135	VAL	10
1	A	136	LYS	5
1	A	59	MET	1

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	69/119 (58%)	60±2 (87±3%)	9±2 (13±3%)	6	48
All	All	690/1190 (58%)	603 (87%)	87 (13%)	6	48

All 20 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	62	LEU	10
1	A	89	LEU	10
1	A	96	LEU	9
1	A	67	LYS	9
1	A	65	THR	8
1	A	136	LYS	8
1	A	105	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	84	THR	4
1	A	108	LYS	3
1	A	111	SER	3
1	A	132	ASP	3
1	A	135	VAL	3
1	A	85	ARG	2
1	A	70	SER	2
1	A	59	MET	1
1	A	134	GLU	1
1	A	68	GLN	1
1	A	76	MET	1
1	A	88	GLU	1
1	A	133	SER	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 88% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping (i)

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

Total number of shifts	940
Number of shifts mapped to atoms	940
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	80	$-0.40 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	74	$0.15 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	72	$-0.01 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	77	$-0.76 \pm 0.49$	None needed (imprecise)

#### 7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 902 atoms were assigned a chemical shift out of a possible 1034. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	376/394 (95%)	156/161 (97%)	146/156 (94%)	74/77 (96%)
Sidechain	492/594 (83%)	328/388 (85%)	164/190 (86%)	0/16 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	34/46 (74%)	17/23 (74%)	17/19 (89%)	0/4 (0%)
Overall	902/1034 (87%)	501/572 (88%)	327/365 (90%)	74/97 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 940 atoms were assigned a chemical shift out of a possible 1073. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	391/409 (96%)	162/167 (97%)	152/162 (94%)	77/80 (96%)
Sidechain	515/618 (83%)	344/404 (85%)	171/198 (86%)	0/16 (0%)
Aromatic	34/46 (74%)	17/23 (74%)	17/19 (89%)	0/4 (0%)
Overall	940/1073 (88%)	523/594 (88%)	340/379 (90%)	77/100 (77%)

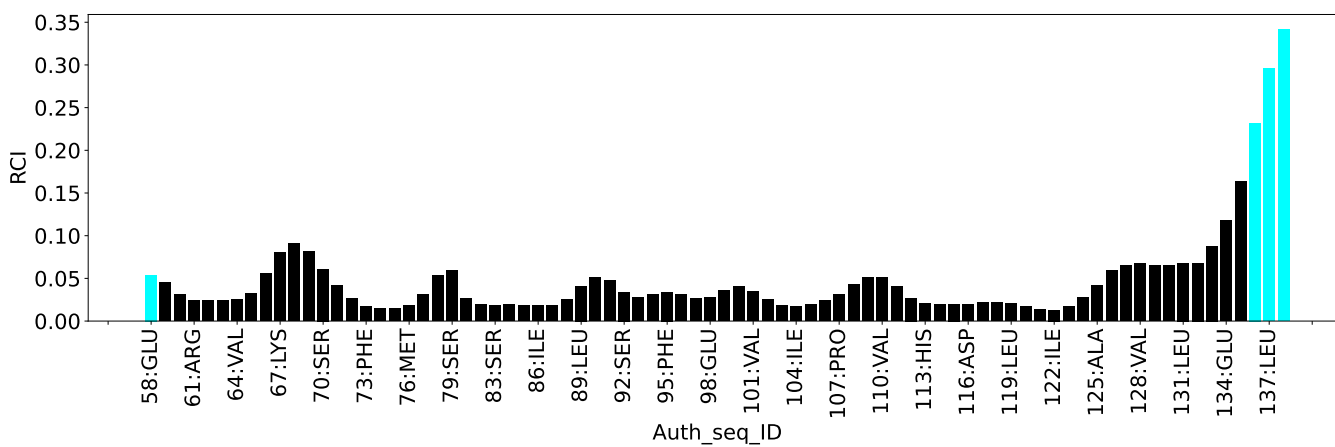
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2018
Intra-residue ( $ i-j =0$ )	617
Sequential ( $ i-j =1$ )	395
Medium range ( $ i-j >1$ and $ i-j <5$ )	359
Long range ( $ i-j \geq 5$ )	647
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	144
Number of unmapped restraints	0
Number of restraints per residue	15.7
Number of long range restraints per residue <sup>1</sup>	4.7

<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)	81.9	0.2
0.2-0.5 (Medium)	167.4	0.5
>0.5 (Large)	203.3	3.8

### 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)	8.9	6.31
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis

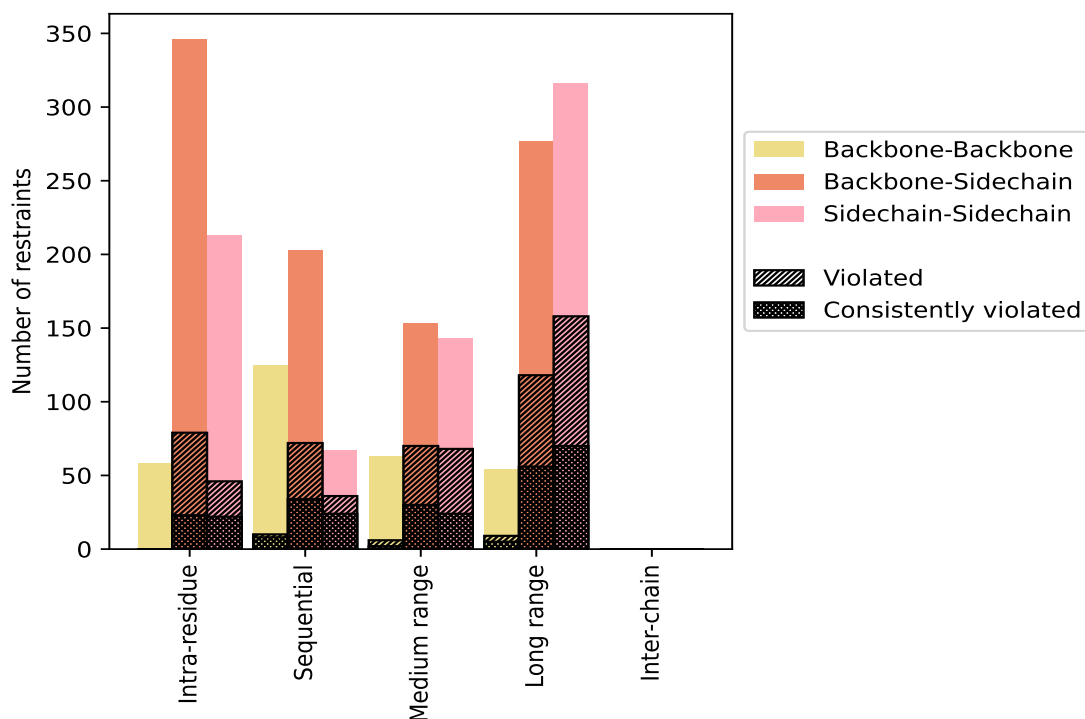
### 9.1 Summary of distance violations

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>617</b>	<b>30.6</b>	<b>125</b>	<b>20.3</b>	<b>6.2</b>	<b>45</b>	<b>7.3</b>	<b>2.2</b>
Backbone-Backbone	58	2.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	346	17.1	79	22.8	3.9	23	6.6	1.1
Sidechain-Sidechain	213	10.6	46	21.6	2.3	22	10.3	1.1
<b>Sequential (<math> i-j =1</math>)</b>	<b>395</b>	<b>19.6</b>	<b>118</b>	<b>29.9</b>	<b>5.8</b>	<b>66</b>	<b>16.7</b>	<b>3.3</b>
Backbone-Backbone	125	6.2	10	8.0	0.5	8	6.4	0.4
Backbone-Sidechain	203	10.1	72	35.5	3.6	34	16.7	1.7
Sidechain-Sidechain	67	3.3	36	53.7	1.8	24	35.8	1.2
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>359</b>	<b>17.8</b>	<b>144</b>	<b>40.1</b>	<b>7.1</b>	<b>56</b>	<b>15.6</b>	<b>2.8</b>
Backbone-Backbone	63	3.1	6	9.5	0.3	2	3.2	0.1
Backbone-Sidechain	153	7.6	70	45.8	3.5	30	19.6	1.5
Sidechain-Sidechain	143	7.1	68	47.6	3.4	24	16.8	1.2
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>647</b>	<b>32.1</b>	<b>285</b>	<b>44.0</b>	<b>14.1</b>	<b>131</b>	<b>20.2</b>	<b>6.5</b>
Backbone-Backbone	54	2.7	9	16.7	0.4	5	9.3	0.2
Backbone-Sidechain	277	13.7	118	42.6	5.8	56	20.2	2.8
Sidechain-Sidechain	316	15.7	158	50.0	7.8	70	22.2	3.5
<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>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>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>2018</b>	<b>100.0</b>	<b>672</b>	<b>33.3</b>	<b>33.3</b>	<b>298</b>	<b>14.8</b>	<b>14.8</b>
Backbone-Backbone	300	14.9	25	8.3	1.2	15	5.0	0.7
Backbone-Sidechain	979	48.5	339	34.6	16.8	143	14.6	7.1
Sidechain-Sidechain	739	36.6	308	41.7	15.3	140	18.9	6.9

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

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



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

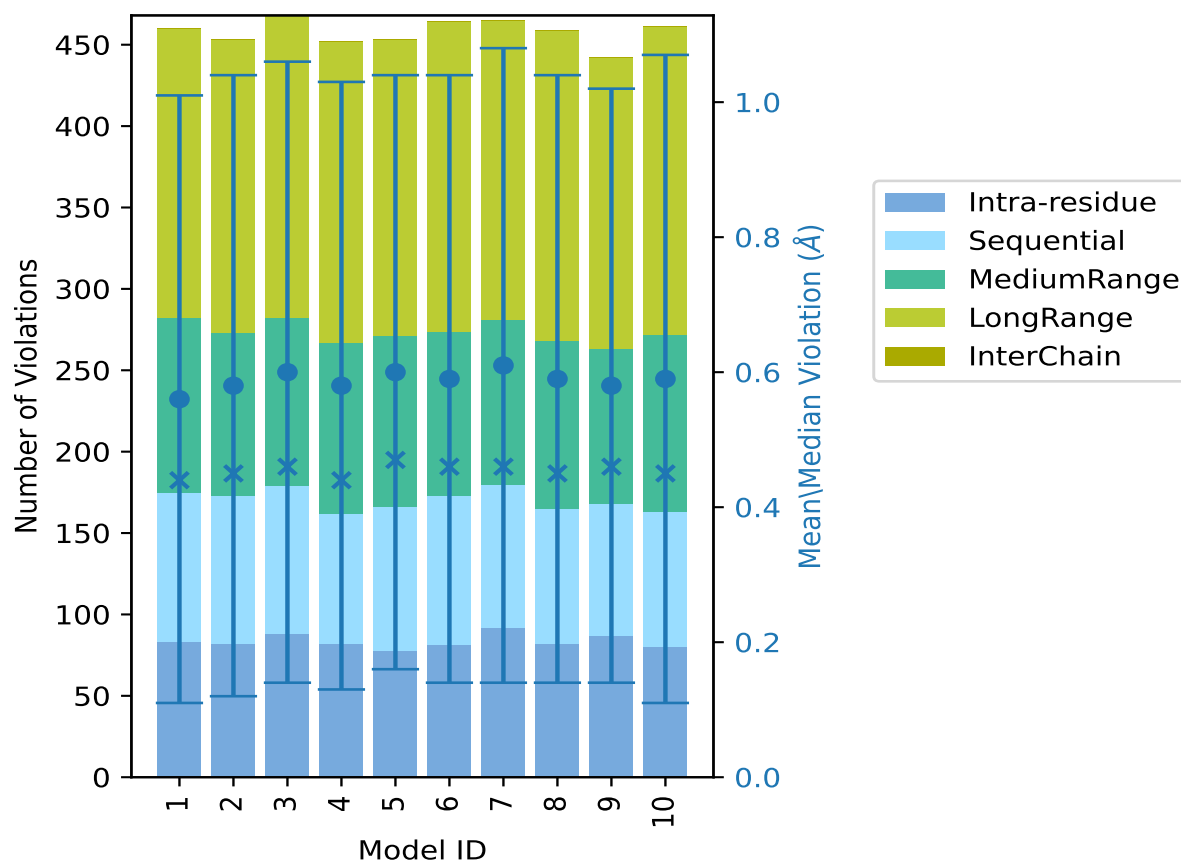
## 9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	83	92	107	178	0	460	0.56	3.62	0.45	0.44
2	82	91	100	180	0	453	0.58	3.26	0.46	0.45
3	88	91	103	186	0	468	0.6	3.11	0.46	0.46
4	82	80	105	185	0	452	0.58	3.19	0.45	0.44
5	78	88	105	182	0	453	0.6	2.76	0.44	0.47
6	81	92	101	190	0	464	0.59	3.06	0.45	0.46
7	92	88	101	184	0	465	0.61	3.25	0.47	0.46
8	82	83	103	191	0	459	0.59	3.47	0.45	0.45
9	87	81	95	179	0	442	0.58	3.54	0.44	0.46
10	80	83	109	189	0	461	0.59	3.8	0.48	0.45

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1346(IR:492, SQ:277, MR:215, LR:362, 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>	%
18	13	24	43	0	98	1	10.0
11	11	17	20	0	59	2	20.0
10	0	4	15	0	29	3	30.0

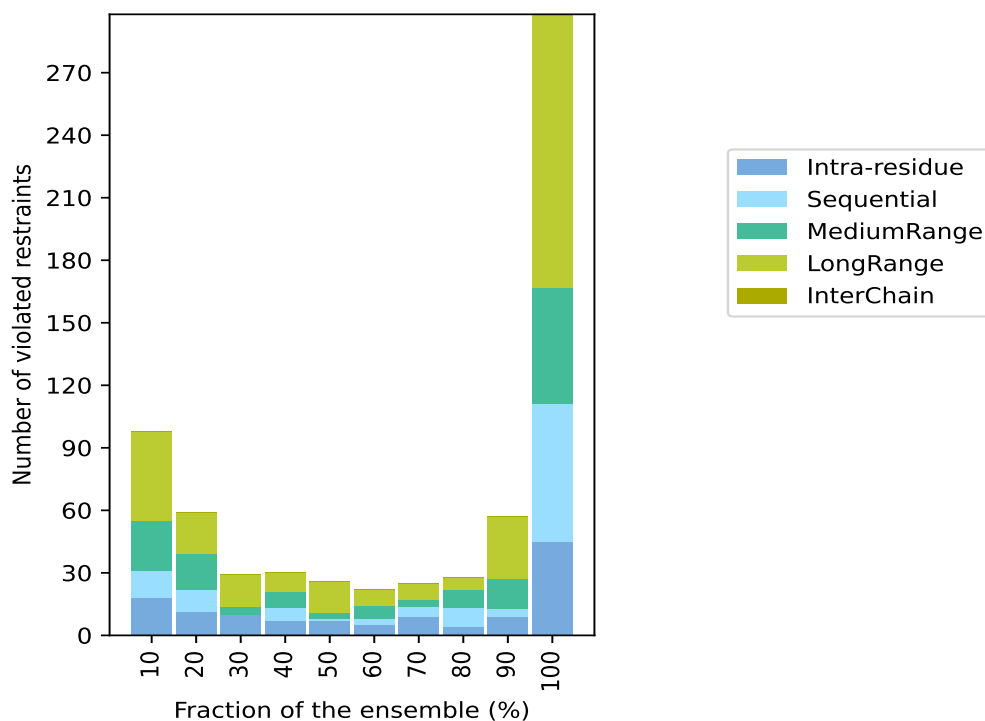
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
7	6	8	9	0	30	4	40.0
7	1	3	15	0	26	5	50.0
5	3	6	8	0	22	6	60.0
9	5	3	8	0	25	7	70.0
4	9	9	6	0	28	8	80.0
9	4	14	30	0	57	9	90.0
45	66	56	131	0	298	10	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

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

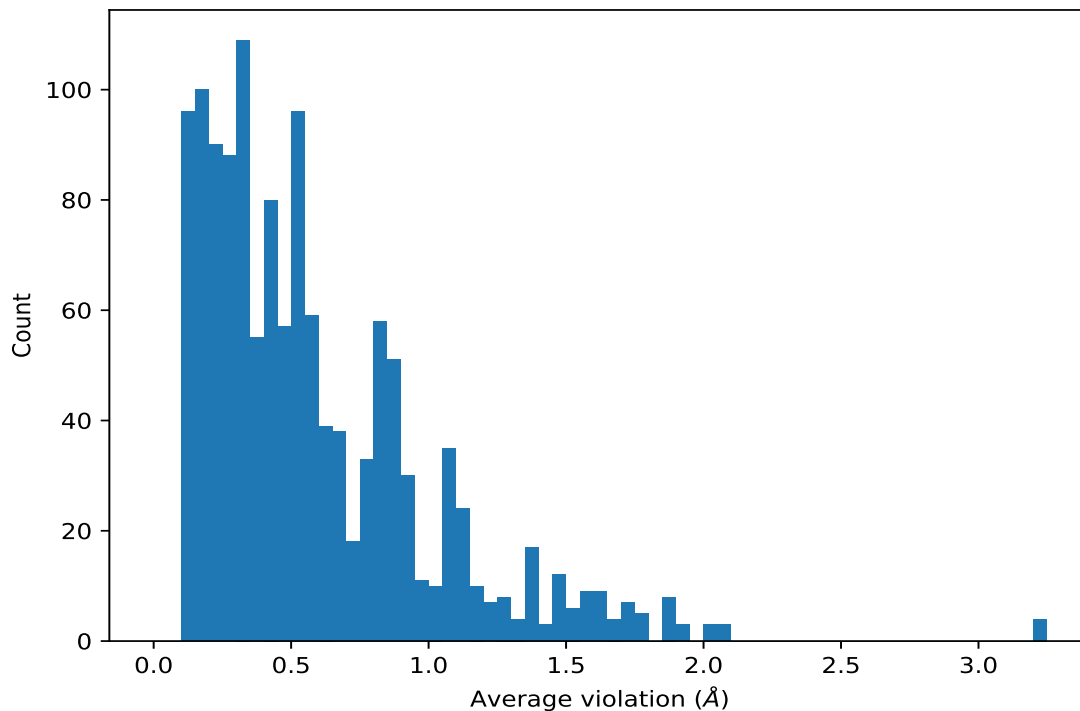


## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1415)	1:128:A:VAL:HG22	1:62:A:LEU:HG	10	3.2	0.29	3.22
(2,1415)	1:128:A:VAL:HG23	1:62:A:LEU:HG	10	3.2	0.29	3.22
(2,1415)	1:128:A:VAL:HG12	1:62:A:LEU:HG	10	3.2	0.29	3.22
(2,1415)	1:128:A:VAL:HG21	1:62:A:LEU:HG	10	3.2	0.29	3.22
(2,1296)	1:86:A:ILE:HG13	1:82:A:PHE:HD1	10	2.09	0.04	2.1
(2,1296)	1:85:A:ARG:H	1:86:A:ILE:HG13	10	2.09	0.04	2.1
(2,1296)	1:86:A:ILE:HG13	1:82:A:PHE:HD2	10	2.09	0.04	2.1
(2,1399)	1:101:A:VAL:HG13	1:104:A:ILE:HB	10	2.04	0.07	2.05
(2,1399)	1:101:A:VAL:HG12	1:104:A:ILE:HB	10	2.04	0.07	2.05
(2,1399)	1:101:A:VAL:HG11	1:104:A:ILE:HB	10	2.04	0.07	2.05
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD13	10	1.91	0.08	1.9
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD12	10	1.91	0.08	1.9
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD11	10	1.91	0.08	1.9
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD21	10	1.9	0.17	2.0
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD22	10	1.9	0.17	2.0

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD23	10	1.9	0.17	2.0
(2,1530)	1:129:A:VAL:HA	1:119:A:LEU:HB2	10	1.9	0.07	1.88
(2,1530)	1:129:A:VAL:HA	1:61:A:ARG:HG2	10	1.9	0.07	1.88
(2,1842)	1:85:A:ARG:H	1:87:A:GLU:HB3	10	1.9	0.14	1.94
(2,1504)	1:70:A:SER:HB3	1:64:A:VAL:HG21	10	1.75	0.25	1.67
(2,1504)	1:70:A:SER:HB3	1:64:A:VAL:HG23	10	1.75	0.25	1.67
(2,1504)	1:70:A:SER:HB3	1:64:A:VAL:HG22	10	1.75	0.25	1.67
(2,1504)	1:70:A:SER:HB2	1:64:A:VAL:HG22	10	1.75	0.25	1.67
(2,1504)	1:70:A:SER:HB2	1:64:A:VAL:HG23	10	1.75	0.25	1.67
(2,846)	1:85:A:ARG:H	1:86:A:ILE:HG13	10	1.71	0.02	1.71
(2,709)	1:119:A:LEU:HB3	1:116:A:ASP:HA	10	1.71	0.07	1.73
(2,1736)	1:71:A:LYS:HE2	1:73:A:PHE:HD2	10	1.68	0.31	1.78
(2,1736)	1:71:A:LYS:HE3	1:73:A:PHE:HD2	10	1.68	0.31	1.78
(2,1736)	1:71:A:LYS:HE3	1:73:A:PHE:HD1	10	1.68	0.31	1.78
(2,1736)	1:71:A:LYS:HE2	1:73:A:PHE:HD1	10	1.68	0.31	1.78
(2,1395)	1:101:A:VAL:HG13	1:73:A:PHE:HE2	10	1.61	0.06	1.6
(2,1395)	1:101:A:VAL:HG12	1:73:A:PHE:HE2	10	1.61	0.06	1.6
(2,1395)	1:101:A:VAL:HG13	1:73:A:PHE:HE1	10	1.61	0.06	1.6
(2,1395)	1:101:A:VAL:HG12	1:73:A:PHE:HE1	10	1.61	0.06	1.6
(2,1395)	1:101:A:VAL:HG11	1:73:A:PHE:HE2	10	1.61	0.06	1.6
(2,1371)	1:101:A:VAL:HG22	1:67:A:LYS:HE3	10	1.6	0.19	1.56
(2,1371)	1:101:A:VAL:HG21	1:67:A:LYS:HE2	10	1.6	0.19	1.56
(2,1371)	1:101:A:VAL:HG22	1:67:A:LYS:HE2	10	1.6	0.19	1.56
(2,1371)	1:101:A:VAL:HG23	1:67:A:LYS:HE2	10	1.6	0.19	1.56
(2,143)	1:93:A:ILE:HG13	1:82:A:PHE:HB2	10	1.59	0.05	1.59
(2,311)	1:135:A:VAL:HG22	1:133:A:SER:HB2	10	1.57	0.21	1.56
(2,311)	1:135:A:VAL:HG21	1:133:A:SER:HB2	10	1.57	0.21	1.56
(2,311)	1:135:A:VAL:HG23	1:133:A:SER:HB2	10	1.57	0.21	1.56
(2,311)	1:135:A:VAL:HG12	1:133:A:SER:HB2	10	1.57	0.21	1.56
(2,403)	1:84:A:THR:HA	1:87:A:GLU:HB3	10	1.57	0.07	1.59
(2,1376)	1:129:A:VAL:HG13	1:127:A:GLY:HA2	10	1.55	0.07	1.52
(2,1376)	1:129:A:VAL:HG12	1:127:A:GLY:HA2	10	1.55	0.07	1.52
(2,1376)	1:129:A:VAL:HG11	1:127:A:GLY:HA2	10	1.55	0.07	1.52
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG23	10	1.54	0.07	1.54
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG21	10	1.54	0.07	1.54
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG22	10	1.54	0.07	1.54
(2,1369)	1:110:A:VAL:HG23	1:86:A:ILE:HA	10	1.51	0.07	1.52
(2,1369)	1:110:A:VAL:HG22	1:86:A:ILE:HA	10	1.51	0.07	1.52
(2,1369)	1:110:A:VAL:HG21	1:86:A:ILE:HA	10	1.51	0.07	1.52
(2,1426)	1:124:A:ALA:HB3	1:117:A:GLN:HB3	10	1.49	0.38	1.38
(2,1426)	1:124:A:ALA:HB2	1:117:A:GLN:HB2	10	1.49	0.38	1.38
(2,1426)	1:124:A:ALA:HB2	1:117:A:GLN:HB3	10	1.49	0.38	1.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1426)	1:124:A:ALA:HB1	1:117:A:GLN:HB3	10	1.49	0.38	1.38
(2,1426)	1:124:A:ALA:HB3	1:117:A:GLN:HB2	10	1.49	0.38	1.38
(2,1435)	1:104:A:ILE:HG23	1:91:A:GLY:HA2	10	1.47	0.08	1.49
(2,1435)	1:104:A:ILE:HG21	1:91:A:GLY:HA2	10	1.47	0.08	1.49
(2,1435)	1:104:A:ILE:HG22	1:91:A:GLY:HA2	10	1.47	0.08	1.49
(2,1482)	1:118:A:LEU:HD23	1:84:A:THR:HB	10	1.47	0.28	1.41
(2,1482)	1:118:A:LEU:HD22	1:84:A:THR:HB	10	1.47	0.28	1.41
(2,1482)	1:97:A:THR:HB	1:96:A:LEU:HD13	10	1.47	0.28	1.41
(2,1482)	1:118:A:LEU:HD21	1:84:A:THR:HB	10	1.47	0.28	1.41
(1,15)	1:136:A:LYS:HD3	1:107:A:PRO:HB2	10	1.43	0.22	1.41
(2,1624)	1:118:A:LEU:HA	1:114:A:ASP:HB2	10	1.4	0.3	1.54
(2,1624)	1:76:A:MET:HG3	1:118:A:LEU:HA	10	1.4	0.3	1.54
(2,1554)	1:86:A:ILE:HA	1:87:A:GLU:HB3	10	1.38	0.15	1.41
(2,1554)	1:86:A:ILE:HA	1:88:A:GLU:HB3	10	1.38	0.15	1.41
(2,1421)	1:125:A:ALA:HB2	1:122:A:ILE:HD11	10	1.38	0.13	1.38
(2,1421)	1:125:A:ALA:HB3	1:122:A:ILE:HD13	10	1.38	0.13	1.38
(2,1421)	1:125:A:ALA:HB1	1:122:A:ILE:HD12	10	1.38	0.13	1.38
(2,1421)	1:125:A:ALA:HB1	1:122:A:ILE:HD11	10	1.38	0.13	1.38
(2,1421)	1:125:A:ALA:HB1	1:122:A:ILE:HD13	10	1.38	0.13	1.38
(2,1421)	1:125:A:ALA:HB3	1:122:A:ILE:HD12	10	1.38	0.13	1.38
(2,1421)	1:125:A:ALA:HB2	1:122:A:ILE:HD12	10	1.38	0.13	1.38
(2,1421)	1:125:A:ALA:HB2	1:122:A:ILE:HD13	10	1.38	0.13	1.38
(2,1933)	1:92:A:SER:H	1:104:A:ILE:HG12	10	1.36	0.08	1.38
(2,1933)	1:92:A:SER:H	1:93:A:ILE:HD13	10	1.36	0.08	1.38
(2,1579)	1:104:A:ILE:HA	1:105:A:GLU:HG2	10	1.36	0.03	1.35
(1,7)	1:107:A:PRO:HB2	1:59:A:MET:HG3	10	1.31	0.14	1.28
(2,1226)	1:66:A:GLU:HB2	1:73:A:PHE:HB3	10	1.3	0.14	1.26
(2,1226)	1:71:A:LYS:HB3	1:72:A:ASN:HB2	10	1.3	0.14	1.26
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD12	10	1.28	0.07	1.3
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD11	10	1.28	0.07	1.3
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD13	10	1.28	0.07	1.3
(2,88)	1:63:A:MET:HB2	1:132:A:ASP:HB2	10	1.25	0.33	1.27
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD23	10	1.25	0.03	1.26
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD21	10	1.25	0.03	1.26
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD22	10	1.25	0.03	1.26
(2,86)	1:63:A:MET:HB2	1:132:A:ASP:HB3	10	1.24	0.26	1.28
(2,1470)	1:86:A:ILE:HD11	1:122:A:ILE:HG13	10	1.23	0.27	1.37
(2,1470)	1:86:A:ILE:HD13	1:122:A:ILE:HG13	10	1.23	0.27	1.37
(2,1470)	1:86:A:ILE:HD12	1:122:A:ILE:HG13	10	1.23	0.27	1.37
(2,1309)	1:118:A:LEU:HD13	1:121:A:ASP:HB3	10	1.22	0.14	1.27
(2,1309)	1:118:A:LEU:HD12	1:113:A:HIS:HB2	10	1.22	0.14	1.27
(2,1309)	1:118:A:LEU:HD11	1:121:A:ASP:HB3	10	1.22	0.14	1.27

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG23	10	1.18	0.04	1.17
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG22	10	1.18	0.04	1.17
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG21	10	1.18	0.04	1.17
(2,237)	1:110:A:VAL:HG13	1:107:A:PRO:HD3	10	1.17	0.08	1.16
(2,237)	1:110:A:VAL:HG11	1:107:A:PRO:HD3	10	1.17	0.08	1.16
(2,237)	1:110:A:VAL:HG12	1:107:A:PRO:HD3	10	1.17	0.08	1.16
(2,1301)	1:118:A:LEU:HG	1:117:A:GLN:HA	10	1.16	0.09	1.17
(2,1701)	1:107:A:PRO:HG3	1:106:A:LEU:HB2	10	1.14	0.03	1.15
(2,1355)	1:123:A:LEU:HD13	1:104:A:ILE:HD12	10	1.14	0.07	1.16
(2,1355)	1:123:A:LEU:HD13	1:104:A:ILE:HD13	10	1.14	0.07	1.16
(2,1355)	1:123:A:LEU:HD12	1:104:A:ILE:HD13	10	1.14	0.07	1.16
(2,1355)	1:123:A:LEU:HD11	1:104:A:ILE:HD11	10	1.14	0.07	1.16
(2,1355)	1:123:A:LEU:HD12	1:104:A:ILE:HD12	10	1.14	0.07	1.16
(2,1451)	1:125:A:ALA:HB2	1:122:A:ILE:HG21	10	1.14	0.1	1.1
(2,1451)	1:125:A:ALA:HB3	1:122:A:ILE:HG22	10	1.14	0.1	1.1
(2,1451)	1:125:A:ALA:HB1	1:122:A:ILE:HG21	10	1.14	0.1	1.1
(2,1451)	1:125:A:ALA:HB1	1:122:A:ILE:HG23	10	1.14	0.1	1.1
(2,1451)	1:125:A:ALA:HB2	1:122:A:ILE:HG22	10	1.14	0.1	1.1
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB3	10	1.14	0.16	1.12
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB2	10	1.14	0.16	1.12
(2,134)	1:120:A:HIS:HB3	1:119:A:LEU:HB3	10	1.14	0.06	1.16
(1,4)	1:58:A:GLU:HG2	1:91:A:GLY:HA3	10	1.13	0.63	0.75
(2,1712)	1:91:A:GLY:HA2	1:86:A:ILE:HB	10	1.13	0.11	1.15
(2,1500)	1:66:A:GLU:HB2	1:70:A:SER:HB2	10	1.12	0.21	1.07
(2,1500)	1:133:A:SER:HB3	1:105:A:GLU:HG3	10	1.12	0.21	1.07
(2,1500)	1:128:A:VAL:HB	1:70:A:SER:HB2	10	1.12	0.21	1.07
(2,1387)	1:84:A:THR:HG23	1:86:A:ILE:HA	10	1.1	0.15	1.06
(2,1387)	1:84:A:THR:HG22	1:86:A:ILE:HA	10	1.1	0.15	1.06
(2,1387)	1:84:A:THR:HG21	1:86:A:ILE:HA	10	1.1	0.15	1.06
(2,1302)	1:62:A:LEU:HG	1:122:A:ILE:HG13	10	1.1	0.27	1.14
(2,1302)	1:62:A:LEU:HG	1:103:A:MET:HG2	10	1.1	0.27	1.14
(2,1360)	1:119:A:LEU:HD21	1:115:A:MET:HG3	10	1.08	0.08	1.08
(2,1360)	1:63:A:MET:HB2	1:96:A:LEU:HD23	10	1.08	0.08	1.08
(2,1360)	1:119:A:LEU:HD22	1:115:A:MET:HG3	10	1.08	0.08	1.08
(2,1360)	1:63:A:MET:HB2	1:96:A:LEU:HD21	10	1.08	0.08	1.08
(2,1360)	1:63:A:MET:HB2	1:96:A:LEU:HD22	10	1.08	0.08	1.08
(2,1374)	1:129:A:VAL:HG11	1:73:A:PHE:HE1	10	1.07	0.14	1.06
(2,1374)	1:129:A:VAL:HG13	1:73:A:PHE:HE1	10	1.07	0.14	1.06
(2,1374)	1:129:A:VAL:HG12	1:73:A:PHE:HE1	10	1.07	0.14	1.06
(2,1374)	1:129:A:VAL:HG13	1:73:A:PHE:HE2	10	1.07	0.14	1.06
(2,1374)	1:129:A:VAL:HG12	1:73:A:PHE:HE2	10	1.07	0.14	1.06
(2,1738)	1:75:A:LYS:HE3	1:95:A:PHE:HE2	10	1.07	0.19	1.09

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1738)	1:71:A:LYS:HE3	1:95:A:PHE:HE2	10	1.07	0.19	1.09
(2,1738)	1:75:A:LYS:HE3	1:95:A:PHE:HE1	10	1.07	0.19	1.09
(2,1738)	1:71:A:LYS:HE2	1:95:A:PHE:HE2	10	1.07	0.19	1.09
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG21	10	1.07	0.07	1.09
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG22	10	1.07	0.07	1.09
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG23	10	1.07	0.07	1.09
(2,1833)	1:137:A:LEU:H	1:135:A:VAL:HB	10	1.06	0.17	1.13
(2,1833)	1:137:A:LEU:H	1:105:A:GLU:HG3	10	1.06	0.17	1.13
(2,1444)	1:86:A:ILE:HG23	1:92:A:SER:HB3	10	1.05	0.11	1.06
(2,1444)	1:93:A:ILE:HG23	1:94:A:SER:HB3	10	1.05	0.11	1.06
(2,1444)	1:86:A:ILE:HG22	1:92:A:SER:HB3	10	1.05	0.11	1.06
(2,1444)	1:86:A:ILE:HG21	1:92:A:SER:HB3	10	1.05	0.11	1.06
(1,29)	1:82:A:PHE:HA	1:86:A:ILE:HG13	10	1.05	0.06	1.04
(2,1386)	1:109:A:THR:HG22	1:58:A:GLU:HG2	10	1.05	0.29	1.02
(2,1386)	1:84:A:THR:HG22	1:88:A:GLU:HB3	10	1.05	0.29	1.02
(2,1386)	1:109:A:THR:HG21	1:58:A:GLU:HG2	10	1.05	0.29	1.02
(2,1386)	1:109:A:THR:HG23	1:58:A:GLU:HG2	10	1.05	0.29	1.02
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD11	10	1.04	0.12	1.0
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD12	10	1.04	0.12	1.0
(2,1506)	1:66:A:GLU:HB2	1:70:A:SER:HB2	10	1.03	0.19	0.99
(2,1506)	1:128:A:VAL:HB	1:70:A:SER:HB2	10	1.03	0.19	0.99
(2,1708)	1:91:A:GLY:HA3	1:60:A:THR:HB	10	1.01	0.12	1.0
(2,1708)	1:91:A:GLY:HA3	1:89:A:LEU:HA	10	1.01	0.12	1.0
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG22	10	0.97	0.25	0.96
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG23	10	0.97	0.25	0.96
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG21	10	0.97	0.25	0.96
(2,1304)	1:118:A:LEU:HD13	1:82:A:PHE:HE1	10	0.97	0.08	0.96
(2,1304)	1:118:A:LEU:HD11	1:82:A:PHE:HE1	10	0.97	0.08	0.96
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB2	10	0.96	0.13	0.95
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB3	10	0.96	0.13	0.95
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB1	10	0.96	0.13	0.95
(2,59)	1:105:A:GLU:HG3	1:59:A:MET:HG3	10	0.94	0.21	1.02
(2,1378)	1:64:A:VAL:HG11	1:129:A:VAL:HA	10	0.94	0.12	0.96
(2,1378)	1:64:A:VAL:HG13	1:129:A:VAL:HA	10	0.94	0.12	0.96
(2,1378)	1:64:A:VAL:HG11	1:101:A:VAL:HA	10	0.94	0.12	0.96
(2,1378)	1:64:A:VAL:HG13	1:101:A:VAL:HA	10	0.94	0.12	0.96
(2,1378)	1:64:A:VAL:HG12	1:129:A:VAL:HA	10	0.94	0.12	0.96
(2,1412)	1:128:A:VAL:HG12	1:126:A:GLY:HA2	10	0.93	0.33	0.9
(2,1412)	1:128:A:VAL:HG11	1:126:A:GLY:HA2	10	0.93	0.33	0.9
(2,1412)	1:128:A:VAL:HG12	1:130:A:GLY:HA2	10	0.93	0.33	0.9
(2,1412)	1:128:A:VAL:HG13	1:126:A:GLY:HA2	10	0.93	0.33	0.9
(2,1412)	1:128:A:VAL:HG23	1:130:A:GLY:HA2	10	0.93	0.33	0.9

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,446)	1:118:A:LEU:HD23	1:81:A:SER:HA	10	0.92	0.1	0.96
(2,446)	1:118:A:LEU:HD21	1:81:A:SER:HA	10	0.92	0.1	0.96
(2,446)	1:118:A:LEU:HD22	1:81:A:SER:HA	10	0.92	0.1	0.96
(2,1446)	1:86:A:ILE:HG22	1:107:A:PRO:HG3	10	0.92	0.09	0.94
(2,1446)	1:86:A:ILE:HG23	1:107:A:PRO:HG3	10	0.92	0.09	0.94
(2,1446)	1:86:A:ILE:HG21	1:107:A:PRO:HG3	10	0.92	0.09	0.94
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG12	10	0.91	0.09	0.91
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG13	10	0.91	0.09	0.91
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG11	10	0.91	0.09	0.91
(2,1867)	1:88:A:GLU:H	1:86:A:ILE:HB	10	0.91	0.06	0.92
(2,679)	1:89:A:LEU:HB3	1:114:A:ASP:HB2	10	0.9	0.15	0.96
(2,1190)	1:107:A:PRO:HB3	1:90:A:GLY:HA2	10	0.9	0.17	0.99
(2,1190)	1:59:A:MET:HG2	1:133:A:SER:HB2	10	0.9	0.17	0.99
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG12	10	0.89	0.1	0.88
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG11	10	0.89	0.1	0.88
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG23	10	0.89	0.1	0.88
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG22	10	0.89	0.1	0.88
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG13	10	0.89	0.1	0.88
(2,946)	1:58:A:GLU:H	1:58:A:GLU:HB2	10	0.89	0.16	0.84
(2,1653)	1:66:A:GLU:HA	1:74:A:SER:HA	10	0.89	0.21	0.82
(2,1805)	1:61:A:ARG:H	1:131:A:LEU:HD11	10	0.89	0.32	0.86
(2,1805)	1:61:A:ARG:H	1:137:A:LEU:HD12	10	0.89	0.32	0.86
(2,1805)	1:61:A:ARG:H	1:131:A:LEU:HD13	10	0.89	0.32	0.86
(2,1805)	1:61:A:ARG:H	1:137:A:LEU:HD23	10	0.89	0.32	0.86
(2,1805)	1:61:A:ARG:H	1:137:A:LEU:HD21	10	0.89	0.32	0.86
(2,1805)	1:61:A:ARG:H	1:131:A:LEU:HD12	10	0.89	0.32	0.86
(2,1805)	1:61:A:ARG:H	1:137:A:LEU:HD11	10	0.89	0.32	0.86
(2,1805)	1:61:A:ARG:H	1:137:A:LEU:HD22	10	0.89	0.32	0.86
(2,586)	1:71:A:LYS:HA	1:66:A:GLU:HB2	10	0.88	0.14	0.88
(2,1379)	1:64:A:VAL:HG13	1:102:A:THR:HG23	10	0.88	0.06	0.86
(2,1379)	1:64:A:VAL:HG12	1:102:A:THR:HG22	10	0.88	0.06	0.86
(2,1379)	1:64:A:VAL:HG12	1:102:A:THR:HG21	10	0.88	0.06	0.86
(2,1379)	1:64:A:VAL:HG11	1:102:A:THR:HG23	10	0.88	0.06	0.86
(2,1379)	1:64:A:VAL:HG13	1:102:A:THR:HG21	10	0.88	0.06	0.86
(2,1379)	1:64:A:VAL:HG11	1:122:A:ILE:HG12	10	0.88	0.06	0.86
(2,623)	1:59:A:MET:HA	1:107:A:PRO:HB2	10	0.88	0.08	0.87
(2,1608)	1:76:A:MET:HA	1:77:A:ALA:HB1	10	0.88	0.03	0.88
(2,1608)	1:76:A:MET:HA	1:77:A:ALA:HB2	10	0.88	0.03	0.88
(2,1608)	1:117:A:GLN:HA	1:118:A:LEU:HD22	10	0.88	0.03	0.88
(2,1608)	1:117:A:GLN:HA	1:118:A:LEU:HD23	10	0.88	0.03	0.88
(2,1608)	1:117:A:GLN:HA	1:118:A:LEU:HD21	10	0.88	0.03	0.88
(2,360)	1:122:A:ILE:HG22	1:127:A:GLY:HA2	10	0.87	0.11	0.86

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,360)	1:122:A:ILE:HG23	1:127:A:GLY:HA2	10	0.87	0.11	0.86
(2,360)	1:122:A:ILE:HG21	1:127:A:GLY:HA2	10	0.87	0.11	0.86
(2,1358)	1:119:A:LEU:HD22	1:121:A:ASP:HB3	10	0.87	0.11	0.89
(2,1358)	1:119:A:LEU:HD21	1:121:A:ASP:HB3	10	0.87	0.11	0.89
(2,1358)	1:119:A:LEU:HD23	1:121:A:ASP:HB3	10	0.87	0.11	0.89
(2,1358)	1:137:A:LEU:HD21	1:136:A:LYS:HE2	10	0.87	0.11	0.89
(2,1866)	1:88:A:GLU:H	1:88:A:GLU:HB3	10	0.87	0.06	0.88
(2,1866)	1:88:A:GLU:H	1:87:A:GLU:HB3	10	0.87	0.06	0.88
(2,1242)	1:120:A:HIS:HB2	1:122:A:ILE:HB	10	0.87	0.02	0.86
(2,1242)	1:120:A:HIS:HB2	1:123:A:LEU:HB3	10	0.87	0.02	0.86
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD22	10	0.86	0.07	0.87
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD23	10	0.86	0.07	0.87
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD21	10	0.86	0.07	0.87
(2,1348)	1:62:A:LEU:HD21	1:115:A:MET:HG3	10	0.86	0.1	0.84
(2,1348)	1:62:A:LEU:HD23	1:115:A:MET:HG3	10	0.86	0.1	0.84
(2,1348)	1:62:A:LEU:HD22	1:115:A:MET:HG3	10	0.86	0.1	0.84
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD12	10	0.86	0.05	0.85
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD11	10	0.86	0.05	0.85
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD13	10	0.86	0.05	0.85
(2,1455)	1:93:A:ILE:HD12	1:78:A:LYS:HD3	10	0.85	0.21	0.88
(2,1455)	1:93:A:ILE:HD13	1:78:A:LYS:HD3	10	0.85	0.21	0.88
(2,1455)	1:93:A:ILE:HD11	1:78:A:LYS:HD3	10	0.85	0.21	0.88
(2,1455)	1:93:A:ILE:HD11	1:85:A:ARG:HG2	10	0.85	0.21	0.88
(2,1578)	1:102:A:THR:HG22	1:93:A:ILE:HA	10	0.85	0.05	0.85
(2,1578)	1:102:A:THR:HG21	1:93:A:ILE:HA	10	0.85	0.05	0.85
(2,1578)	1:102:A:THR:HG23	1:93:A:ILE:HA	10	0.85	0.05	0.85
(2,1433)	1:77:A:ALA:HB3	1:78:A:LYS:HB2	10	0.84	0.27	0.93
(2,1433)	1:77:A:ALA:HB1	1:78:A:LYS:HB2	10	0.84	0.27	0.93
(2,1433)	1:77:A:ALA:HB2	1:78:A:LYS:HB2	10	0.84	0.27	0.93
(2,1433)	1:77:A:ALA:HB3	1:76:A:MET:HG2	10	0.84	0.27	0.93
(2,1741)	1:136:A:LYS:HE2	1:136:A:LYS:HA	10	0.84	0.52	0.7
(2,1741)	1:71:A:LYS:HE2	1:72:A:ASN:HA	10	0.84	0.52	0.7
(2,1432)	1:124:A:ALA:HB3	1:123:A:LEU:HB3	10	0.82	0.04	0.84
(2,1432)	1:124:A:ALA:HB2	1:123:A:LEU:HB3	10	0.82	0.04	0.84
(2,1432)	1:124:A:ALA:HB1	1:123:A:LEU:HB3	10	0.82	0.04	0.84
(2,1406)	1:135:A:VAL:HG13	1:107:A:PRO:HD3	10	0.82	0.2	0.9
(2,1406)	1:135:A:VAL:HG12	1:107:A:PRO:HD3	10	0.82	0.2	0.9
(2,1406)	1:135:A:VAL:HG11	1:107:A:PRO:HD3	10	0.82	0.2	0.9
(2,1657)	1:61:A:ARG:HG2	1:105:A:GLU:HA	10	0.82	0.04	0.82
(2,1657)	1:105:A:GLU:HA	1:106:A:LEU:HB3	10	0.82	0.04	0.82
(2,1071)	1:86:A:ILE:H	1:86:A:ILE:HG13	10	0.82	0.03	0.82
(2,867)	1:87:A:GLU:H	1:86:A:ILE:HG13	10	0.81	0.06	0.82

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1431)	1:124:A:ALA:HB2	1:76:A:MET:HG3	10	0.81	0.24	0.73
(2,1431)	1:124:A:ALA:HB1	1:76:A:MET:HG3	10	0.81	0.24	0.73
(2,1431)	1:124:A:ALA:HB3	1:76:A:MET:HG3	10	0.81	0.24	0.73
(2,612)	1:77:A:ALA:HA	1:76:A:MET:HB2	10	0.81	0.03	0.8
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD13	10	0.8	0.04	0.8
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD12	10	0.8	0.04	0.8
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD11	10	0.8	0.04	0.8
(2,375)	1:64:A:VAL:HG13	1:122:A:ILE:HD11	10	0.8	0.11	0.82
(2,375)	1:64:A:VAL:HG12	1:122:A:ILE:HD13	10	0.8	0.11	0.82
(2,375)	1:64:A:VAL:HG13	1:122:A:ILE:HD12	10	0.8	0.11	0.82
(2,375)	1:64:A:VAL:HG11	1:122:A:ILE:HD12	10	0.8	0.11	0.82
(2,375)	1:64:A:VAL:HG11	1:122:A:ILE:HD13	10	0.8	0.11	0.82
(2,1388)	1:84:A:THR:HG23	1:85:A:ARG:HD2	10	0.8	0.23	0.72
(2,1388)	1:109:A:THR:HG23	1:108:A:LYS:HE3	10	0.8	0.23	0.72
(2,1388)	1:109:A:THR:HG21	1:108:A:LYS:HE3	10	0.8	0.23	0.72
(2,1388)	1:84:A:THR:HG21	1:85:A:ARG:HD2	10	0.8	0.23	0.72
(2,1388)	1:84:A:THR:HG22	1:85:A:ARG:HD2	10	0.8	0.23	0.72
(2,1298)	1:86:A:ILE:HG13	1:85:A:ARG:HA	10	0.79	0.02	0.79
(2,329)	1:125:A:ALA:HB2	1:122:A:ILE:HG21	10	0.79	0.1	0.74
(2,329)	1:125:A:ALA:HB3	1:122:A:ILE:HG22	10	0.79	0.1	0.74
(2,329)	1:125:A:ALA:HB1	1:122:A:ILE:HG21	10	0.79	0.1	0.74
(2,329)	1:125:A:ALA:HB1	1:122:A:ILE:HG23	10	0.79	0.1	0.74
(2,329)	1:125:A:ALA:HB2	1:122:A:ILE:HG22	10	0.79	0.1	0.74
(2,1705)	1:126:A:GLY:HA3	1:73:A:PHE:HA	10	0.77	0.1	0.76
(2,1705)	1:126:A:GLY:HA3	1:69:A:GLU:HA	10	0.77	0.1	0.76
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB3	10	0.76	0.57	0.46
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB2	10	0.76	0.57	0.46
(2,1311)	1:89:A:LEU:HD11	1:107:A:PRO:HG3	10	0.75	0.13	0.81
(2,1311)	1:89:A:LEU:HD13	1:107:A:PRO:HG3	10	0.75	0.13	0.81
(2,1311)	1:89:A:LEU:HD12	1:107:A:PRO:HG3	10	0.75	0.13	0.81
(2,1714)	1:106:A:LEU:HB2	1:91:A:GLY:HA2	10	0.75	0.12	0.8
(1,60)	1:119:A:LEU:H	1:114:A:ASP:HB2	10	0.75	0.21	0.84
(2,65)	1:107:A:PRO:HB2	1:107:A:PRO:HD2	10	0.75	0.01	0.75
(2,1524)	1:136:A:LYS:HD2	1:135:A:VAL:HA	10	0.74	0.31	0.72
(2,1524)	1:110:A:VAL:HA	1:89:A:LEU:HB2	10	0.74	0.31	0.72
(2,294)	1:64:A:VAL:HG13	1:102:A:THR:HG23	10	0.74	0.06	0.74
(2,294)	1:64:A:VAL:HG12	1:102:A:THR:HG22	10	0.74	0.06	0.74
(2,294)	1:64:A:VAL:HG12	1:102:A:THR:HG21	10	0.74	0.06	0.74
(2,294)	1:64:A:VAL:HG11	1:102:A:THR:HG23	10	0.74	0.06	0.74
(2,294)	1:64:A:VAL:HG13	1:102:A:THR:HG21	10	0.74	0.06	0.74
(2,294)	1:64:A:VAL:HG11	1:102:A:THR:HG21	10	0.74	0.06	0.74
(2,1212)	1:108:A:LYS:HB3	1:109:A:THR:HG22	10	0.71	0.07	0.74

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1212)	1:108:A:LYS:HB3	1:109:A:THR:HG23	10	0.71	0.07	0.74
(2,1212)	1:108:A:LYS:HB3	1:109:A:THR:HG21	10	0.71	0.07	0.74
(2,1212)	1:128:A:VAL:HB	1:65:A:THR:HG23	10	0.71	0.07	0.74
(2,1212)	1:128:A:VAL:HB	1:65:A:THR:HG21	10	0.71	0.07	0.74
(2,296)	1:101:A:VAL:HG13	1:94:A:SER:HB2	10	0.7	0.08	0.72
(2,296)	1:101:A:VAL:HG12	1:94:A:SER:HB2	10	0.7	0.08	0.72
(2,296)	1:101:A:VAL:HG11	1:94:A:SER:HB2	10	0.7	0.08	0.72
(2,1325)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	10	0.7	0.61	0.42
(2,282)	1:97:A:THR:HG21	1:78:A:LYS:HE2	10	0.69	0.16	0.72
(2,282)	1:97:A:THR:HG23	1:78:A:LYS:HE2	10	0.69	0.16	0.72
(2,282)	1:97:A:THR:HG22	1:78:A:LYS:HE2	10	0.69	0.16	0.72
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD11	10	0.68	0.49	0.55
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD12	10	0.68	0.49	0.55
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD13	10	0.68	0.49	0.55
(2,240)	1:110:A:VAL:HG12	1:89:A:LEU:HB2	10	0.68	0.17	0.67
(2,240)	1:110:A:VAL:HG13	1:89:A:LEU:HB2	10	0.68	0.17	0.67
(2,240)	1:110:A:VAL:HG11	1:89:A:LEU:HB2	10	0.68	0.17	0.67
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG12	10	0.68	0.13	0.68
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG11	10	0.68	0.13	0.68
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG13	10	0.68	0.13	0.68
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG11	10	0.67	0.1	0.68
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG13	10	0.67	0.1	0.68
(2,1910)	1:89:A:LEU:H	1:84:A:THR:HG22	10	0.67	0.1	0.68
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG12	10	0.67	0.1	0.68
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG23	10	0.67	0.11	0.64
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG22	10	0.67	0.11	0.64
(2,1445)	1:87:A:GLU:HG3	1:86:A:ILE:HG22	10	0.67	0.11	0.64
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG21	10	0.67	0.11	0.64
(2,1208)	1:66:A:GLU:HB3	1:74:A:SER:HA	10	0.66	0.21	0.64
(2,1532)	1:87:A:GLU:HB3	1:83:A:SER:HA	10	0.66	0.29	0.68
(2,1546)	1:95:A:PHE:HE2	1:102:A:THR:HA	10	0.66	0.12	0.69
(2,1546)	1:95:A:PHE:HE1	1:102:A:THR:HA	10	0.66	0.12	0.69
(1,45)	1:125:A:ALA:HA	1:127:A:GLY:HA2	10	0.66	0.04	0.66
(2,1846)	1:106:A:LEU:H	1:105:A:GLU:HG3	10	0.65	0.1	0.66
(2,1465)	1:122:A:ILE:HD12	1:120:A:HIS:HA	10	0.65	0.06	0.64
(2,1465)	1:122:A:ILE:HD11	1:120:A:HIS:HA	10	0.65	0.06	0.64
(2,1465)	1:122:A:ILE:HD13	1:120:A:HIS:HA	10	0.65	0.06	0.64
(2,1419)	1:64:A:VAL:HG22	1:122:A:ILE:HG13	10	0.64	0.08	0.62
(2,1419)	1:64:A:VAL:HG21	1:122:A:ILE:HG13	10	0.64	0.08	0.62
(2,1419)	1:64:A:VAL:HG23	1:122:A:ILE:HG13	10	0.64	0.08	0.62
(2,1450)	1:122:A:ILE:HG23	1:119:A:LEU:HA	10	0.64	0.05	0.64
(2,1450)	1:122:A:ILE:HG21	1:119:A:LEU:HA	10	0.64	0.05	0.64

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1450)	1:122:A:ILE:HG22	1:119:A:LEU:HA	10	0.64	0.05	0.64
(2,1763)	1:82:A:PHE:HB2	1:85:A:ARG:HB3	10	0.64	0.11	0.64
(2,1420)	1:64:A:VAL:HG23	1:62:A:LEU:HG	10	0.63	0.06	0.62
(2,1420)	1:64:A:VAL:HG22	1:62:A:LEU:HG	10	0.63	0.06	0.62
(2,1420)	1:64:A:VAL:HG21	1:62:A:LEU:HG	10	0.63	0.06	0.62
(2,1462)	1:122:A:ILE:HD13	1:118:A:LEU:HB3	10	0.62	0.05	0.62
(2,1462)	1:122:A:ILE:HD12	1:118:A:LEU:HB3	10	0.62	0.05	0.62
(2,1462)	1:122:A:ILE:HD11	1:118:A:LEU:HB3	10	0.62	0.05	0.62
(2,1475)	1:102:A:THR:HB	1:64:A:VAL:HA	10	0.62	0.04	0.62
(2,1475)	1:102:A:THR:HB	1:95:A:PHE:HA	10	0.62	0.04	0.62
(2,387)	1:86:A:ILE:HD12	1:85:A:ARG:HD2	10	0.61	0.03	0.62
(2,387)	1:86:A:ILE:HD11	1:85:A:ARG:HD2	10	0.61	0.03	0.62
(2,387)	1:86:A:ILE:HD13	1:85:A:ARG:HD2	10	0.61	0.03	0.62
(2,1418)	1:64:A:VAL:HG21	1:127:A:GLY:HA2	10	0.61	0.26	0.6
(2,1418)	1:64:A:VAL:HG23	1:127:A:GLY:HA2	10	0.61	0.26	0.6
(2,1418)	1:64:A:VAL:HG22	1:127:A:GLY:HA2	10	0.61	0.26	0.6
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD22	10	0.6	0.16	0.66
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD21	10	0.6	0.16	0.66
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD23	10	0.6	0.16	0.66
(1,8)	1:107:A:PRO:HB2	1:90:A:GLY:HA2	10	0.6	0.16	0.62
(2,1525)	1:86:A:ILE:HG22	1:110:A:VAL:HA	10	0.59	0.09	0.62
(2,1525)	1:86:A:ILE:HG21	1:110:A:VAL:HA	10	0.59	0.09	0.62
(2,1525)	1:86:A:ILE:HG23	1:110:A:VAL:HA	10	0.59	0.09	0.62
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG21	10	0.59	0.13	0.59
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG23	10	0.59	0.13	0.59
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG13	10	0.59	0.13	0.59
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG22	10	0.59	0.13	0.59
(2,288)	1:110:A:VAL:HG21	1:113:A:HIS:HB2	10	0.59	0.05	0.59
(2,288)	1:110:A:VAL:HG23	1:113:A:HIS:HB2	10	0.59	0.05	0.59
(2,288)	1:110:A:VAL:HG22	1:113:A:HIS:HB2	10	0.59	0.05	0.59
(2,1617)	1:79:A:SER:HA	1:78:A:LYS:HB3	10	0.59	0.1	0.58
(2,1526)	1:95:A:PHE:HD1	1:94:A:SER:HA	10	0.58	0.14	0.62
(2,1526)	1:95:A:PHE:HD1	1:102:A:THR:HA	10	0.58	0.14	0.62
(2,200)	1:118:A:LEU:HD13	1:86:A:ILE:HA	10	0.58	0.04	0.6
(2,200)	1:118:A:LEU:HD11	1:86:A:ILE:HA	10	0.58	0.04	0.6
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG13	10	0.58	0.1	0.58
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG12	10	0.58	0.1	0.58
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG11	10	0.58	0.1	0.58
(2,1667)	1:123:A:LEU:HD23	1:124:A:ALA:HA	10	0.57	0.03	0.58
(2,1667)	1:123:A:LEU:HD21	1:124:A:ALA:HA	10	0.57	0.03	0.58
(2,1667)	1:123:A:LEU:HD22	1:124:A:ALA:HA	10	0.57	0.03	0.58
(2,186)	1:96:A:LEU:HG	1:103:A:MET:HG2	10	0.57	0.65	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,436)	1:93:A:ILE:HG23	1:82:A:PHE:HD2	10	0.57	0.12	0.62
(2,436)	1:93:A:ILE:HG21	1:82:A:PHE:HD2	10	0.57	0.12	0.62
(2,436)	1:93:A:ILE:HG22	1:82:A:PHE:HD2	10	0.57	0.12	0.62
(2,1635)	1:114:A:ASP:HA	1:115:A:MET:HA	10	0.56	0.07	0.6
(2,1635)	1:114:A:ASP:HA	1:118:A:LEU:HA	10	0.56	0.07	0.6
(2,331)	1:125:A:ALA:HB3	1:121:A:ASP:HB3	10	0.56	0.17	0.47
(2,331)	1:125:A:ALA:HB1	1:121:A:ASP:HB3	10	0.56	0.17	0.47
(2,331)	1:125:A:ALA:HB2	1:121:A:ASP:HB3	10	0.56	0.17	0.47
(2,1774)	1:104:A:ILE:HB	1:103:A:MET:HG3	10	0.55	0.38	0.35
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD13	10	0.55	0.12	0.58
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD11	10	0.55	0.12	0.58
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD12	10	0.55	0.12	0.58
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB3	10	0.55	0.09	0.55
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB2	10	0.55	0.09	0.55
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG21	10	0.54	0.13	0.57
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG22	10	0.54	0.13	0.57
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG23	10	0.54	0.13	0.57
(2,1523)	1:135:A:VAL:HA	1:58:A:GLU:HG2	10	0.54	0.19	0.58
(2,1523)	1:110:A:VAL:HA	1:107:A:PRO:HG3	10	0.54	0.19	0.58
(2,1904)	1:66:A:GLU:H	1:71:A:LYS:HD3	10	0.54	0.33	0.51
(2,353)	1:86:A:ILE:HG21	1:104:A:ILE:HG23	10	0.53	0.05	0.55
(2,353)	1:86:A:ILE:HG23	1:104:A:ILE:HG23	10	0.53	0.05	0.55
(2,353)	1:86:A:ILE:HG21	1:104:A:ILE:HG21	10	0.53	0.05	0.55
(2,353)	1:86:A:ILE:HG21	1:104:A:ILE:HG22	10	0.53	0.05	0.55
(2,353)	1:86:A:ILE:HG23	1:104:A:ILE:HG21	10	0.53	0.05	0.55
(2,353)	1:86:A:ILE:HG22	1:104:A:ILE:HG23	10	0.53	0.05	0.55
(2,353)	1:86:A:ILE:HG23	1:104:A:ILE:HG22	10	0.53	0.05	0.55
(2,560)	1:70:A:SER:HB2	1:70:A:SER:HA	10	0.53	0.13	0.6
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG13	10	0.53	0.15	0.58
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG12	10	0.53	0.15	0.58
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG11	10	0.53	0.15	0.58
(2,1456)	1:104:A:ILE:HD11	1:93:A:ILE:HA	10	0.53	0.08	0.52
(2,1456)	1:104:A:ILE:HD12	1:93:A:ILE:HA	10	0.53	0.08	0.52
(2,1862)	1:121:A:ASP:H	1:116:A:ASP:HA	10	0.53	0.09	0.56
(2,1460)	1:104:A:ILE:HD11	1:102:A:THR:HB	10	0.53	0.06	0.52
(2,1460)	1:104:A:ILE:HD12	1:102:A:THR:HB	10	0.53	0.06	0.52
(2,1460)	1:104:A:ILE:HD13	1:102:A:THR:HB	10	0.53	0.06	0.52
(2,1417)	1:64:A:VAL:HG23	1:62:A:LEU:HA	10	0.53	0.16	0.57
(2,1417)	1:64:A:VAL:HG22	1:62:A:LEU:HA	10	0.53	0.16	0.57
(2,1417)	1:64:A:VAL:HG21	1:102:A:THR:HA	10	0.53	0.16	0.57
(2,1417)	1:64:A:VAL:HG22	1:102:A:THR:HA	10	0.53	0.16	0.57
(2,1417)	1:64:A:VAL:HG21	1:62:A:LEU:HA	10	0.53	0.16	0.57

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD21	10	0.52	0.11	0.48
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD22	10	0.52	0.11	0.48
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD23	10	0.52	0.11	0.48
(2,333)	1:124:A:ALA:HB2	1:76:A:MET:HG3	10	0.52	0.24	0.44
(2,333)	1:124:A:ALA:HB1	1:76:A:MET:HG3	10	0.52	0.24	0.44
(2,333)	1:124:A:ALA:HB3	1:76:A:MET:HG3	10	0.52	0.24	0.44
(2,1380)	1:64:A:VAL:HG11	1:128:A:VAL:HG23	10	0.52	0.22	0.46
(2,1380)	1:64:A:VAL:HG13	1:128:A:VAL:HG21	10	0.52	0.22	0.46
(2,1380)	1:64:A:VAL:HG13	1:128:A:VAL:HG23	10	0.52	0.22	0.46
(2,1380)	1:64:A:VAL:HG13	1:128:A:VAL:HG22	10	0.52	0.22	0.46
(2,1380)	1:64:A:VAL:HG12	1:128:A:VAL:HG22	10	0.52	0.22	0.46
(2,1380)	1:64:A:VAL:HG11	1:128:A:VAL:HG21	10	0.52	0.22	0.46
(2,1380)	1:64:A:VAL:HG12	1:128:A:VAL:HG21	10	0.52	0.22	0.46
(2,1675)	1:101:A:VAL:HG13	1:103:A:MET:HA	10	0.51	0.07	0.51
(2,1675)	1:101:A:VAL:HG12	1:103:A:MET:HA	10	0.51	0.07	0.51
(2,1675)	1:101:A:VAL:HG11	1:103:A:MET:HA	10	0.51	0.07	0.51
(2,264)	1:65:A:THR:HG23	1:64:A:VAL:HG12	10	0.51	0.25	0.46
(2,264)	1:65:A:THR:HG22	1:64:A:VAL:HG11	10	0.51	0.25	0.46
(2,264)	1:65:A:THR:HG21	1:64:A:VAL:HG12	10	0.51	0.25	0.46
(2,264)	1:65:A:THR:HG23	1:64:A:VAL:HG11	10	0.51	0.25	0.46
(2,264)	1:65:A:THR:HG21	1:64:A:VAL:HG13	10	0.51	0.25	0.46
(2,264)	1:65:A:THR:HG23	1:64:A:VAL:HG13	10	0.51	0.25	0.46
(2,264)	1:65:A:THR:HG21	1:64:A:VAL:HG11	10	0.51	0.25	0.46
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG21	10	0.51	0.16	0.56
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG23	10	0.51	0.16	0.56
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG22	10	0.51	0.16	0.56
(2,1626)	1:118:A:LEU:HA	1:85:A:ARG:HG2	10	0.51	0.06	0.5
(2,1367)	1:65:A:THR:HG21	1:100:A:GLY:HA2	10	0.51	0.16	0.52
(2,1367)	1:65:A:THR:HG23	1:100:A:GLY:HA2	10	0.51	0.16	0.52
(2,1367)	1:65:A:THR:HG22	1:100:A:GLY:HA2	10	0.51	0.16	0.52
(2,275)	1:64:A:VAL:HG12	1:102:A:THR:HB	10	0.5	0.06	0.5
(2,275)	1:64:A:VAL:HG13	1:102:A:THR:HB	10	0.5	0.06	0.5
(2,275)	1:64:A:VAL:HG11	1:102:A:THR:HB	10	0.5	0.06	0.5
(2,1171)	1:112:A:GLU:HG3	1:112:A:GLU:HB2	10	0.5	0.05	0.52
(2,1171)	1:58:A:GLU:HG2	1:58:A:GLU:HB3	10	0.5	0.05	0.52
(2,1171)	1:58:A:GLU:HG2	1:107:A:PRO:HB2	10	0.5	0.05	0.52
(2,1171)	1:88:A:GLU:HG2	1:88:A:GLU:HB2	10	0.5	0.05	0.52
(2,1670)	1:82:A:PHE:HA	1:77:A:ALA:HA	10	0.5	0.05	0.52
(2,1670)	1:77:A:ALA:HA	1:78:A:LYS:HA	10	0.5	0.05	0.52
(2,1769)	1:121:A:ASP:HB2	1:82:A:PHE:HA	10	0.5	0.05	0.49
(2,241)	1:106:A:LEU:HD22	1:110:A:VAL:HG13	10	0.5	0.05	0.49
(2,241)	1:106:A:LEU:HD22	1:110:A:VAL:HG11	10	0.5	0.05	0.49

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,241)	1:106:A:LEU:HD22	1:110:A:VAL:HG12	10	0.5	0.05	0.49
(2,241)	1:106:A:LEU:HD23	1:110:A:VAL:HG11	10	0.5	0.05	0.49
(2,241)	1:106:A:LEU:HD23	1:110:A:VAL:HG12	10	0.5	0.05	0.49
(2,241)	1:106:A:LEU:HD21	1:110:A:VAL:HG13	10	0.5	0.05	0.49
(2,241)	1:106:A:LEU:HD21	1:110:A:VAL:HG11	10	0.5	0.05	0.49
(2,871)	1:87:A:GLU:H	1:92:A:SER:HB3	10	0.49	0.03	0.5
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG11	10	0.49	0.09	0.49
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG13	10	0.49	0.09	0.49
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG12	10	0.49	0.09	0.49
(2,1925)	1:130:A:GLY:H	1:128:A:VAL:HG12	10	0.49	0.09	0.49
(2,1274)	1:122:A:ILE:HG13	1:119:A:LEU:HB2	10	0.49	0.05	0.48
(2,1471)	1:86:A:ILE:HD12	1:89:A:LEU:HB2	10	0.49	0.14	0.46
(2,1471)	1:86:A:ILE:HD13	1:89:A:LEU:HB2	10	0.49	0.14	0.46
(2,1471)	1:86:A:ILE:HD11	1:89:A:LEU:HB2	10	0.49	0.14	0.46
(2,1627)	1:95:A:PHE:HA	1:101:A:VAL:HB	10	0.49	0.1	0.5
(2,1178)	1:85:A:ARG:H	1:86:A:ILE:HB	10	0.48	0.04	0.48
(2,1345)	1:110:A:VAL:HG12	1:114:A:ASP:HB2	10	0.48	0.27	0.38
(2,1345)	1:110:A:VAL:HG13	1:114:A:ASP:HB2	10	0.48	0.27	0.38
(2,1345)	1:110:A:VAL:HG11	1:114:A:ASP:HB2	10	0.48	0.27	0.38
(2,1345)	1:107:A:PRO:HB3	1:110:A:VAL:HG11	10	0.48	0.27	0.38
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG21	10	0.48	0.1	0.52
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG23	10	0.48	0.1	0.52
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG22	10	0.48	0.1	0.52
(2,664)	1:118:A:LEU:HD23	1:85:A:ARG:HD3	10	0.47	0.01	0.48
(2,664)	1:118:A:LEU:HD22	1:85:A:ARG:HD3	10	0.47	0.01	0.48
(2,664)	1:118:A:LEU:HD21	1:85:A:ARG:HD3	10	0.47	0.01	0.48
(2,1700)	1:107:A:PRO:HD2	1:106:A:LEU:HB2	10	0.47	0.02	0.47
(2,1702)	1:106:A:LEU:HB2	1:86:A:ILE:HB	10	0.47	0.03	0.48
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD1	10	0.47	0.04	0.46
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD2	10	0.47	0.04	0.46
(2,340)	1:124:A:ALA:HB2	1:121:A:ASP:HB2	10	0.46	0.08	0.48
(2,340)	1:124:A:ALA:HB1	1:121:A:ASP:HB2	10	0.46	0.08	0.48
(2,340)	1:124:A:ALA:HB3	1:121:A:ASP:HB2	10	0.46	0.08	0.48
(2,1324)	1:115:A:MET:HG3	1:108:A:LYS:HG3	10	0.46	0.23	0.43
(2,728)	1:124:A:ALA:HB3	1:120:A:HIS:HB2	10	0.46	0.09	0.48
(2,728)	1:124:A:ALA:HB2	1:120:A:HIS:HB2	10	0.46	0.09	0.48
(2,728)	1:124:A:ALA:HB1	1:120:A:HIS:HB2	10	0.46	0.09	0.48
(2,1516)	1:107:A:PRO:HA	1:59:A:MET:HB3	10	0.46	0.16	0.48
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG23	10	0.45	0.09	0.48
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG21	10	0.45	0.09	0.48
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG22	10	0.45	0.09	0.48
(2,646)	1:106:A:LEU:HG	1:107:A:PRO:HD3	10	0.45	0.08	0.45

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1572)	1:82:A:PHE:HE2	1:77:A:ALA:HA	10	0.45	0.09	0.42
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD12	10	0.45	0.03	0.44
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD11	10	0.45	0.03	0.44
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD13	10	0.45	0.03	0.44
(2,1439)	1:104:A:ILE:HG21	1:105:A:GLU:HG2	10	0.45	0.1	0.42
(2,1439)	1:104:A:ILE:HG22	1:105:A:GLU:HG2	10	0.45	0.1	0.42
(2,1439)	1:104:A:ILE:HG23	1:105:A:GLU:HG2	10	0.45	0.1	0.42
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD12	10	0.44	0.09	0.42
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD21	10	0.44	0.09	0.42
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD23	10	0.44	0.09	0.42
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD13	10	0.44	0.09	0.42
(2,934)	1:60:A:THR:H	1:60:A:THR:HG21	10	0.44	0.04	0.44
(2,934)	1:60:A:THR:H	1:60:A:THR:HG23	10	0.44	0.04	0.44
(2,934)	1:60:A:THR:H	1:60:A:THR:HG22	10	0.44	0.04	0.44
(2,1890)	1:76:A:MET:H	1:77:A:ALA:HA	10	0.43	0.02	0.44
(2,1404)	1:102:A:THR:HG23	1:77:A:ALA:HA	10	0.43	0.15	0.48
(2,1404)	1:102:A:THR:HG22	1:77:A:ALA:HA	10	0.43	0.15	0.48
(2,1404)	1:102:A:THR:HG21	1:77:A:ALA:HA	10	0.43	0.15	0.48
(2,1711)	1:104:A:ILE:HG23	1:91:A:GLY:HA2	10	0.43	0.08	0.45
(2,1711)	1:104:A:ILE:HG21	1:91:A:GLY:HA2	10	0.43	0.08	0.45
(2,1711)	1:104:A:ILE:HG22	1:91:A:GLY:HA2	10	0.43	0.08	0.45
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG22	10	0.43	0.04	0.44
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG23	10	0.43	0.04	0.44
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG21	10	0.43	0.04	0.44
(2,1344)	1:123:A:LEU:HD22	1:129:A:VAL:HG23	10	0.42	0.22	0.34
(2,1344)	1:123:A:LEU:HD23	1:129:A:VAL:HG21	10	0.42	0.22	0.34
(2,1344)	1:106:A:LEU:HD21	1:62:A:LEU:HD21	10	0.42	0.22	0.34
(2,1344)	1:123:A:LEU:HD22	1:129:A:VAL:HG22	10	0.42	0.22	0.34
(2,1344)	1:123:A:LEU:HD21	1:129:A:VAL:HG22	10	0.42	0.22	0.34
(2,1344)	1:123:A:LEU:HD22	1:129:A:VAL:HG21	10	0.42	0.22	0.34
(2,1344)	1:123:A:LEU:HD21	1:129:A:VAL:HG21	10	0.42	0.22	0.34
(2,1344)	1:123:A:LEU:HD23	1:129:A:VAL:HG23	10	0.42	0.22	0.34
(2,1651)	1:104:A:ILE:HG21	1:61:A:ARG:HA	10	0.42	0.1	0.42
(2,1651)	1:104:A:ILE:HG22	1:61:A:ARG:HA	10	0.42	0.1	0.42
(2,1651)	1:104:A:ILE:HG23	1:61:A:ARG:HA	10	0.42	0.1	0.42
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD11	10	0.42	0.07	0.42
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD12	10	0.42	0.07	0.42
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD13	10	0.42	0.07	0.42
(2,633)	1:120:A:HIS:HB2	1:120:A:HIS:HD2	10	0.41	0.01	0.41
(2,1582)	1:104:A:ILE:HD13	1:104:A:ILE:HA	10	0.41	0.03	0.4
(2,1582)	1:104:A:ILE:HD11	1:104:A:ILE:HA	10	0.41	0.03	0.4
(2,1582)	1:104:A:ILE:HD12	1:104:A:ILE:HA	10	0.41	0.03	0.4

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1429)	1:77:A:ALA:HB3	1:74:A:SER:HA	10	0.4	0.06	0.42
(2,1429)	1:77:A:ALA:HB1	1:74:A:SER:HA	10	0.4	0.06	0.42
(2,1429)	1:77:A:ALA:HB2	1:74:A:SER:HA	10	0.4	0.06	0.42
(2,1351)	1:118:A:LEU:HD23	1:85:A:ARG:HD3	10	0.4	0.01	0.4
(2,1351)	1:118:A:LEU:HD22	1:85:A:ARG:HD3	10	0.4	0.01	0.4
(2,1351)	1:118:A:LEU:HD21	1:85:A:ARG:HD3	10	0.4	0.01	0.4
(2,1042)	1:89:A:LEU:H	1:88:A:GLU:HB3	10	0.4	0.14	0.4
(2,1545)	1:95:A:PHE:HE2	1:95:A:PHE:HA	10	0.4	0.06	0.41
(2,1545)	1:95:A:PHE:HE1	1:95:A:PHE:HA	10	0.4	0.06	0.41
(2,1540)	1:135:A:VAL:HA	1:109:A:THR:H	10	0.39	0.05	0.4
(2,1434)	1:86:A:ILE:HG22	1:106:A:LEU:HD13	10	0.39	0.11	0.4
(2,1434)	1:86:A:ILE:HG21	1:106:A:LEU:HD13	10	0.39	0.11	0.4
(2,1434)	1:86:A:ILE:HG22	1:106:A:LEU:HD11	10	0.39	0.11	0.4
(2,1434)	1:86:A:ILE:HG22	1:106:A:LEU:HD12	10	0.39	0.11	0.4
(2,1434)	1:86:A:ILE:HG23	1:106:A:LEU:HD13	10	0.39	0.11	0.4
(2,1434)	1:86:A:ILE:HG21	1:106:A:LEU:HD12	10	0.39	0.11	0.4
(2,1434)	1:86:A:ILE:HG21	1:106:A:LEU:HD11	10	0.39	0.11	0.4
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG21	10	0.39	0.09	0.41
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG22	10	0.39	0.09	0.41
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG23	10	0.39	0.09	0.41
(2,570)	1:121:A:ASP:HA	1:120:A:HIS:HB2	10	0.39	0.02	0.39
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG11	10	0.39	0.14	0.39
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG13	10	0.39	0.14	0.39
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG12	10	0.39	0.14	0.39
(2,193)	1:106:A:LEU:HD13	1:106:A:LEU:HA	10	0.38	0.02	0.38
(2,193)	1:106:A:LEU:HD11	1:106:A:LEU:HA	10	0.38	0.02	0.38
(2,193)	1:106:A:LEU:HD12	1:106:A:LEU:HA	10	0.38	0.02	0.38
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG13	10	0.38	0.02	0.38
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG12	10	0.38	0.02	0.38
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG21	10	0.38	0.02	0.38
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG22	10	0.38	0.02	0.38
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG23	10	0.38	0.02	0.38
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG11	10	0.38	0.02	0.38
(2,1721)	1:85:A:ARG:HA	1:85:A:ARG:HD2	10	0.38	0.04	0.38
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD21	10	0.38	0.05	0.38
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD23	10	0.38	0.05	0.38
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD22	10	0.38	0.05	0.38
(2,706)	1:122:A:ILE:HG22	1:123:A:LEU:HB2	10	0.38	0.02	0.39
(2,706)	1:122:A:ILE:HG23	1:123:A:LEU:HB2	10	0.38	0.02	0.39
(2,706)	1:122:A:ILE:HG21	1:123:A:LEU:HB2	10	0.38	0.02	0.39
(2,1601)	1:112:A:GLU:HA	1:111:A:SER:HA	10	0.38	0.03	0.37
(2,1601)	1:111:A:SER:HA	1:110:A:VAL:HA	10	0.38	0.03	0.37

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1694)	1:106:A:LEU:HD23	1:107:A:PRO:HD2	10	0.38	0.06	0.4
(2,1694)	1:106:A:LEU:HD21	1:107:A:PRO:HD2	10	0.38	0.06	0.4
(2,1694)	1:106:A:LEU:HD22	1:107:A:PRO:HD2	10	0.38	0.06	0.4
(2,1285)	1:93:A:ILE:HG12	1:92:A:SER:HA	10	0.37	0.08	0.35
(2,1043)	1:89:A:LEU:H	1:89:A:LEU:HB3	10	0.37	0.04	0.37
(2,1488)	1:92:A:SER:HB2	1:93:A:ILE:HB	10	0.37	0.04	0.35
(2,626)	1:64:A:VAL:HG12	1:63:A:MET:HA	10	0.36	0.03	0.36
(2,626)	1:64:A:VAL:HG11	1:63:A:MET:HA	10	0.36	0.03	0.36
(2,626)	1:64:A:VAL:HG13	1:63:A:MET:HA	10	0.36	0.03	0.36
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB3	10	0.36	0.14	0.36
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB2	10	0.36	0.14	0.36
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG11	10	0.35	0.06	0.38
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG12	10	0.35	0.06	0.38
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG13	10	0.35	0.06	0.38
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG21	10	0.35	0.05	0.32
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG23	10	0.35	0.05	0.32
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG22	10	0.35	0.05	0.32
(2,230)	1:62:A:LEU:HD11	1:122:A:ILE:HG12	10	0.34	0.02	0.34
(2,230)	1:62:A:LEU:HD13	1:122:A:ILE:HG12	10	0.34	0.02	0.34
(2,230)	1:62:A:LEU:HD12	1:122:A:ILE:HG12	10	0.34	0.02	0.34
(2,369)	1:104:A:ILE:HD12	1:122:A:ILE:HG13	10	0.34	0.01	0.34
(2,369)	1:104:A:ILE:HD13	1:122:A:ILE:HG13	10	0.34	0.01	0.34
(2,369)	1:104:A:ILE:HD11	1:122:A:ILE:HG13	10	0.34	0.01	0.34
(2,530)	1:88:A:GLU:HA	1:88:A:GLU:HB2	10	0.34	0.02	0.35
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG22	10	0.34	0.05	0.35
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG21	10	0.34	0.05	0.35
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG23	10	0.34	0.05	0.35
(2,1581)	1:104:A:ILE:HA	1:93:A:ILE:HG13	10	0.34	0.12	0.35
(2,1932)	1:92:A:SER:H	1:93:A:ILE:HG13	10	0.34	0.05	0.34
(2,1012)	1:119:A:LEU:H	1:119:A:LEU:HB3	10	0.33	0.01	0.33
(2,744)	1:105:A:GLU:H	1:105:A:GLU:HG2	10	0.33	0.03	0.33
(2,246)	1:123:A:LEU:HD13	1:127:A:GLY:HA2	10	0.33	0.09	0.34
(2,246)	1:123:A:LEU:HD12	1:127:A:GLY:HA2	10	0.33	0.09	0.34
(2,246)	1:123:A:LEU:HD11	1:127:A:GLY:HA2	10	0.33	0.09	0.34
(1,13)	1:120:A:HIS:HB2	1:122:A:ILE:HG13	10	0.33	0.03	0.32
(2,1225)	1:115:A:MET:HB2	1:107:A:PRO:HD2	10	0.33	0.03	0.32
(2,307)	1:102:A:THR:HG22	1:64:A:VAL:HB	10	0.32	0.04	0.32
(2,307)	1:102:A:THR:HG21	1:64:A:VAL:HB	10	0.32	0.04	0.32
(2,307)	1:102:A:THR:HG23	1:64:A:VAL:HB	10	0.32	0.04	0.32
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG23	10	0.32	0.01	0.32
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG21	10	0.32	0.01	0.32
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG22	10	0.32	0.01	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1443)	1:86:A:ILE:HG23	1:87:A:GLU:HA	10	0.32	0.06	0.3
(2,1443)	1:86:A:ILE:HG22	1:87:A:GLU:HA	10	0.32	0.06	0.3
(2,1443)	1:86:A:ILE:HG21	1:87:A:GLU:HA	10	0.32	0.06	0.3
(2,1363)	1:96:A:LEU:HB2	1:96:A:LEU:HD21	10	0.31	0.01	0.32
(2,1363)	1:131:A:LEU:HG	1:131:A:LEU:HD22	10	0.31	0.01	0.32
(2,1363)	1:96:A:LEU:HG	1:96:A:LEU:HD23	10	0.31	0.01	0.32
(2,1363)	1:96:A:LEU:HG	1:96:A:LEU:HD21	10	0.31	0.01	0.32
(2,1363)	1:137:A:LEU:HG	1:137:A:LEU:HD22	10	0.31	0.01	0.32
(2,1363)	1:96:A:LEU:HB2	1:96:A:LEU:HD22	10	0.31	0.01	0.32
(2,1363)	1:131:A:LEU:HG	1:131:A:LEU:HD21	10	0.31	0.01	0.32
(2,374)	1:104:A:ILE:HD12	1:122:A:ILE:HG21	10	0.31	0.04	0.3
(2,374)	1:104:A:ILE:HD12	1:122:A:ILE:HG22	10	0.31	0.04	0.3
(2,374)	1:104:A:ILE:HD13	1:122:A:ILE:HG21	10	0.31	0.04	0.3
(2,374)	1:104:A:ILE:HD13	1:122:A:ILE:HG23	10	0.31	0.04	0.3
(2,374)	1:104:A:ILE:HD11	1:122:A:ILE:HG21	10	0.31	0.04	0.3
(2,374)	1:104:A:ILE:HD13	1:122:A:ILE:HG22	10	0.31	0.04	0.3
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB3	10	0.31	0.11	0.32
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB1	10	0.31	0.11	0.32
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB2	10	0.31	0.11	0.32
(2,343)	1:86:A:ILE:HG23	1:91:A:GLY:HA2	10	0.3	0.05	0.29
(2,343)	1:86:A:ILE:HG22	1:91:A:GLY:HA2	10	0.3	0.05	0.29
(2,343)	1:86:A:ILE:HG21	1:91:A:GLY:HA2	10	0.3	0.05	0.29
(2,1297)	1:86:A:ILE:HG13	1:82:A:PHE:HZ	10	0.3	0.09	0.29
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG13	10	0.29	0.0	0.29
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG12	10	0.29	0.0	0.29
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG22	10	0.29	0.0	0.29
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG21	10	0.29	0.0	0.29
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD21	10	0.28	0.06	0.3
(2,1874)	1:123:A:LEU:H	1:129:A:VAL:HG12	10	0.28	0.06	0.3
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD23	10	0.28	0.06	0.3
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD22	10	0.28	0.06	0.3
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG23	10	0.28	0.06	0.3
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG21	10	0.28	0.06	0.3
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG22	10	0.28	0.06	0.3
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG21	10	0.28	0.01	0.27
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG23	10	0.28	0.01	0.27
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG22	10	0.28	0.01	0.27
(2,1930)	1:92:A:SER:H	1:105:A:GLU:HG2	10	0.28	0.05	0.28
(2,1481)	1:84:A:THR:HG21	1:84:A:THR:HB	10	0.27	0.01	0.28
(2,1481)	1:84:A:THR:HG23	1:84:A:THR:HB	10	0.27	0.01	0.28
(2,1481)	1:84:A:THR:HG22	1:84:A:THR:HB	10	0.27	0.01	0.28
(2,1481)	1:97:A:THR:HG22	1:97:A:THR:HB	10	0.27	0.01	0.28

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1891)	1:116:A:ASP:H	1:115:A:MET:HB2	10	0.27	0.1	0.31
(2,1648)	1:136:A:LYS:HG3	1:136:A:LYS:HA	10	0.27	0.11	0.24
(2,1648)	1:136:A:LYS:HG2	1:136:A:LYS:HA	10	0.27	0.11	0.24
(2,1334)	1:137:A:LEU:HG	1:137:A:LEU:HD13	10	0.26	0.02	0.27
(2,1334)	1:131:A:LEU:HG	1:131:A:LEU:HD11	10	0.26	0.02	0.27
(2,1334)	1:137:A:LEU:HD12	1:137:A:LEU:HB3	10	0.26	0.02	0.27
(2,1334)	1:131:A:LEU:HG	1:131:A:LEU:HD13	10	0.26	0.02	0.27
(2,1334)	1:137:A:LEU:HG	1:137:A:LEU:HD12	10	0.26	0.02	0.27
(2,1334)	1:137:A:LEU:HD11	1:137:A:LEU:HB3	10	0.26	0.02	0.27
(2,1676)	1:63:A:MET:HG2	1:63:A:MET:HA	10	0.26	0.03	0.27
(2,1676)	1:63:A:MET:HG3	1:63:A:MET:HA	10	0.26	0.03	0.27
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD12	10	0.26	0.01	0.26
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD11	10	0.26	0.01	0.26
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD13	10	0.26	0.01	0.26
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD22	10	0.26	0.08	0.26
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD21	10	0.26	0.08	0.26
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD23	10	0.26	0.08	0.26
(2,1939)	1:127:A:GLY:H	1:122:A:ILE:HB	10	0.26	0.09	0.28
(2,1261)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	10	0.25	0.03	0.26
(2,1261)	1:71:A:LYS:HD2	1:71:A:LYS:HG3	10	0.25	0.03	0.26
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG21	10	0.25	0.01	0.25
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG22	10	0.25	0.01	0.25
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG23	10	0.25	0.01	0.25
(2,385)	1:86:A:ILE:HD12	1:85:A:ARG:HA	10	0.24	0.03	0.24
(2,385)	1:86:A:ILE:HD11	1:85:A:ARG:HA	10	0.24	0.03	0.24
(2,385)	1:86:A:ILE:HD13	1:85:A:ARG:HA	10	0.24	0.03	0.24
(2,1658)	1:60:A:THR:HG21	1:105:A:GLU:HA	10	0.24	0.07	0.25
(2,1658)	1:60:A:THR:HG23	1:105:A:GLU:HA	10	0.24	0.07	0.25
(2,1658)	1:60:A:THR:HG22	1:105:A:GLU:HA	10	0.24	0.07	0.25
(2,1291)	1:118:A:LEU:HG	1:118:A:LEU:HD21	10	0.24	0.01	0.24
(2,1291)	1:131:A:LEU:HG	1:131:A:LEU:HD22	10	0.24	0.01	0.24
(2,1291)	1:118:A:LEU:HG	1:118:A:LEU:HD23	10	0.24	0.01	0.24
(2,1291)	1:96:A:LEU:HG	1:96:A:LEU:HD23	10	0.24	0.01	0.24
(2,1291)	1:96:A:LEU:HG	1:96:A:LEU:HD13	10	0.24	0.01	0.24
(2,1291)	1:96:A:LEU:HG	1:96:A:LEU:HD11	10	0.24	0.01	0.24
(2,1291)	1:131:A:LEU:HG	1:131:A:LEU:HD21	10	0.24	0.01	0.24
(2,1291)	1:96:A:LEU:HG	1:96:A:LEU:HD21	10	0.24	0.01	0.24
(2,1062)	1:120:A:HIS:H	1:119:A:LEU:HB3	10	0.23	0.05	0.25
(2,359)	1:122:A:ILE:HG23	1:64:A:VAL:HA	10	0.22	0.08	0.24
(2,359)	1:122:A:ILE:HG21	1:64:A:VAL:HA	10	0.22	0.08	0.24
(2,359)	1:122:A:ILE:HG22	1:64:A:VAL:HA	10	0.22	0.08	0.24
(2,1935)	1:78:A:LYS:H	1:78:A:LYS:HB3	10	0.22	0.05	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1765)	1:116:A:ASP:HA	1:116:A:ASP:HB3	10	0.22	0.01	0.22
(2,1686)	1:120:A:HIS:HD2	1:123:A:LEU:HA	10	0.22	0.03	0.21
(2,1555)	1:86:A:ILE:HB	1:86:A:ILE:HA	10	0.21	0.01	0.22
(2,1555)	1:86:A:ILE:HA	1:89:A:LEU:HB3	10	0.21	0.01	0.22
(2,1541)	1:81:A:SER:HB3	1:81:A:SER:HA	10	0.21	0.02	0.21
(2,1541)	1:81:A:SER:HB2	1:81:A:SER:HA	10	0.21	0.02	0.21
(2,1567)	1:99:A:THR:HA	1:100:A:GLY:HA2	10	0.21	0.02	0.21
(2,400)	1:109:A:THR:HG23	1:109:A:THR:HB	10	0.21	0.01	0.21
(2,400)	1:109:A:THR:HG21	1:109:A:THR:HB	10	0.21	0.01	0.21
(2,400)	1:109:A:THR:HG22	1:109:A:THR:HB	10	0.21	0.01	0.21
(2,1863)	1:121:A:ASP:H	1:122:A:ILE:HB	10	0.2	0.02	0.21
(2,1306)	1:106:A:LEU:HD11	1:106:A:LEU:HG	10	0.2	0.01	0.2
(2,1306)	1:106:A:LEU:HD12	1:106:A:LEU:HG	10	0.2	0.01	0.2
(2,1306)	1:106:A:LEU:HD13	1:106:A:LEU:HG	10	0.2	0.01	0.2
(2,1144)	1:126:A:GLY:H	1:127:A:GLY:HA2	10	0.2	0.06	0.22
(2,1337)	1:137:A:LEU:HG	1:137:A:LEU:HD13	10	0.19	0.02	0.2
(2,1337)	1:96:A:LEU:HG	1:96:A:LEU:HD13	10	0.19	0.02	0.2
(2,1337)	1:96:A:LEU:HG	1:96:A:LEU:HD11	10	0.19	0.02	0.2
(2,1337)	1:137:A:LEU:HD12	1:137:A:LEU:HB3	10	0.19	0.02	0.2
(2,1337)	1:131:A:LEU:HG	1:131:A:LEU:HD13	10	0.19	0.02	0.2
(2,1337)	1:137:A:LEU:HD11	1:137:A:LEU:HB3	10	0.19	0.02	0.2
(2,1856)	1:94:A:SER:H	1:93:A:ILE:HB	10	0.19	0.07	0.18
(2,262)	1:65:A:THR:HG21	1:65:A:THR:HB	10	0.18	0.02	0.19
(2,262)	1:65:A:THR:HG23	1:65:A:THR:HB	10	0.18	0.02	0.19
(2,262)	1:65:A:THR:HG22	1:65:A:THR:HB	10	0.18	0.02	0.19
(2,464)	1:101:A:VAL:HG12	1:101:A:VAL:HA	10	0.18	0.06	0.16
(2,464)	1:101:A:VAL:HG11	1:101:A:VAL:HA	10	0.18	0.06	0.16
(2,464)	1:101:A:VAL:HG13	1:101:A:VAL:HA	10	0.18	0.06	0.16
(2,1566)	1:99:A:THR:HA	1:100:A:GLY:HA3	10	0.18	0.02	0.18
(2,1566)	1:99:A:THR:HA	1:98:A:GLU:HA	10	0.18	0.02	0.18
(2,1047)	1:79:A:SER:H	1:82:A:PHE:HD2	10	0.18	0.04	0.19
(2,414)	1:92:A:SER:HB3	1:92:A:SER:HA	10	0.18	0.02	0.18
(2,322)	1:64:A:VAL:HG13	1:64:A:VAL:HG22	10	0.17	0.02	0.18
(2,322)	1:64:A:VAL:HG12	1:64:A:VAL:HG21	10	0.17	0.02	0.18
(2,322)	1:64:A:VAL:HG12	1:64:A:VAL:HG23	10	0.17	0.02	0.18
(2,322)	1:64:A:VAL:HG11	1:64:A:VAL:HG23	10	0.17	0.02	0.18
(2,322)	1:64:A:VAL:HG13	1:64:A:VAL:HG23	10	0.17	0.02	0.18
(2,659)	1:90:A:GLY:HA2	1:89:A:LEU:HA	10	0.17	0.01	0.17
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG21	10	0.17	0.01	0.17
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG23	10	0.17	0.01	0.17
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG22	10	0.17	0.01	0.17
(2,1384)	1:84:A:THR:HG21	1:84:A:THR:HB	10	0.17	0.01	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1384)	1:109:A:THR:HG21	1:109:A:THR:HA	10	0.17	0.01	0.17
(2,1384)	1:84:A:THR:HG22	1:84:A:THR:HB	10	0.17	0.01	0.17
(2,1384)	1:109:A:THR:HG22	1:109:A:THR:HA	10	0.17	0.01	0.17
(2,1384)	1:84:A:THR:HG23	1:84:A:THR:HB	10	0.17	0.01	0.17
(2,1600)	1:79:A:SER:HB2	1:79:A:SER:HA	10	0.16	0.02	0.16
(2,195)	1:89:A:LEU:HG	1:89:A:LEU:HA	10	0.16	0.01	0.15
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD13	10	0.14	0.02	0.14
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD12	10	0.14	0.02	0.14
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD11	10	0.14	0.02	0.14
(2,1193)	1:129:A:VAL:HB	1:129:A:VAL:HG11	10	0.13	0.01	0.13
(2,1193)	1:129:A:VAL:HB	1:129:A:VAL:HG13	10	0.13	0.01	0.13
(2,1193)	1:128:A:VAL:HB	1:128:A:VAL:HG13	10	0.13	0.01	0.13
(2,1193)	1:129:A:VAL:HB	1:129:A:VAL:HG12	10	0.13	0.01	0.13
(2,1484)	1:122:A:ILE:HA	1:123:A:LEU:HA	10	0.13	0.01	0.13
(2,608)	1:124:A:ALA:HB3	1:124:A:ALA:HA	10	0.13	0.01	0.12
(2,608)	1:124:A:ALA:HB1	1:124:A:ALA:HA	10	0.13	0.01	0.12
(2,608)	1:124:A:ALA:HB2	1:124:A:ALA:HA	10	0.13	0.01	0.12
(2,1921)	1:86:A:ILE:H	1:85:A:ARG:HA	10	0.12	0.0	0.12
(2,569)	1:95:A:PHE:HD1	1:94:A:SER:HA	10	0.12	0.01	0.11
(2,569)	1:95:A:PHE:HD2	1:94:A:SER:HA	10	0.12	0.01	0.11
(2,156)	1:107:A:PRO:HG2	1:107:A:PRO:HD3	10	0.11	0.01	0.11
(2,1268)	1:78:A:LYS:HD3	1:74:A:SER:HB3	9	1.89	0.51	2.0
(2,1268)	1:78:A:LYS:HD2	1:74:A:SER:HB3	9	1.89	0.51	2.0
(2,1231)	1:76:A:MET:HG2	1:82:A:PHE:HE1	9	1.03	0.18	1.09
(2,1231)	1:76:A:MET:HG2	1:82:A:PHE:HE2	9	1.03	0.18	1.09
(2,1908)	1:84:A:THR:H	1:88:A:GLU:HG3	9	1.02	0.36	1.07
(2,1908)	1:84:A:THR:H	1:87:A:GLU:HG2	9	1.02	0.36	1.07
(2,1258)	1:136:A:LYS:HD3	1:59:A:MET:HA	9	0.98	0.17	0.95
(2,1258)	1:136:A:LYS:HD2	1:59:A:MET:HA	9	0.98	0.17	0.95
(2,1176)	1:66:A:GLU:HG3	1:128:A:VAL:HG23	9	0.94	0.37	1.01
(2,1176)	1:87:A:GLU:HG2	1:86:A:ILE:HG12	9	0.94	0.37	1.01
(2,1176)	1:66:A:GLU:HG3	1:128:A:VAL:HG22	9	0.94	0.37	1.01
(2,1176)	1:66:A:GLU:HG3	1:128:A:VAL:HG21	9	0.94	0.37	1.01
(2,1176)	1:66:A:GLU:HG3	1:101:A:VAL:HG11	9	0.94	0.37	1.01
(2,1861)	1:77:A:ALA:H	1:78:A:LYS:HE3	9	0.89	0.38	0.99
(2,216)	1:96:A:LEU:HD13	1:103:A:MET:HA	9	0.82	0.05	0.81
(2,216)	1:96:A:LEU:HD11	1:103:A:MET:HA	9	0.82	0.05	0.81
(2,216)	1:96:A:LEU:HD12	1:103:A:MET:HA	9	0.82	0.05	0.81
(2,1401)	1:84:A:THR:HG23	1:89:A:LEU:HD23	9	0.76	0.39	0.68
(2,1401)	1:84:A:THR:HG22	1:89:A:LEU:HD23	9	0.76	0.39	0.68
(2,1401)	1:84:A:THR:HG22	1:89:A:LEU:HD22	9	0.76	0.39	0.68
(2,1401)	1:84:A:THR:HG23	1:89:A:LEU:HD22	9	0.76	0.39	0.68

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1401)	1:84:A:THR:HG23	1:118:A:LEU:HD21	9	0.76	0.39	0.68
(2,1401)	1:84:A:THR:HG22	1:89:A:LEU:HD21	9	0.76	0.39	0.68
(2,1401)	1:84:A:THR:HG21	1:89:A:LEU:HD22	9	0.76	0.39	0.68
(2,1478)	1:98:A:GLU:HG3	1:97:A:THR:HB	9	0.66	0.18	0.64
(2,1478)	1:97:A:THR:HB	1:78:A:LYS:HE2	9	0.66	0.18	0.64
(2,1393)	1:110:A:VAL:HG23	1:119:A:LEU:HG	9	0.63	0.12	0.63
(2,1393)	1:60:A:THR:HG22	1:62:A:LEU:HB3	9	0.63	0.12	0.63
(2,1393)	1:60:A:THR:HG23	1:62:A:LEU:HB3	9	0.63	0.12	0.63
(2,1393)	1:60:A:THR:HG21	1:62:A:LEU:HB3	9	0.63	0.12	0.63
(2,1424)	1:125:A:ALA:HB1	1:72:A:ASN:HB3	9	0.61	0.1	0.61
(2,1424)	1:125:A:ALA:HB2	1:72:A:ASN:HB3	9	0.61	0.1	0.61
(2,1424)	1:73:A:PHE:HB3	1:125:A:ALA:HB3	9	0.61	0.1	0.61
(2,1424)	1:73:A:PHE:HB3	1:125:A:ALA:HB1	9	0.61	0.1	0.61
(2,1424)	1:73:A:PHE:HB3	1:125:A:ALA:HB2	9	0.61	0.1	0.61
(1,46)	1:108:A:LYS:HE3	1:59:A:MET:HA	9	0.6	0.6	0.23
(2,1682)	1:62:A:LEU:HA	1:103:A:MET:HG3	9	0.6	0.46	0.4
(2,1682)	1:62:A:LEU:HA	1:63:A:MET:HB2	9	0.6	0.46	0.4
(2,1759)	1:82:A:PHE:HB3	1:85:A:ARG:HG3	9	0.58	0.08	0.58
(1,11)	1:66:A:GLU:HB3	1:101:A:VAL:HA	9	0.58	0.13	0.63
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG23	9	0.56	0.69	0.32
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG21	9	0.56	0.69	0.32
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG22	9	0.56	0.69	0.32
(2,459)	1:77:A:ALA:HB3	1:74:A:SER:HB3	9	0.54	0.07	0.56
(2,459)	1:77:A:ALA:HB1	1:74:A:SER:HB3	9	0.54	0.07	0.56
(2,459)	1:77:A:ALA:HB2	1:74:A:SER:HB3	9	0.54	0.07	0.56
(2,1860)	1:77:A:ALA:H	1:76:A:MET:HG2	9	0.53	0.08	0.55
(2,494)	1:65:A:THR:HG21	1:99:A:THR:HA	9	0.53	0.08	0.56
(2,494)	1:65:A:THR:HG23	1:99:A:THR:HA	9	0.53	0.08	0.56
(2,494)	1:65:A:THR:HG22	1:99:A:THR:HA	9	0.53	0.08	0.56
(2,1238)	1:134:A:GLU:HB3	1:131:A:LEU:HA	9	0.5	0.46	0.34
(2,1661)	1:134:A:GLU:HB3	1:131:A:LEU:HA	9	0.5	0.45	0.34
(2,1661)	1:132:A:ASP:HA	1:103:A:MET:HB3	9	0.5	0.45	0.34
(2,1544)	1:74:A:SER:HB3	1:75:A:LYS:HG2	9	0.47	0.32	0.27
(2,1544)	1:74:A:SER:HB3	1:71:A:LYS:HG2	9	0.47	0.32	0.27
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD22	9	0.46	0.05	0.44
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD23	9	0.46	0.05	0.44
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD21	9	0.46	0.05	0.44
(2,1438)	1:104:A:ILE:HG21	1:62:A:LEU:HB2	9	0.43	0.07	0.46
(2,1438)	1:104:A:ILE:HG22	1:62:A:LEU:HB2	9	0.43	0.07	0.46
(2,1438)	1:104:A:ILE:HG23	1:62:A:LEU:HB2	9	0.43	0.07	0.46
(2,1396)	1:101:A:VAL:HG12	1:65:A:THR:HA	9	0.43	0.13	0.44
(2,1396)	1:101:A:VAL:HG13	1:63:A:MET:HA	9	0.43	0.13	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1396)	1:101:A:VAL:HG11	1:65:A:THR:HA	9	0.43	0.13	0.44
(2,1396)	1:101:A:VAL:HG23	1:65:A:THR:HA	9	0.43	0.13	0.44
(2,1396)	1:101:A:VAL:HG12	1:63:A:MET:HA	9	0.43	0.13	0.44
(2,1396)	1:101:A:VAL:HG13	1:65:A:THR:HA	9	0.43	0.13	0.44
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD23	9	0.41	0.07	0.41
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD21	9	0.41	0.07	0.41
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD22	9	0.41	0.07	0.41
(2,1940)	1:127:A:GLY:H	1:123:A:LEU:HG	9	0.38	0.12	0.4
(2,1294)	1:106:A:LEU:HG	1:90:A:GLY:HA3	9	0.35	0.08	0.36
(2,318)	1:64:A:VAL:HG22	1:102:A:THR:HB	9	0.35	0.09	0.38
(2,318)	1:64:A:VAL:HG21	1:102:A:THR:HB	9	0.35	0.09	0.38
(2,318)	1:64:A:VAL:HG23	1:102:A:THR:HB	9	0.35	0.09	0.38
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB1	9	0.35	0.12	0.38
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB2	9	0.35	0.12	0.38
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB3	9	0.35	0.12	0.38
(2,36)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	9	0.35	0.02	0.36
(2,1381)	1:64:A:VAL:HG13	1:125:A:ALA:HB2	9	0.35	0.15	0.42
(2,1381)	1:64:A:VAL:HG12	1:125:A:ALA:HB3	9	0.35	0.15	0.42
(2,1381)	1:64:A:VAL:HG13	1:125:A:ALA:HB3	9	0.35	0.15	0.42
(2,1381)	1:64:A:VAL:HG12	1:125:A:ALA:HB1	9	0.35	0.15	0.42
(2,1381)	1:64:A:VAL:HG11	1:125:A:ALA:HB3	9	0.35	0.15	0.42
(2,1381)	1:64:A:VAL:HG11	1:125:A:ALA:HB1	9	0.35	0.15	0.42
(2,1381)	1:64:A:VAL:HG12	1:125:A:ALA:HB2	9	0.35	0.15	0.42
(2,1557)	1:95:A:PHE:HE2	1:102:A:THR:HB	9	0.32	0.11	0.34
(2,1557)	1:95:A:PHE:HE1	1:102:A:THR:HB	9	0.32	0.11	0.34
(2,1662)	1:131:A:LEU:HA	1:61:A:ARG:HA	9	0.32	0.13	0.28
(2,624)	1:101:A:VAL:HG13	1:63:A:MET:HA	9	0.31	0.11	0.3
(2,624)	1:101:A:VAL:HG12	1:63:A:MET:HA	9	0.31	0.11	0.3
(2,624)	1:101:A:VAL:HG11	1:63:A:MET:HA	9	0.31	0.11	0.3
(2,1288)	1:137:A:LEU:HG	1:132:A:ASP:HA	9	0.31	0.09	0.33
(2,1796)	1:96:A:LEU:H	1:101:A:VAL:HB	9	0.3	0.05	0.31
(2,1796)	1:96:A:LEU:H	1:96:A:LEU:HB3	9	0.3	0.05	0.31
(2,279)	1:64:A:VAL:HG13	1:122:A:ILE:HG21	9	0.3	0.1	0.3
(2,279)	1:64:A:VAL:HG12	1:122:A:ILE:HG22	9	0.3	0.1	0.3
(2,279)	1:64:A:VAL:HG12	1:122:A:ILE:HG23	9	0.3	0.1	0.3
(2,279)	1:64:A:VAL:HG11	1:122:A:ILE:HG22	9	0.3	0.1	0.3
(2,279)	1:64:A:VAL:HG11	1:122:A:ILE:HG23	9	0.3	0.1	0.3
(2,724)	1:128:A:VAL:HG21	1:65:A:THR:HB	9	0.28	0.12	0.23
(2,724)	1:128:A:VAL:HG22	1:65:A:THR:HB	9	0.28	0.12	0.23
(2,724)	1:128:A:VAL:HG23	1:65:A:THR:HB	9	0.28	0.12	0.23
(2,990)	1:59:A:MET:H	1:59:A:MET:HB3	9	0.27	0.05	0.27
(2,1922)	1:86:A:ILE:H	1:87:A:GLU:HB2	9	0.26	0.05	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1321)	1:62:A:LEU:HD11	1:82:A:PHE:HZ	9	0.26	0.07	0.26
(2,1321)	1:62:A:LEU:HD13	1:82:A:PHE:HZ	9	0.26	0.07	0.26
(2,1321)	1:62:A:LEU:HD12	1:82:A:PHE:HZ	9	0.26	0.07	0.26
(2,1628)	1:95:A:PHE:HA	1:96:A:LEU:HB2	9	0.25	0.02	0.25
(1,3)	1:122:A:ILE:HB	1:62:A:LEU:HB2	9	0.24	0.05	0.22
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB3	9	0.22	0.04	0.23
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB2	9	0.22	0.04	0.23
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB1	9	0.22	0.04	0.23
(2,364)	1:104:A:ILE:HD11	1:82:A:PHE:HE2	9	0.21	0.05	0.23
(2,364)	1:104:A:ILE:HD12	1:82:A:PHE:HE2	9	0.21	0.05	0.23
(2,364)	1:104:A:ILE:HD13	1:82:A:PHE:HE2	9	0.21	0.05	0.23
(2,1531)	1:87:A:GLU:HG3	1:83:A:SER:HA	9	0.19	0.04	0.21
(2,788)	1:73:A:PHE:H	1:73:A:PHE:HD2	9	0.19	0.06	0.15
(2,788)	1:73:A:PHE:H	1:73:A:PHE:HD1	9	0.19	0.06	0.15
(2,1253)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	9	0.18	0.05	0.17
(2,564)	1:95:A:PHE:HD2	1:95:A:PHE:HA	9	0.18	0.05	0.21
(2,564)	1:95:A:PHE:HD1	1:95:A:PHE:HA	9	0.18	0.05	0.21
(2,1791)	1:103:A:MET:H	1:103:A:MET:HB3	9	0.17	0.02	0.18
(2,1602)	1:118:A:LEU:HG	1:118:A:LEU:HA	9	0.17	0.03	0.16
(2,918)	1:71:A:LYS:H	1:67:A:LYS:HA	9	0.17	0.02	0.17
(2,1240)	1:120:A:HIS:HB3	1:122:A:ILE:HG13	9	0.15	0.04	0.15
(1,47)	1:103:A:MET:H	1:95:A:PHE:HB3	9	0.15	0.03	0.14
(2,479)	1:128:A:VAL:HG13	1:128:A:VAL:HA	9	0.14	0.03	0.14
(2,479)	1:128:A:VAL:HG12	1:128:A:VAL:HA	9	0.14	0.03	0.14
(2,479)	1:128:A:VAL:HG11	1:128:A:VAL:HA	9	0.14	0.03	0.14
(2,1611)	1:104:A:ILE:HG12	1:82:A:PHE:HZ	9	0.14	0.02	0.14
(2,394)	1:99:A:THR:HB	1:98:A:GLU:HB3	8	1.16	0.07	1.15
(2,1056)	1:113:A:HIS:H	1:114:A:ASP:HB3	8	1.08	0.06	1.08
(2,727)	1:111:A:SER:HB3	1:114:A:ASP:HB3	8	0.89	0.13	0.94
(2,1357)	1:96:A:LEU:HD23	1:61:A:ARG:HD2	8	0.82	0.56	0.64
(2,1357)	1:96:A:LEU:HD22	1:61:A:ARG:HD3	8	0.82	0.56	0.64
(2,1357)	1:96:A:LEU:HD23	1:61:A:ARG:HD3	8	0.82	0.56	0.64
(2,1357)	1:96:A:LEU:HD21	1:61:A:ARG:HD3	8	0.82	0.56	0.64
(2,1332)	1:119:A:LEU:HD12	1:119:A:LEU:HA	8	0.81	0.11	0.84
(2,1332)	1:119:A:LEU:HD11	1:119:A:LEU:HA	8	0.81	0.11	0.84
(2,1332)	1:119:A:LEU:HD13	1:119:A:LEU:HA	8	0.81	0.11	0.84
(2,1332)	1:137:A:LEU:HD11	1:133:A:SER:HB3	8	0.81	0.11	0.84
(2,1332)	1:137:A:LEU:HD12	1:133:A:SER:HB3	8	0.81	0.11	0.84
(2,258)	1:89:A:LEU:HD22	1:114:A:ASP:HB2	8	0.75	0.06	0.76
(2,258)	1:89:A:LEU:HD21	1:114:A:ASP:HB2	8	0.75	0.06	0.76
(2,258)	1:89:A:LEU:HD23	1:114:A:ASP:HB2	8	0.75	0.06	0.76
(2,1032)	1:84:A:THR:H	1:84:A:THR:HG23	8	0.73	0.19	0.76

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1032)	1:84:A:THR:H	1:84:A:THR:HG22	8	0.73	0.19	0.76
(2,1032)	1:84:A:THR:H	1:84:A:THR:HG21	8	0.73	0.19	0.76
(2,1726)	1:127:A:GLY:HA2	1:128:A:VAL:HB	8	0.57	0.01	0.56
(2,1607)	1:76:A:MET:HA	1:75:A:LYS:HG2	8	0.55	0.12	0.54
(2,1607)	1:76:A:MET:HA	1:78:A:LYS:HG3	8	0.55	0.12	0.54
(2,759)	1:111:A:SER:H	1:114:A:ASP:HB3	8	0.52	0.03	0.5
(2,1364)	1:119:A:LEU:HD22	1:104:A:ILE:HG12	8	0.5	0.1	0.47
(2,1364)	1:119:A:LEU:HD21	1:104:A:ILE:HG12	8	0.5	0.1	0.47
(2,1364)	1:119:A:LEU:HD23	1:104:A:ILE:HG12	8	0.5	0.1	0.47
(2,1224)	1:115:A:MET:HB3	1:111:A:SER:HB2	8	0.5	0.35	0.37
(2,1224)	1:115:A:MET:HB3	1:109:A:THR:HA	8	0.5	0.35	0.37
(2,1915)	1:79:A:SER:H	1:78:A:LYS:HG3	8	0.44	0.11	0.46
(2,1770)	1:116:A:ASP:HB2	1:112:A:GLU:HB3	8	0.43	0.12	0.4
(2,1770)	1:116:A:ASP:HB2	1:112:A:GLU:HB2	8	0.43	0.12	0.4
(2,1770)	1:116:A:ASP:HB2	1:115:A:MET:HB2	8	0.43	0.12	0.4
(2,1752)	1:78:A:LYS:HE2	1:75:A:LYS:HA	8	0.42	0.14	0.44
(2,1752)	1:74:A:SER:HA	1:78:A:LYS:HE2	8	0.42	0.14	0.44
(2,1683)	1:131:A:LEU:HD22	1:62:A:LEU:HA	8	0.39	0.16	0.36
(2,1683)	1:131:A:LEU:HD12	1:62:A:LEU:HA	8	0.39	0.16	0.36
(2,1683)	1:131:A:LEU:HD11	1:62:A:LEU:HA	8	0.39	0.16	0.36
(2,267)	1:110:A:VAL:HG23	1:114:A:ASP:HB3	8	0.33	0.03	0.33
(2,267)	1:110:A:VAL:HG22	1:114:A:ASP:HB3	8	0.33	0.03	0.33
(2,267)	1:110:A:VAL:HG21	1:114:A:ASP:HB3	8	0.33	0.03	0.33
(2,1159)	1:72:A:ASN:HB3	1:76:A:MET:HB3	8	0.3	0.12	0.36
(2,1159)	1:72:A:ASN:HB2	1:76:A:MET:HB3	8	0.3	0.12	0.36
(2,962)	1:114:A:ASP:H	1:114:A:ASP:HB3	8	0.29	0.01	0.29
(2,225)	1:115:A:MET:HG3	1:119:A:LEU:HD13	8	0.26	0.1	0.26
(2,225)	1:115:A:MET:HG3	1:119:A:LEU:HD12	8	0.26	0.1	0.26
(2,225)	1:115:A:MET:HG3	1:119:A:LEU:HD11	8	0.26	0.1	0.26
(2,299)	1:101:A:VAL:HG13	1:102:A:THR:HA	8	0.23	0.06	0.22
(2,299)	1:101:A:VAL:HG12	1:102:A:THR:HA	8	0.23	0.06	0.22
(2,299)	1:101:A:VAL:HG11	1:102:A:THR:HA	8	0.23	0.06	0.22
(2,1819)	1:136:A:LYS:H	1:58:A:GLU:HA	8	0.21	0.06	0.22
(2,506)	1:118:A:LEU:HD23	1:82:A:PHE:HE1	8	0.2	0.04	0.2
(2,506)	1:118:A:LEU:HD22	1:82:A:PHE:HE1	8	0.2	0.04	0.2
(2,506)	1:118:A:LEU:HD21	1:82:A:PHE:HE1	8	0.2	0.04	0.2
(2,295)	1:101:A:VAL:HG13	1:103:A:MET:HA	8	0.18	0.05	0.16
(2,295)	1:101:A:VAL:HG12	1:103:A:MET:HA	8	0.18	0.05	0.16
(2,295)	1:101:A:VAL:HG11	1:103:A:MET:HA	8	0.18	0.05	0.16
(2,521)	1:86:A:ILE:HG23	1:87:A:GLU:HA	8	0.17	0.05	0.15
(2,521)	1:86:A:ILE:HG22	1:87:A:GLU:HA	8	0.17	0.05	0.15
(2,177)	1:123:A:LEU:HG	1:122:A:ILE:HG22	8	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,177)	1:123:A:LEU:HG	1:122:A:ILE:HG21	8	0.15	0.03	0.16
(2,177)	1:123:A:LEU:HG	1:122:A:ILE:HG23	8	0.15	0.03	0.16
(2,794)	1:82:A:PHE:H	1:82:A:PHE:HD1	8	0.14	0.03	0.14
(2,256)	1:89:A:LEU:HD21	1:89:A:LEU:HA	8	0.13	0.02	0.13
(2,256)	1:89:A:LEU:HD23	1:89:A:LEU:HA	8	0.13	0.02	0.13
(2,256)	1:89:A:LEU:HD22	1:89:A:LEU:HA	8	0.13	0.02	0.13
(2,1343)	1:137:A:LEU:HD11	1:136:A:LYS:HE2	7	1.71	0.87	1.44
(2,1343)	1:137:A:LEU:HD12	1:136:A:LYS:HE3	7	1.71	0.87	1.44
(2,1343)	1:137:A:LEU:HD13	1:136:A:LYS:HE3	7	1.71	0.87	1.44
(2,1343)	1:137:A:LEU:HD11	1:136:A:LYS:HE3	7	1.71	0.87	1.44
(2,1343)	1:106:A:LEU:HD21	1:113:A:HIS:HB2	7	1.71	0.87	1.44
(2,1425)	1:138:A:ALA:HB2	1:108:A:LYS:HG3	7	1.08	0.33	1.02
(2,1425)	1:138:A:ALA:HB1	1:108:A:LYS:HG3	7	1.08	0.33	1.02
(2,1425)	1:138:A:ALA:HB3	1:61:A:ARG:HG3	7	1.08	0.33	1.02
(2,1425)	1:138:A:ALA:HB1	1:61:A:ARG:HG3	7	1.08	0.33	1.02
(2,1425)	1:138:A:ALA:HB2	1:61:A:ARG:HG3	7	1.08	0.33	1.02
(2,1174)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	7	1.06	0.38	0.99
(2,131)	1:136:A:LYS:HD3	1:58:A:GLU:HG3	7	0.94	0.41	0.88
(2,1154)	1:72:A:ASN:HB2	1:73:A:PHE:HD1	7	0.85	0.69	0.37
(2,1154)	1:72:A:ASN:HB2	1:73:A:PHE:HD2	7	0.85	0.69	0.37
(2,943)	1:58:A:GLU:H	1:59:A:MET:H	7	0.8	0.19	0.85
(2,1257)	1:75:A:LYS:HD3	1:78:A:LYS:HE2	7	0.78	0.52	0.62
(2,1257)	1:136:A:LYS:HD2	1:59:A:MET:HG2	7	0.78	0.52	0.62
(2,1257)	1:136:A:LYS:HD3	1:58:A:GLU:HG3	7	0.78	0.52	0.62
(2,1269)	1:78:A:LYS:HD2	1:75:A:LYS:HE2	7	0.44	0.22	0.46
(2,1269)	1:78:A:LYS:HD3	1:75:A:LYS:HE3	7	0.44	0.22	0.46
(2,1269)	1:78:A:LYS:HD2	1:75:A:LYS:HE3	7	0.44	0.22	0.46
(2,121)	1:58:A:GLU:HB3	1:59:A:MET:HA	7	0.42	0.05	0.43
(2,182)	1:137:A:LEU:HG	1:61:A:ARG:HD3	7	0.42	0.15	0.36
(2,182)	1:137:A:LEU:HG	1:61:A:ARG:HD2	7	0.42	0.15	0.36
(2,604)	1:131:A:LEU:HD22	1:131:A:LEU:HA	7	0.35	0.1	0.33
(2,604)	1:131:A:LEU:HD21	1:131:A:LEU:HA	7	0.35	0.1	0.33
(2,604)	1:131:A:LEU:HD23	1:131:A:LEU:HA	7	0.35	0.1	0.33
(2,1249)	1:117:A:GLN:HB2	1:113:A:HIS:HA	7	0.35	0.1	0.32
(2,1249)	1:117:A:GLN:HB2	1:114:A:ASP:HA	7	0.35	0.1	0.32
(2,1317)	1:78:A:LYS:HG3	1:78:A:LYS:HA	7	0.33	0.05	0.34
(2,813)	1:137:A:LEU:H	1:137:A:LEU:HD12	7	0.32	0.05	0.32
(2,813)	1:137:A:LEU:H	1:137:A:LEU:HD11	7	0.32	0.05	0.32
(2,813)	1:137:A:LEU:H	1:137:A:LEU:HD13	7	0.32	0.05	0.32
(2,592)	1:61:A:ARG:HA	1:61:A:ARG:HD2	7	0.31	0.06	0.31
(2,649)	1:70:A:SER:HB2	1:126:A:GLY:HA3	7	0.31	0.17	0.24
(2,219)	1:75:A:LYS:HG3	1:75:A:LYS:HA	7	0.26	0.04	0.27

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1881)	1:114:A:ASP:H	1:115:A:MET:HB3	7	0.23	0.04	0.23
(2,28)	1:87:A:GLU:HG2	1:87:A:GLU:HB3	7	0.22	0.13	0.18
(2,1553)	1:60:A:THR:HA	1:59:A:MET:HG2	7	0.22	0.09	0.25
(2,1553)	1:60:A:THR:HA	1:107:A:PRO:HB3	7	0.22	0.09	0.25
(2,1814)	1:62:A:LEU:H	1:62:A:LEU:HB3	7	0.21	0.04	0.24
(2,1814)	1:62:A:LEU:H	1:104:A:ILE:HB	7	0.21	0.04	0.24
(2,1383)	1:96:A:LEU:HB3	1:97:A:THR:HG23	7	0.21	0.07	0.18
(2,1383)	1:66:A:GLU:HB2	1:97:A:THR:HG21	7	0.21	0.07	0.18
(2,1383)	1:66:A:GLU:HB2	1:97:A:THR:HG22	7	0.21	0.07	0.18
(2,1383)	1:96:A:LEU:HB3	1:97:A:THR:HG22	7	0.21	0.07	0.18
(2,1785)	1:103:A:MET:H	1:103:A:MET:HG2	7	0.19	0.05	0.18
(2,365)	1:93:A:ILE:HD11	1:82:A:PHE:HD2	7	0.16	0.02	0.16
(2,365)	1:93:A:ILE:HD12	1:82:A:PHE:HD2	7	0.16	0.02	0.16
(2,365)	1:93:A:ILE:HD13	1:82:A:PHE:HD2	7	0.16	0.02	0.16
(2,291)	1:60:A:THR:HG22	1:60:A:THR:HA	7	0.15	0.02	0.15
(2,291)	1:60:A:THR:HG21	1:60:A:THR:HA	7	0.15	0.02	0.15
(2,291)	1:60:A:THR:HG23	1:60:A:THR:HA	7	0.15	0.02	0.15
(2,139)	1:71:A:LYS:HD3	1:74:A:SER:HA	6	1.45	0.08	1.45
(2,1256)	1:75:A:LYS:HD3	1:78:A:LYS:HE3	6	0.81	0.54	0.78
(2,1149)	1:58:A:GLU:H	1:58:A:GLU:HG2	6	0.71	0.42	0.78
(2,1252)	1:136:A:LYS:HD3	1:59:A:MET:HG2	6	0.7	0.38	0.73
(2,1252)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	6	0.7	0.38	0.73
(1,24)	1:75:A:LYS:HG3	1:78:A:LYS:HE3	6	0.67	0.29	0.68
(2,472)	1:82:A:PHE:HA	1:84:A:THR:HG23	6	0.47	0.25	0.42
(2,472)	1:82:A:PHE:HA	1:84:A:THR:HG22	6	0.47	0.25	0.42
(2,472)	1:82:A:PHE:HA	1:84:A:THR:HG21	6	0.47	0.25	0.42
(2,1372)	1:89:A:LEU:HD21	1:88:A:GLU:HB3	6	0.41	0.07	0.45
(2,1372)	1:89:A:LEU:HD23	1:88:A:GLU:HB3	6	0.41	0.07	0.45
(2,1372)	1:103:A:MET:HG2	1:101:A:VAL:HG13	6	0.41	0.07	0.45
(2,1372)	1:103:A:MET:HG2	1:101:A:VAL:HG12	6	0.41	0.07	0.45
(2,1372)	1:89:A:LEU:HD22	1:88:A:GLU:HB3	6	0.41	0.07	0.45
(2,72)	1:59:A:MET:HG3	1:136:A:LYS:HB3	6	0.38	0.42	0.2
(2,1673)	1:93:A:ILE:HD11	1:77:A:ALA:HA	6	0.34	0.09	0.36
(2,1673)	1:93:A:ILE:HD13	1:77:A:ALA:HA	6	0.34	0.09	0.36
(2,1649)	1:78:A:LYS:HD3	1:78:A:LYS:HA	6	0.3	0.21	0.24
(2,1649)	1:78:A:LYS:HG3	1:78:A:LYS:HA	6	0.3	0.21	0.24
(2,1649)	1:78:A:LYS:HD2	1:78:A:LYS:HA	6	0.3	0.21	0.24
(2,1305)	1:118:A:LEU:HD13	1:85:A:ARG:HA	6	0.21	0.04	0.2
(2,1305)	1:118:A:LEU:HD11	1:85:A:ARG:HA	6	0.21	0.04	0.2
(2,1949)	1:90:A:GLY:H	1:107:A:PRO:HG3	6	0.21	0.06	0.22
(2,1514)	1:86:A:ILE:HD11	1:82:A:PHE:HD1	6	0.2	0.07	0.2
(2,1514)	1:86:A:ILE:HD12	1:82:A:PHE:HD1	6	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)
(2,1514)	1:86:A:ILE:HD13	1:82:A:PHE:HD1	6	0.2	0.07	0.2
(1,41)	1:105:A:GLU:HA	1:132:A:ASP:HB2	6	0.19	0.07	0.2
(2,1597)	1:75:A:LYS:HB3	1:75:A:LYS:HA	6	0.18	0.06	0.16
(2,1597)	1:75:A:LYS:HB2	1:75:A:LYS:HA	6	0.18	0.06	0.16
(2,1209)	1:110:A:VAL:HB	1:106:A:LEU:HG	6	0.18	0.07	0.17
(2,1295)	1:106:A:LEU:HG	1:89:A:LEU:HB3	6	0.18	0.05	0.16
(2,1680)	1:104:A:ILE:HD13	1:63:A:MET:HA	6	0.18	0.02	0.17
(2,1680)	1:104:A:ILE:HD11	1:63:A:MET:HA	6	0.18	0.02	0.17
(2,1680)	1:104:A:ILE:HD12	1:63:A:MET:HA	6	0.18	0.02	0.17
(1,43)	1:132:A:ASP:HA	1:103:A:MET:HG2	6	0.15	0.03	0.15
(2,1685)	1:62:A:LEU:HA	1:103:A:MET:HB3	6	0.14	0.02	0.13
(2,617)	1:103:A:MET:HG2	1:103:A:MET:HA	6	0.14	0.01	0.14
(2,546)	1:119:A:LEU:HA	1:119:A:LEU:HB2	6	0.1	0.0	0.1
(2,1223)	1:115:A:MET:HB3	1:106:A:LEU:HD22	5	0.62	0.23	0.73
(2,1223)	1:115:A:MET:HB3	1:106:A:LEU:HD23	5	0.62	0.23	0.73
(2,1223)	1:115:A:MET:HB3	1:106:A:LEU:HD21	5	0.62	0.23	0.73
(2,1223)	1:103:A:MET:HG2	1:101:A:VAL:HG13	5	0.62	0.23	0.73
(2,1223)	1:103:A:MET:HG2	1:96:A:LEU:HD21	5	0.62	0.23	0.73
(2,1810)	1:136:A:LYS:H	1:136:A:LYS:HD2	5	0.48	0.17	0.52
(2,1810)	1:136:A:LYS:H	1:136:A:LYS:HD3	5	0.48	0.17	0.52
(2,1222)	1:76:A:MET:HG3	1:77:A:ALA:HB1	5	0.34	0.17	0.3
(2,1222)	1:76:A:MET:HG3	1:77:A:ALA:HB3	5	0.34	0.17	0.3
(2,1222)	1:76:A:MET:HG3	1:77:A:ALA:HB2	5	0.34	0.17	0.3
(2,330)	1:64:A:VAL:HG13	1:125:A:ALA:HB2	5	0.33	0.06	0.31
(2,330)	1:64:A:VAL:HG12	1:125:A:ALA:HB3	5	0.33	0.06	0.31
(2,330)	1:64:A:VAL:HG12	1:125:A:ALA:HB1	5	0.33	0.06	0.31
(2,330)	1:64:A:VAL:HG11	1:125:A:ALA:HB3	5	0.33	0.06	0.31
(2,167)	1:61:A:ARG:HG2	1:105:A:GLU:HA	5	0.33	0.42	0.13
(2,1740)	1:128:A:VAL:HG21	1:67:A:LYS:HE3	5	0.33	0.34	0.16
(2,1740)	1:128:A:VAL:HG22	1:67:A:LYS:HE2	5	0.33	0.34	0.16
(2,1740)	1:128:A:VAL:HG23	1:67:A:LYS:HE2	5	0.33	0.34	0.16
(2,1153)	1:72:A:ASN:HB3	1:76:A:MET:HG2	5	0.26	0.15	0.17
(2,688)	1:108:A:LYS:HD3	1:108:A:LYS:HE3	5	0.23	0.02	0.24
(1,23)	1:93:A:ILE:HG12	1:78:A:LYS:HG2	5	0.23	0.23	0.12
(2,433)	1:76:A:MET:HG3	1:82:A:PHE:HD1	5	0.22	0.11	0.16
(2,630)	1:77:A:ALA:HA	1:93:A:ILE:HG23	5	0.22	0.06	0.25
(2,630)	1:77:A:ALA:HA	1:93:A:ILE:HG22	5	0.22	0.06	0.25
(2,1403)	1:102:A:THR:HG23	1:74:A:SER:HA	5	0.19	0.09	0.14
(2,1403)	1:102:A:THR:HG22	1:74:A:SER:HA	5	0.19	0.09	0.14
(2,1403)	1:102:A:THR:HG21	1:74:A:SER:HA	5	0.19	0.09	0.14
(2,363)	1:93:A:ILE:HD11	1:77:A:ALA:HA	5	0.19	0.04	0.19
(2,363)	1:93:A:ILE:HD13	1:77:A:ALA:HA	5	0.19	0.04	0.19

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1181)	1:101:A:VAL:HB	1:103:A:MET:HA	5	0.19	0.05	0.16
(2,1184)	1:59:A:MET:HB3	1:90:A:GLY:HA2	5	0.18	0.06	0.14
(2,1642)	1:72:A:ASN:HA	1:72:A:ASN:HB3	5	0.17	0.03	0.17
(2,1642)	1:72:A:ASN:HB2	1:72:A:ASN:HA	5	0.17	0.03	0.17
(2,308)	1:102:A:THR:HG23	1:104:A:ILE:HG13	5	0.16	0.02	0.16
(2,308)	1:102:A:THR:HG22	1:104:A:ILE:HG13	5	0.16	0.02	0.16
(2,933)	1:60:A:THR:H	1:106:A:LEU:HB3	5	0.15	0.05	0.12
(2,1892)	1:65:A:THR:H	1:128:A:VAL:HB	5	0.15	0.03	0.14
(2,1230)	1:71:A:LYS:HB2	1:71:A:LYS:HE3	5	0.14	0.02	0.15
(2,1230)	1:71:A:LYS:HB2	1:71:A:LYS:HE2	5	0.14	0.02	0.15
(2,1928)	1:83:A:SER:H	1:85:A:ARG:HB3	5	0.13	0.03	0.12
(2,514)	1:115:A:MET:HG3	1:112:A:GLU:HA	5	0.13	0.01	0.12
(2,598)	1:66:A:GLU:HA	1:73:A:PHE:HD2	5	0.12	0.01	0.12
(2,598)	1:66:A:GLU:HA	1:73:A:PHE:HD1	5	0.12	0.01	0.12
(2,1329)	1:136:A:LYS:HG2	1:136:A:LYS:HD2	5	0.12	0.01	0.12
(2,1365)	1:89:A:LEU:HG	1:89:A:LEU:HD23	5	0.12	0.0	0.12
(2,1365)	1:89:A:LEU:HG	1:89:A:LEU:HD22	5	0.12	0.0	0.12
(2,48)	1:86:A:ILE:HB	1:86:A:ILE:HD11	5	0.11	0.01	0.11
(2,48)	1:86:A:ILE:HB	1:86:A:ILE:HD13	5	0.11	0.01	0.11
(2,48)	1:86:A:ILE:HB	1:86:A:ILE:HD12	5	0.11	0.01	0.11
(2,6)	1:72:A:ASN:HB2	1:126:A:GLY:HA2	4	0.97	0.5	1.21
(2,587)	1:71:A:LYS:HD3	1:71:A:LYS:HA	4	0.56	0.07	0.6
(2,1265)	1:78:A:LYS:HD3	1:78:A:LYS:HA	4	0.54	0.26	0.5
(2,1265)	1:78:A:LYS:HD2	1:78:A:LYS:HA	4	0.54	0.26	0.5
(2,1148)	1:58:A:GLU:H	1:58:A:GLU:HB3	4	0.52	0.03	0.52
(2,812)	1:137:A:LEU:H	1:60:A:THR:HG23	4	0.45	0.2	0.5
(2,812)	1:137:A:LEU:H	1:60:A:THR:HG21	4	0.45	0.2	0.5
(2,812)	1:137:A:LEU:H	1:60:A:THR:HG22	4	0.45	0.2	0.5
(2,1502)	1:133:A:SER:HB3	1:136:A:LYS:HB2	4	0.44	0.34	0.34
(2,1502)	1:70:A:SER:HB2	1:71:A:LYS:HD3	4	0.44	0.34	0.34
(2,870)	1:87:A:GLU:H	1:84:A:THR:HG22	4	0.38	0.04	0.38
(2,870)	1:87:A:GLU:H	1:84:A:THR:HG23	4	0.38	0.04	0.38
(2,870)	1:87:A:GLU:H	1:84:A:THR:HG21	4	0.38	0.04	0.38
(2,1878)	1:58:A:GLU:H	1:90:A:GLY:HA2	4	0.35	0.17	0.36
(2,1747)	1:78:A:LYS:HE3	1:75:A:LYS:HA	4	0.28	0.08	0.26
(2,523)	1:87:A:GLU:HG3	1:87:A:GLU:HA	4	0.27	0.23	0.14
(2,1408)	1:135:A:VAL:HG23	1:134:A:GLU:HA	4	0.26	0.16	0.2
(2,1408)	1:135:A:VAL:HG22	1:134:A:GLU:HA	4	0.26	0.16	0.2
(2,1408)	1:135:A:VAL:HG21	1:134:A:GLU:HA	4	0.26	0.16	0.2
(2,1408)	1:135:A:VAL:HG12	1:58:A:GLU:HA	4	0.26	0.16	0.2
(2,1618)	1:79:A:SER:HA	1:78:A:LYS:HB2	4	0.26	0.17	0.2
(2,1739)	1:75:A:LYS:HG3	1:75:A:LYS:HE3	4	0.24	0.08	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1739)	1:71:A:LYS:HE2	1:71:A:LYS:HG3	4	0.24	0.08	0.22
(2,352)	1:104:A:ILE:HG21	1:73:A:PHE:HZ	4	0.24	0.06	0.22
(2,352)	1:104:A:ILE:HG23	1:73:A:PHE:HZ	4	0.24	0.06	0.22
(2,341)	1:77:A:ALA:HB3	1:78:A:LYS:HA	4	0.2	0.09	0.16
(2,341)	1:77:A:ALA:HB1	1:78:A:LYS:HA	4	0.2	0.09	0.16
(2,341)	1:77:A:ALA:HB2	1:78:A:LYS:HA	4	0.2	0.09	0.16
(1,36)	1:85:A:ARG:HA	1:88:A:GLU:HB3	4	0.19	0.09	0.16
(2,1764)	1:116:A:ASP:HB3	1:117:A:GLN:HB2	4	0.19	0.02	0.19
(2,1416)	1:64:A:VAL:HG22	1:73:A:PHE:HE1	4	0.18	0.05	0.19
(2,1416)	1:64:A:VAL:HG21	1:73:A:PHE:HE2	4	0.18	0.05	0.19
(2,1416)	1:64:A:VAL:HG23	1:73:A:PHE:HE2	4	0.18	0.05	0.19
(2,1715)	1:85:A:ARG:HD3	1:82:A:PHE:HE1	4	0.17	0.05	0.17
(2,1474)	1:99:A:THR:HB	1:101:A:VAL:HB	4	0.17	0.03	0.17
(2,1594)	1:89:A:LEU:HG	1:111:A:SER:HA	4	0.16	0.02	0.16
(2,1323)	1:75:A:LYS:HG3	1:75:A:LYS:HE3	4	0.15	0.05	0.13
(2,1323)	1:75:A:LYS:HG3	1:75:A:LYS:HE2	4	0.15	0.05	0.13
(2,595)	1:60:A:THR:HG23	1:61:A:ARG:HA	4	0.14	0.01	0.14
(2,595)	1:60:A:THR:HG21	1:61:A:ARG:HA	4	0.14	0.01	0.14
(2,595)	1:60:A:THR:HG22	1:61:A:ARG:HA	4	0.14	0.01	0.14
(2,868)	1:87:A:GLU:H	1:86:A:ILE:HG22	4	0.14	0.0	0.14
(2,868)	1:87:A:GLU:H	1:86:A:ILE:HG23	4	0.14	0.0	0.14
(2,231)	1:123:A:LEU:HD22	1:120:A:HIS:HA	4	0.14	0.01	0.14
(2,231)	1:123:A:LEU:HD21	1:120:A:HIS:HA	4	0.14	0.01	0.14
(2,1097)	1:92:A:SER:H	1:92:A:SER:HB3	4	0.13	0.01	0.12
(2,1391)	1:60:A:THR:HG23	1:61:A:ARG:HA	4	0.13	0.01	0.13
(2,1391)	1:60:A:THR:HG21	1:61:A:ARG:HA	4	0.13	0.01	0.13
(2,1391)	1:60:A:THR:HG22	1:61:A:ARG:HA	4	0.13	0.01	0.13
(2,1088)	1:83:A:SER:H	1:82:A:PHE:HB2	4	0.12	0.01	0.12
(2,995)	1:125:A:ALA:H	1:126:A:GLY:HA2	4	0.12	0.01	0.12
(2,18)	1:122:A:ILE:HB	1:120:A:HIS:HA	4	0.11	0.0	0.11
(2,597)	1:61:A:ARG:HA	1:103:A:MET:HG3	3	1.35	0.19	1.41
(2,1177)	1:58:A:GLU:HG2	1:107:A:PRO:HD3	3	1.26	0.11	1.22
(2,528)	1:78:A:LYS:HG2	1:75:A:LYS:HA	3	1.2	0.16	1.24
(2,1327)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	3	1.19	0.53	1.48
(2,689)	1:108:A:LYS:HG3	1:108:A:LYS:HE3	3	0.87	0.04	0.87
(2,1599)	1:75:A:LYS:HG2	1:75:A:LYS:HA	3	0.85	0.04	0.83
(2,1331)	1:137:A:LEU:HD11	1:137:A:LEU:HA	3	0.78	0.37	0.52
(2,1331)	1:137:A:LEU:HD12	1:137:A:LEU:HA	3	0.78	0.37	0.52
(2,34)	1:58:A:GLU:HG2	1:135:A:VAL:HG13	3	0.75	0.34	0.54
(2,34)	1:58:A:GLU:HG2	1:135:A:VAL:HG12	3	0.75	0.34	0.54
(2,772)	1:62:A:LEU:H	1:103:A:MET:HG3	3	0.71	0.15	0.77
(2,1507)	1:133:A:SER:HB3	1:61:A:ARG:HB3	3	0.58	0.32	0.75

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1507)	1:133:A:SER:HB3	1:138:A:ALA:HB1	3	0.58	0.32	0.75
(2,687)	1:108:A:LYS:HE3	1:60:A:THR:HA	3	0.55	0.25	0.44
(1,6)	1:101:A:VAL:HB	1:103:A:MET:HG2	3	0.51	0.24	0.64
(2,1341)	1:136:A:LYS:HG2	1:58:A:GLU:HG2	3	0.41	0.18	0.39
(2,1341)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	3	0.41	0.18	0.39
(2,1743)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	3	0.34	0.22	0.21
(2,1743)	1:75:A:LYS:HG2	1:75:A:LYS:HE2	3	0.34	0.22	0.21
(2,580)	1:134:A:GLU:HA	1:62:A:LEU:HD22	3	0.32	0.26	0.14
(2,580)	1:134:A:GLU:HA	1:62:A:LEU:HD23	3	0.32	0.26	0.14
(2,654)	1:72:A:ASN:HB2	1:126:A:GLY:HA3	3	0.31	0.09	0.35
(2,243)	1:123:A:LEU:HD11	1:128:A:VAL:HA	3	0.28	0.14	0.21
(2,106)	1:103:A:MET:HG2	1:94:A:SER:HB2	3	0.24	0.03	0.25
(2,132)	1:75:A:LYS:HD3	1:75:A:LYS:HA	3	0.23	0.12	0.16
(2,583)	1:136:A:LYS:HA	1:133:A:SER:HB2	3	0.22	0.12	0.16
(2,1423)	1:125:A:ALA:HB3	1:126:A:GLY:HA2	3	0.2	0.05	0.21
(2,1423)	1:125:A:ALA:HB1	1:126:A:GLY:HA2	3	0.2	0.05	0.21
(2,1784)	1:104:A:ILE:H	1:103:A:MET:HG3	3	0.18	0.05	0.17
(2,1272)	1:78:A:LYS:HB2	1:78:A:LYS:HD2	3	0.17	0.03	0.17
(2,1800)	1:105:A:GLU:H	1:86:A:ILE:HG23	3	0.15	0.06	0.12
(2,1800)	1:105:A:GLU:H	1:86:A:ILE:HG21	3	0.15	0.06	0.12
(2,326)	1:125:A:ALA:HB1	1:125:A:ALA:HA	3	0.14	0.02	0.15
(2,326)	1:125:A:ALA:HB2	1:125:A:ALA:HA	3	0.14	0.02	0.15
(2,202)	1:118:A:LEU:HD11	1:114:A:ASP:HB2	3	0.14	0.02	0.14
(2,202)	1:118:A:LEU:HD12	1:114:A:ASP:HB2	3	0.14	0.02	0.14
(2,500)	1:82:A:PHE:HE1	1:119:A:LEU:HA	3	0.14	0.0	0.14
(2,458)	1:74:A:SER:HA	1:74:A:SER:HB3	3	0.11	0.0	0.11
(2,1349)	1:118:A:LEU:HG	1:118:A:LEU:HD23	3	0.11	0.0	0.11
(2,1349)	1:118:A:LEU:HG	1:118:A:LEU:HD22	3	0.11	0.0	0.11
(1,14)	1:69:A:GLU:HB3	1:65:A:THR:HB	2	1.42	0.05	1.42
(2,221)	1:71:A:LYS:HG3	1:67:A:LYS:HA	2	1.4	0.03	1.4
(2,1248)	1:67:A:LYS:HD3	1:69:A:GLU:HB3	2	1.33	0.22	1.33
(2,1509)	1:110:A:VAL:HA	1:114:A:ASP:HB2	2	0.84	0.03	0.84
(2,265)	1:110:A:VAL:HG23	1:114:A:ASP:HB2	2	0.64	0.03	0.64
(2,265)	1:110:A:VAL:HG22	1:114:A:ASP:HB2	2	0.64	0.03	0.64
(2,223)	1:131:A:LEU:HD13	1:131:A:LEU:HA	2	0.63	0.02	0.63
(2,223)	1:131:A:LEU:HD12	1:131:A:LEU:HA	2	0.63	0.02	0.63
(2,133)	1:67:A:LYS:HD3	1:69:A:GLU:HB3	2	0.59	0.23	0.59
(2,137)	1:69:A:GLU:HB2	1:69:A:GLU:HA	2	0.59	0.0	0.59
(2,257)	1:89:A:LEU:HD22	1:114:A:ASP:HB3	2	0.58	0.03	0.58
(2,257)	1:89:A:LEU:HD21	1:114:A:ASP:HB3	2	0.58	0.03	0.58
(2,1204)	1:59:A:MET:HG3	1:58:A:GLU:HA	2	0.54	0.34	0.54
(2,589)	1:71:A:LYS:HG2	1:71:A:LYS:HA	2	0.43	0.02	0.43

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1254)	1:136:A:LYS:HD2	1:135:A:VAL:HA	2	0.42	0.15	0.42
(2,1254)	1:136:A:LYS:HD3	1:135:A:VAL:HA	2	0.42	0.15	0.42
(2,286)	1:88:A:GLU:HG3	1:84:A:THR:HG23	2	0.39	0.24	0.39
(2,286)	1:88:A:GLU:HG3	1:84:A:THR:HG21	2	0.39	0.24	0.39
(2,51)	1:103:A:MET:HB2	1:61:A:ARG:HG2	2	0.38	0.28	0.38
(2,103)	1:103:A:MET:HG3	1:61:A:ARG:HD3	2	0.35	0.17	0.35
(2,103)	1:103:A:MET:HG3	1:61:A:ARG:HD2	2	0.35	0.17	0.35
(2,807)	1:67:A:LYS:H	1:71:A:LYS:HG3	2	0.32	0.12	0.32
(2,845)	1:85:A:ARG:H	1:84:A:THR:HG22	2	0.31	0.02	0.31
(2,287)	1:84:A:THR:HG22	1:85:A:ARG:HD3	2	0.3	0.04	0.3
(2,463)	1:101:A:VAL:HA	1:65:A:THR:HG21	2	0.3	0.03	0.3
(2,1768)	1:89:A:LEU:HB2	1:114:A:ASP:HB3	2	0.3	0.01	0.3
(2,489)	1:95:A:PHE:HE2	1:78:A:LYS:HE3	2	0.29	0.12	0.29
(2,1749)	1:95:A:PHE:HE2	1:78:A:LYS:HE3	2	0.27	0.12	0.27
(2,1643)	1:58:A:GLU:HA	1:59:A:MET:HG2	2	0.26	0.1	0.26
(2,1643)	1:58:A:GLU:HA	1:58:A:GLU:HG3	2	0.26	0.1	0.26
(2,538)	1:120:A:HIS:HB2	1:117:A:GLN:HA	2	0.24	0.03	0.24
(2,702)	1:123:A:LEU:HB2	1:129:A:VAL:HG21	2	0.24	0.12	0.24
(2,1339)	1:106:A:LEU:HD22	1:135:A:VAL:HG12	2	0.24	0.08	0.24
(2,1339)	1:106:A:LEU:HD23	1:135:A:VAL:HG12	2	0.24	0.08	0.24
(2,1849)	1:106:A:LEU:H	1:104:A:ILE:HG21	2	0.24	0.0	0.24
(2,1849)	1:106:A:LEU:H	1:104:A:ILE:HG22	2	0.24	0.0	0.24
(2,488)	1:74:A:SER:HB3	1:95:A:PHE:HE2	2	0.22	0.06	0.22
(2,1637)	1:116:A:ASP:HA	1:116:A:ASP:HB3	2	0.22	0.01	0.22
(2,1200)	1:136:A:LYS:HB3	1:59:A:MET:HA	2	0.2	0.08	0.2
(2,749)	1:61:A:ARG:H	1:61:A:ARG:HD2	2	0.19	0.02	0.19
(2,749)	1:61:A:ARG:H	1:61:A:ARG:HD3	2	0.19	0.02	0.19
(2,1669)	1:73:A:PHE:HE2	1:77:A:ALA:HA	2	0.19	0.05	0.19
(2,1436)	1:104:A:ILE:HG21	1:62:A:LEU:HG	2	0.18	0.02	0.18
(2,1560)	1:78:A:LYS:HG3	1:95:A:PHE:HE2	2	0.18	0.02	0.18
(2,1560)	1:95:A:PHE:HE2	1:97:A:THR:HG21	2	0.18	0.02	0.18
(2,1247)	1:68:A:GLN:HB3	1:67:A:LYS:HA	2	0.16	0.04	0.16
(2,54)	1:129:A:VAL:HB	1:122:A:ILE:HG22	2	0.16	0.04	0.16
(2,54)	1:129:A:VAL:HB	1:122:A:ILE:HG21	2	0.16	0.04	0.16
(2,1362)	1:101:A:VAL:HB	1:96:A:LEU:HD23	2	0.16	0.0	0.16
(2,1362)	1:96:A:LEU:HB3	1:96:A:LEU:HD22	2	0.16	0.0	0.16
(2,1623)	1:115:A:MET:HA	1:119:A:LEU:HG	2	0.16	0.02	0.16
(2,1755)	1:104:A:ILE:HB	1:102:A:THR:HB	2	0.16	0.04	0.16
(2,1827)	1:95:A:PHE:H	1:93:A:ILE:HB	2	0.16	0.01	0.16
(2,405)	1:64:A:VAL:HG13	1:122:A:ILE:HA	2	0.16	0.02	0.16
(2,405)	1:64:A:VAL:HG11	1:122:A:ILE:HA	2	0.16	0.02	0.16
(2,642)	1:113:A:HIS:HB2	1:113:A:HIS:HD2	2	0.16	0.04	0.16

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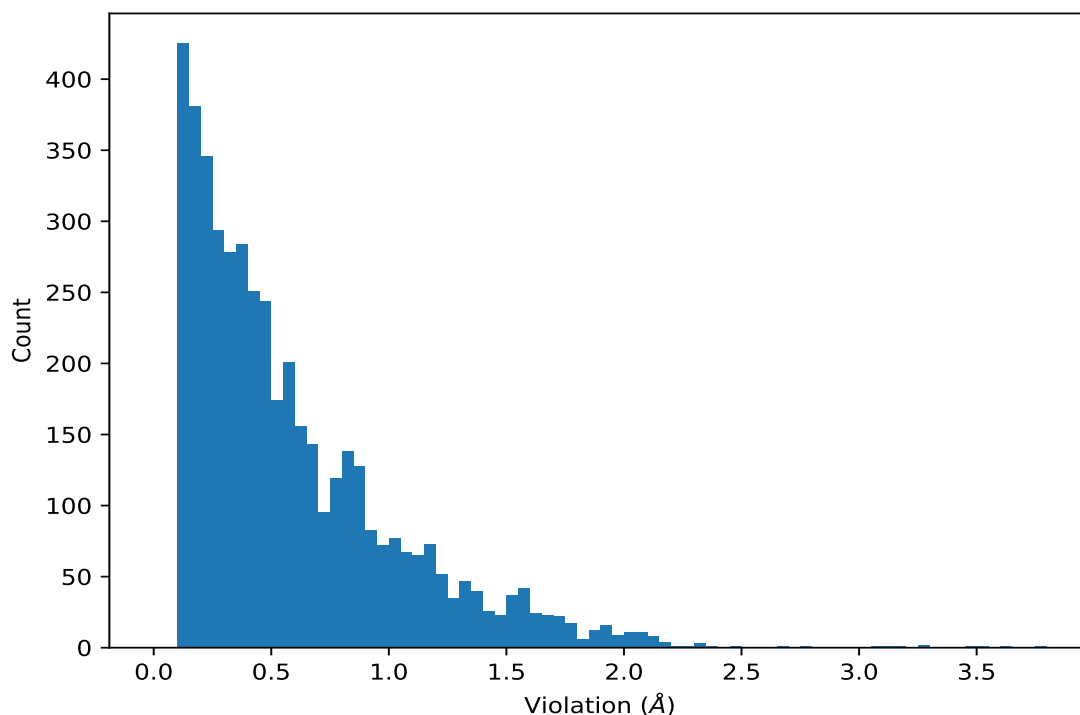
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,893)	1:115:A:MET:H	1:114:A:ASP:HB3	2	0.16	0.02	0.16
(2,932)	1:60:A:THR:H	1:59:A:MET:HB2	2	0.16	0.02	0.16
(2,1615)	1:64:A:VAL:HB	1:73:A:PHE:HZ	2	0.16	0.04	0.16
(2,290)	1:60:A:THR:HG23	1:62:A:LEU:HA	2	0.15	0.01	0.15
(2,290)	1:60:A:THR:HG22	1:62:A:LEU:HA	2	0.15	0.01	0.15
(2,1914)	1:79:A:SER:H	1:78:A:LYS:HB3	2	0.15	0.03	0.15
(2,293)	1:110:A:VAL:HG23	1:106:A:LEU:HG	2	0.12	0.02	0.12
(2,366)	1:93:A:ILE:HD11	1:82:A:PHE:HB2	2	0.12	0.01	0.12
(2,366)	1:93:A:ILE:HD13	1:82:A:PHE:HB2	2	0.12	0.01	0.12
(2,1290)	1:118:A:LEU:HG	1:114:A:ASP:HB2	2	0.12	0.02	0.12
(2,259)	1:97:A:THR:HG23	1:96:A:LEU:HA	2	0.12	0.02	0.12
(2,259)	1:97:A:THR:HG21	1:96:A:LEU:HA	2	0.12	0.02	0.12
(2,484)	1:86:A:ILE:HG13	1:86:A:ILE:HA	2	0.12	0.01	0.12
(2,625)	1:64:A:VAL:HG23	1:63:A:MET:HA	2	0.12	0.01	0.12
(2,625)	1:64:A:VAL:HG22	1:63:A:MET:HA	2	0.12	0.01	0.12
(2,1353)	1:118:A:LEU:HD23	1:118:A:LEU:HD13	2	0.12	0.0	0.12
(2,1353)	1:118:A:LEU:HD22	1:118:A:LEU:HD11	2	0.12	0.0	0.12
(2,373)	1:104:A:ILE:HD12	1:122:A:ILE:HD13	2	0.12	0.02	0.12
(2,373)	1:104:A:ILE:HD13	1:122:A:ILE:HD11	2	0.12	0.02	0.12
(2,817)	1:110:A:VAL:H	1:107:A:PRO:HG2	2	0.12	0.0	0.12
(2,154)	1:107:A:PRO:HG3	1:106:A:LEU:HA	2	0.11	0.0	0.11
(2,1659)	1:104:A:ILE:HG22	1:105:A:GLU:HA	2	0.11	0.0	0.11
(2,869)	1:87:A:GLU:H	1:86:A:ILE:HD11	2	0.1	0.0	0.1
(2,869)	1:87:A:GLU:H	1:86:A:ILE:HD13	2	0.1	0.0	0.1

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

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

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1343)	1:106:A:LEU:HD21	1:113:A:HIS:HB2	10	3.8
(2,1415)	1:128:A:VAL:HG22	1:62:A:LEU:HG	1	3.62
(2,1415)	1:128:A:VAL:HG23	1:62:A:LEU:HG	9	3.54
(2,1415)	1:128:A:VAL:HG23	1:62:A:LEU:HG	8	3.47
(2,1415)	1:128:A:VAL:HG23	1:62:A:LEU:HG	2	3.26
(2,1415)	1:128:A:VAL:HG21	1:62:A:LEU:HG	7	3.25
(2,1415)	1:128:A:VAL:HG12	1:62:A:LEU:HG	4	3.19
(2,1415)	1:128:A:VAL:HG22	1:62:A:LEU:HG	3	3.11
(2,1415)	1:128:A:VAL:HG12	1:62:A:LEU:HG	6	3.06
(2,1415)	1:128:A:VAL:HG21	1:62:A:LEU:HG	5	2.76
(2,1415)	1:128:A:VAL:HG23	1:62:A:LEU:HG	10	2.69
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG23	8	2.45
(1,4)	1:58:A:GLU:HG2	1:91:A:GLY:HA3	10	2.37
(2,1268)	1:78:A:LYS:HD2	1:74:A:SER:HB3	2	2.33
(2,1268)	1:78:A:LYS:HD3	1:74:A:SER:HB3	1	2.31
(2,1504)	1:70:A:SER:HB3	1:64:A:VAL:HG22	4	2.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1426)	1:124:A:ALA:HB3	1:117:A:GLN:HB2	10	2.28
(2,1357)	1:96:A:LEU:HD23	1:61:A:ARG:HD2	7	2.23
(2,1268)	1:78:A:LYS:HD2	1:74:A:SER:HB3	3	2.18
(2,1268)	1:78:A:LYS:HD3	1:74:A:SER:HB3	7	2.18
(2,1426)	1:124:A:ALA:HB2	1:117:A:GLN:HB2	2	2.17
(2,1296)	1:85:A:ARG:H	1:86:A:ILE:HG13	9	2.15
(2,1399)	1:101:A:VAL:HG13	1:104:A:ILE:HB	8	2.14
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD13	7	2.14
(2,1399)	1:101:A:VAL:HG13	1:104:A:ILE:HB	4	2.12
(2,1296)	1:85:A:ARG:H	1:86:A:ILE:HG13	8	2.12
(2,1296)	1:86:A:ILE:HG13	1:82:A:PHE:HD1	3	2.11
(2,1296)	1:86:A:ILE:HG13	1:82:A:PHE:HD2	10	2.11
(2,1296)	1:86:A:ILE:HG13	1:82:A:PHE:HD2	5	2.1
(2,1296)	1:86:A:ILE:HG13	1:82:A:PHE:HD2	7	2.1
(2,1399)	1:101:A:VAL:HG13	1:104:A:ILE:HB	5	2.09
(2,1296)	1:86:A:ILE:HG13	1:82:A:PHE:HD1	2	2.09
(2,1296)	1:86:A:ILE:HG13	1:82:A:PHE:HD1	1	2.07
(2,1296)	1:85:A:ARG:H	1:86:A:ILE:HG13	4	2.07
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD21	1	2.06
(2,1399)	1:101:A:VAL:HG13	1:104:A:ILE:HB	1	2.06
(2,1399)	1:101:A:VAL:HG12	1:104:A:ILE:HB	6	2.06
(2,1842)	1:85:A:ARG:H	1:87:A:GLU:HB3	7	2.05
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD23	6	2.05
(2,1530)	1:129:A:VAL:HA	1:119:A:LEU:HB2	10	2.05
(2,1399)	1:101:A:VAL:HG13	1:104:A:ILE:HB	2	2.05
(2,1399)	1:101:A:VAL:HG11	1:104:A:ILE:HB	9	2.04
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD13	3	2.04
(2,1842)	1:85:A:ARG:H	1:87:A:GLU:HB3	8	2.03
(2,1736)	1:71:A:LYS:HE3	1:73:A:PHE:HD2	3	2.03
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD21	4	2.03
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD22	5	2.02
(2,1842)	1:85:A:ARG:H	1:87:A:GLU:HB3	1	2.01
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD21	7	2.01
(2,1842)	1:85:A:ARG:H	1:87:A:GLU:HB3	6	2.0
(2,1268)	1:78:A:LYS:HD2	1:74:A:SER:HB3	10	2.0
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD12	9	2.0
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD23	8	1.99
(2,1399)	1:101:A:VAL:HG12	1:104:A:ILE:HB	3	1.99
(2,1504)	1:70:A:SER:HB2	1:64:A:VAL:HG22	7	1.98
(2,1296)	1:86:A:ILE:HG13	1:82:A:PHE:HD1	6	1.98
(2,1504)	1:70:A:SER:HB3	1:64:A:VAL:HG22	10	1.97
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD12	2	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:58:A:GLU:HG2	1:91:A:GLY:HA3	2	1.97
(2,1842)	1:85:A:ARG:H	1:87:A:GLU:HB3	3	1.95
(2,1399)	1:101:A:VAL:HG12	1:104:A:ILE:HB	10	1.95
(2,1530)	1:129:A:VAL:HA	1:119:A:LEU:HB2	2	1.94
(2,1530)	1:129:A:VAL:HA	1:61:A:ARG:HG2	3	1.94
(2,1371)	1:101:A:VAL:HG22	1:67:A:LYS:HE3	1	1.94
(2,1482)	1:97:A:THR:HB	1:96:A:LEU:HD13	4	1.93
(2,1842)	1:85:A:ARG:H	1:87:A:GLU:HB3	2	1.92
(2,1530)	1:129:A:VAL:HA	1:61:A:ARG:HG2	9	1.92
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD12	10	1.92
(2,1736)	1:71:A:LYS:HE2	1:73:A:PHE:HD2	2	1.91
(2,1736)	1:71:A:LYS:HE2	1:73:A:PHE:HD1	6	1.91
(2,1325)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	10	1.91
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD13	8	1.91
(2,311)	1:135:A:VAL:HG23	1:133:A:SER:HB2	7	1.91
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD21	3	1.9
(2,1399)	1:101:A:VAL:HG12	1:104:A:ILE:HB	7	1.9
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD13	4	1.9
(1,4)	1:58:A:GLU:HG2	1:91:A:GLY:HA3	3	1.9
(2,1530)	1:129:A:VAL:HA	1:119:A:LEU:HB2	5	1.89
(2,1482)	1:118:A:LEU:HD21	1:84:A:THR:HB	10	1.89
(2,1530)	1:129:A:VAL:HA	1:119:A:LEU:HB2	7	1.88
(2,1530)	1:129:A:VAL:HA	1:119:A:LEU:HB2	1	1.87
(2,1530)	1:129:A:VAL:HA	1:119:A:LEU:HB2	6	1.87
(2,1530)	1:129:A:VAL:HA	1:119:A:LEU:HB2	8	1.87
(2,1268)	1:78:A:LYS:HD3	1:74:A:SER:HB3	6	1.87
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD11	7	1.87
(2,1842)	1:85:A:ARG:H	1:87:A:GLU:HB3	5	1.86
(2,1268)	1:78:A:LYS:HD2	1:74:A:SER:HB3	4	1.86
(2,1908)	1:84:A:THR:H	1:87:A:GLU:HG2	7	1.85
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD13	1	1.85
(2,402)	1:84:A:THR:HB	1:88:A:GLU:HG3	7	1.83
(2,1257)	1:75:A:LYS:HD3	1:78:A:LYS:HE2	5	1.81
(2,1371)	1:101:A:VAL:HG21	1:67:A:LYS:HE2	4	1.8
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD11	5	1.8
(2,660)	1:91:A:GLY:HA2	1:86:A:ILE:HD11	6	1.8
(2,311)	1:135:A:VAL:HG22	1:133:A:SER:HB2	1	1.8
(2,1736)	1:71:A:LYS:HE2	1:73:A:PHE:HD2	1	1.79
(2,1371)	1:101:A:VAL:HG22	1:67:A:LYS:HE2	3	1.79
(2,311)	1:135:A:VAL:HG12	1:133:A:SER:HB2	5	1.79
(2,1842)	1:85:A:ARG:H	1:87:A:GLU:HB3	4	1.78
(2,1781)	1:66:A:GLU:HG3	1:73:A:PHE:HB2	10	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1736)	1:71:A:LYS:HE3	1:73:A:PHE:HD2	5	1.78
(2,709)	1:119:A:LEU:HB3	1:116:A:ASP:HA	7	1.78
(2,1842)	1:85:A:ARG:H	1:87:A:GLU:HB3	10	1.77
(2,1736)	1:71:A:LYS:HE3	1:73:A:PHE:HD1	4	1.77
(2,709)	1:119:A:LEU:HB3	1:116:A:ASP:HA	6	1.77
(2,88)	1:63:A:MET:HB2	1:132:A:ASP:HB2	8	1.77
(2,1530)	1:129:A:VAL:HA	1:119:A:LEU:HB2	4	1.76
(2,709)	1:119:A:LEU:HB3	1:116:A:ASP:HA	9	1.76
(1,15)	1:136:A:LYS:HD3	1:107:A:PRO:HB2	2	1.76
(2,1395)	1:101:A:VAL:HG13	1:73:A:PHE:HE2	5	1.75
(2,1238)	1:134:A:GLU:HB3	1:131:A:LEU:HA	3	1.75
(2,846)	1:85:A:ARG:H	1:86:A:ILE:HG13	9	1.75
(2,1741)	1:136:A:LYS:HE2	1:136:A:LYS:HA	5	1.74
(2,1325)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	2	1.74
(2,846)	1:85:A:ARG:H	1:86:A:ILE:HG13	7	1.74
(2,709)	1:119:A:LEU:HB3	1:116:A:ASP:HA	8	1.74
(2,131)	1:136:A:LYS:HD3	1:58:A:GLU:HG3	3	1.74
(2,1504)	1:70:A:SER:HB3	1:64:A:VAL:HG21	1	1.73
(2,846)	1:85:A:ARG:H	1:86:A:ILE:HG13	5	1.73
(2,709)	1:119:A:LEU:HB3	1:116:A:ASP:HA	1	1.73
(2,709)	1:119:A:LEU:HB3	1:116:A:ASP:HA	5	1.73
(2,846)	1:85:A:ARG:H	1:86:A:ILE:HG13	3	1.72
(2,709)	1:119:A:LEU:HB3	1:116:A:ASP:HA	4	1.72
(2,1736)	1:71:A:LYS:HE3	1:73:A:PHE:HD1	7	1.71
(2,1661)	1:132:A:ASP:HA	1:103:A:MET:HB3	3	1.71
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD21	2	1.71
(2,846)	1:85:A:ARG:H	1:86:A:ILE:HG13	1	1.71
(2,846)	1:85:A:ARG:H	1:86:A:ILE:HG13	6	1.71
(2,846)	1:85:A:ARG:H	1:86:A:ILE:HG13	8	1.71
(2,846)	1:85:A:ARG:H	1:86:A:ILE:HG13	10	1.71
(2,709)	1:119:A:LEU:HB3	1:116:A:ASP:HA	3	1.71
(1,15)	1:136:A:LYS:HD3	1:107:A:PRO:HB2	1	1.71
(2,1482)	1:118:A:LEU:HD21	1:84:A:THR:HB	6	1.7
(2,846)	1:85:A:ARG:H	1:86:A:ILE:HG13	2	1.7
(2,1376)	1:129:A:VAL:HG11	1:127:A:GLY:HA2	10	1.69
(2,1268)	1:78:A:LYS:HD3	1:74:A:SER:HB3	5	1.69
(2,1256)	1:75:A:LYS:HD3	1:78:A:LYS:HE3	7	1.69
(2,1154)	1:72:A:ASN:HB2	1:73:A:PHE:HD2	6	1.69
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD21	9	1.68
(2,1504)	1:70:A:SER:HB3	1:64:A:VAL:HG22	8	1.68
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB3	6	1.68
(2,186)	1:96:A:LEU:HG	1:103:A:MET:HG2	5	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1741)	1:136:A:LYS:HE2	1:136:A:LYS:HA	10	1.67
(2,1504)	1:70:A:SER:HB3	1:64:A:VAL:HG21	3	1.66
(2,1395)	1:101:A:VAL:HG13	1:73:A:PHE:HE2	8	1.66
(2,1376)	1:129:A:VAL:HG12	1:127:A:GLY:HA2	7	1.66
(2,1226)	1:66:A:GLU:HB2	1:73:A:PHE:HB3	10	1.66
(2,846)	1:85:A:ARG:H	1:86:A:ILE:HG13	4	1.66
(2,311)	1:135:A:VAL:HG23	1:133:A:SER:HB2	9	1.66
(2,143)	1:93:A:ILE:HG13	1:82:A:PHE:HB2	6	1.66
(2,143)	1:93:A:ILE:HG13	1:82:A:PHE:HB2	7	1.66
(1,46)	1:108:A:LYS:HE3	1:59:A:MET:HA	8	1.66
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG23	1	1.65
(2,1371)	1:101:A:VAL:HG22	1:67:A:LYS:HE2	9	1.65
(2,1327)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	10	1.65
(2,1154)	1:72:A:ASN:HB2	1:73:A:PHE:HD1	2	1.65
(2,86)	1:63:A:MET:HB2	1:132:A:ASP:HB3	1	1.65
(2,1425)	1:138:A:ALA:HB2	1:108:A:LYS:HG3	1	1.64
(2,403)	1:84:A:THR:HA	1:87:A:GLU:HB3	8	1.64
(2,186)	1:96:A:LEU:HG	1:103:A:MET:HG2	6	1.64
(2,88)	1:63:A:MET:HB2	1:132:A:ASP:HB2	7	1.64
(2,1736)	1:71:A:LYS:HE3	1:73:A:PHE:HD2	8	1.63
(2,1504)	1:70:A:SER:HB3	1:64:A:VAL:HG23	6	1.63
(2,1395)	1:101:A:VAL:HG13	1:73:A:PHE:HE1	4	1.63
(2,403)	1:84:A:THR:HA	1:87:A:GLU:HB3	7	1.63
(2,1421)	1:125:A:ALA:HB2	1:122:A:ILE:HD12	8	1.62
(2,1412)	1:128:A:VAL:HG23	1:130:A:GLY:HA2	10	1.62
(2,403)	1:84:A:THR:HA	1:87:A:GLU:HB3	5	1.62
(1,15)	1:136:A:LYS:HD3	1:107:A:PRO:HB2	6	1.62
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG22	5	1.61
(2,1504)	1:70:A:SER:HB3	1:64:A:VAL:HG23	5	1.61
(2,1395)	1:101:A:VAL:HG13	1:73:A:PHE:HE2	2	1.61
(2,1395)	1:101:A:VAL:HG12	1:73:A:PHE:HE1	7	1.61
(2,1386)	1:84:A:THR:HG22	1:88:A:GLU:HB3	3	1.61
(2,403)	1:84:A:THR:HA	1:87:A:GLU:HB3	10	1.61
(2,1500)	1:66:A:GLU:HB2	1:70:A:SER:HB2	9	1.6
(2,1395)	1:101:A:VAL:HG13	1:73:A:PHE:HE2	1	1.6
(2,311)	1:135:A:VAL:HG23	1:133:A:SER:HB2	6	1.6
(2,143)	1:93:A:ILE:HG13	1:82:A:PHE:HB2	1	1.6
(2,143)	1:93:A:ILE:HG13	1:82:A:PHE:HB2	4	1.6
(2,143)	1:93:A:ILE:HG13	1:82:A:PHE:HB2	10	1.6
(2,1842)	1:85:A:ARG:H	1:87:A:GLU:HB3	9	1.59
(2,1591)	1:113:A:HIS:HA	1:118:A:LEU:HD23	10	1.59
(2,1435)	1:104:A:ILE:HG23	1:91:A:GLY:HA2	1	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1395)	1:101:A:VAL:HG12	1:73:A:PHE:HE1	6	1.59
(2,1369)	1:110:A:VAL:HG23	1:86:A:ILE:HA	8	1.59
(2,1369)	1:110:A:VAL:HG23	1:86:A:ILE:HA	9	1.59
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB3	3	1.59
(2,709)	1:119:A:LEU:HB3	1:116:A:ASP:HA	2	1.59
(2,403)	1:84:A:THR:HA	1:87:A:GLU:HB3	3	1.59
(2,403)	1:84:A:THR:HA	1:87:A:GLU:HB3	6	1.59
(2,1624)	1:118:A:LEU:HA	1:114:A:ASP:HB2	5	1.58
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG21	6	1.58
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG21	9	1.58
(2,1343)	1:137:A:LEU:HD11	1:136:A:LYS:HE2	4	1.58
(2,709)	1:119:A:LEU:HB3	1:116:A:ASP:HA	10	1.58
(2,403)	1:84:A:THR:HA	1:87:A:GLU:HB3	2	1.58
(2,143)	1:93:A:ILE:HG13	1:82:A:PHE:HB2	3	1.58
(2,143)	1:93:A:ILE:HG13	1:82:A:PHE:HB2	5	1.58
(2,1624)	1:118:A:LEU:HA	1:114:A:ASP:HB2	1	1.57
(2,1624)	1:118:A:LEU:HA	1:114:A:ASP:HB2	3	1.57
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG22	7	1.57
(2,1395)	1:101:A:VAL:HG11	1:73:A:PHE:HE2	9	1.57
(2,1371)	1:101:A:VAL:HG23	1:67:A:LYS:HE2	7	1.57
(2,1369)	1:110:A:VAL:HG22	1:86:A:ILE:HA	4	1.57
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB3	2	1.57
(2,86)	1:63:A:MET:HB2	1:132:A:ASP:HB3	7	1.57
(2,1624)	1:118:A:LEU:HA	1:114:A:ASP:HB2	6	1.56
(2,1435)	1:104:A:ILE:HG23	1:91:A:GLY:HA2	8	1.56
(2,1395)	1:101:A:VAL:HG12	1:73:A:PHE:HE1	10	1.56
(2,1376)	1:129:A:VAL:HG12	1:127:A:GLY:HA2	4	1.56
(2,1154)	1:72:A:ASN:HB2	1:73:A:PHE:HD1	3	1.56
(2,403)	1:84:A:THR:HA	1:87:A:GLU:HB3	1	1.56
(2,1624)	1:118:A:LEU:HA	1:114:A:ASP:HB2	8	1.55
(2,1554)	1:86:A:ILE:HA	1:87:A:GLU:HB3	6	1.55
(2,1395)	1:101:A:VAL:HG12	1:73:A:PHE:HE2	3	1.55
(2,1376)	1:129:A:VAL:HG11	1:127:A:GLY:HA2	3	1.55
(2,1371)	1:101:A:VAL:HG23	1:67:A:LYS:HE2	6	1.55
(2,1248)	1:67:A:LYS:HD3	1:69:A:GLU:HB3	4	1.55
(2,609)	1:96:A:LEU:HA	1:96:A:LEU:HD11	7	1.55
(2,597)	1:61:A:ARG:HA	1:103:A:MET:HG3	8	1.55
(2,143)	1:93:A:ILE:HG13	1:82:A:PHE:HB2	2	1.55
(2,139)	1:71:A:LYS:HD3	1:74:A:SER:HA	2	1.55
(2,1302)	1:62:A:LEU:HG	1:122:A:ILE:HG13	7	1.54
(2,88)	1:63:A:MET:HB2	1:132:A:ASP:HB2	9	1.54
(1,46)	1:108:A:LYS:HE3	1:59:A:MET:HA	10	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1624)	1:76:A:MET:HG3	1:118:A:LEU:HA	7	1.53
(2,1554)	1:86:A:ILE:HA	1:87:A:GLU:HB3	1	1.53
(2,1554)	1:86:A:ILE:HA	1:87:A:GLU:HB3	5	1.53
(2,1431)	1:124:A:ALA:HB1	1:76:A:MET:HG3	6	1.53
(2,1376)	1:129:A:VAL:HG13	1:127:A:GLY:HA2	8	1.53
(2,1369)	1:110:A:VAL:HG23	1:86:A:ILE:HA	1	1.53
(2,1369)	1:110:A:VAL:HG21	1:86:A:ILE:HA	10	1.53
(2,143)	1:93:A:ILE:HG13	1:82:A:PHE:HB2	9	1.53
(2,1624)	1:118:A:LEU:HA	1:114:A:ASP:HB2	4	1.52
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG22	4	1.52
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG23	10	1.52
(2,1435)	1:104:A:ILE:HG22	1:91:A:GLY:HA2	9	1.52
(2,1376)	1:129:A:VAL:HG12	1:127:A:GLY:HA2	6	1.52
(2,1369)	1:110:A:VAL:HG22	1:86:A:ILE:HA	7	1.52
(2,139)	1:71:A:LYS:HD3	1:74:A:SER:HA	3	1.52
(1,7)	1:107:A:PRO:HB2	1:59:A:MET:HG3	4	1.52
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG23	3	1.51
(2,1401)	1:84:A:THR:HG22	1:89:A:LEU:HD23	2	1.51
(2,1369)	1:110:A:VAL:HG21	1:86:A:ILE:HA	6	1.51
(2,1343)	1:137:A:LEU:HD11	1:136:A:LYS:HE3	9	1.51
(2,311)	1:135:A:VAL:HG21	1:133:A:SER:HB2	4	1.51
(2,143)	1:93:A:ILE:HG13	1:82:A:PHE:HB2	8	1.51
(2,2)	1:95:A:PHE:HB2	1:78:A:LYS:HD3	9	1.51
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG21	2	1.5
(2,1482)	1:118:A:LEU:HD23	1:84:A:THR:HB	1	1.5
(2,1435)	1:104:A:ILE:HG23	1:91:A:GLY:HA2	6	1.5
(2,1386)	1:84:A:THR:HG22	1:88:A:GLU:HB3	2	1.5
(2,1376)	1:129:A:VAL:HG12	1:127:A:GLY:HA2	2	1.5
(2,1376)	1:129:A:VAL:HG11	1:127:A:GLY:HA2	5	1.5
(2,1371)	1:101:A:VAL:HG21	1:67:A:LYS:HE2	8	1.5
(2,1174)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	2	1.5
(2,403)	1:84:A:THR:HA	1:87:A:GLU:HB3	9	1.5
(2,139)	1:71:A:LYS:HD3	1:74:A:SER:HA	6	1.5
(1,15)	1:136:A:LYS:HD3	1:107:A:PRO:HB2	3	1.5
(2,1624)	1:118:A:LEU:HA	1:114:A:ASP:HB2	9	1.49
(2,1504)	1:70:A:SER:HB3	1:64:A:VAL:HG23	2	1.49
(2,1435)	1:104:A:ILE:HG21	1:91:A:GLY:HA2	5	1.49
(2,1435)	1:104:A:ILE:HG22	1:91:A:GLY:HA2	7	1.49
(2,1933)	1:92:A:SER:H	1:104:A:ILE:HG12	9	1.48
(2,1421)	1:125:A:ALA:HB1	1:122:A:ILE:HD12	7	1.48
(2,1376)	1:129:A:VAL:HG11	1:127:A:GLY:HA2	9	1.48
(2,1369)	1:110:A:VAL:HG23	1:86:A:ILE:HA	3	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1327)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	2	1.48
(1,7)	1:107:A:PRO:HB2	1:59:A:MET:HG3	10	1.48
(2,311)	1:135:A:VAL:HG21	1:133:A:SER:HB2	8	1.47
(1,14)	1:69:A:GLU:HB3	1:65:A:THR:HB	4	1.47
(1,7)	1:107:A:PRO:HB2	1:59:A:MET:HG3	2	1.47
(2,1482)	1:118:A:LEU:HD23	1:84:A:THR:HB	5	1.46
(2,1435)	1:104:A:ILE:HG22	1:91:A:GLY:HA2	4	1.46
(2,1421)	1:125:A:ALA:HB1	1:122:A:ILE:HD11	4	1.46
(2,1376)	1:129:A:VAL:HG13	1:127:A:GLY:HA2	1	1.46
(2,1736)	1:71:A:LYS:HE3	1:73:A:PHE:HD2	9	1.45
(2,1504)	1:70:A:SER:HB2	1:64:A:VAL:HG23	9	1.45
(2,1470)	1:86:A:ILE:HD11	1:122:A:ILE:HG13	8	1.45
(2,1371)	1:101:A:VAL:HG23	1:67:A:LYS:HE2	5	1.45
(2,1176)	1:66:A:GLU:HG3	1:128:A:VAL:HG22	5	1.45
(1,15)	1:136:A:LYS:HD3	1:107:A:PRO:HB2	8	1.45
(2,1554)	1:86:A:ILE:HA	1:88:A:GLU:HB3	8	1.44
(2,1369)	1:110:A:VAL:HG23	1:86:A:ILE:HA	2	1.44
(2,1343)	1:137:A:LEU:HD13	1:136:A:LYS:HE3	6	1.44
(2,1174)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	6	1.44
(2,311)	1:135:A:VAL:HG21	1:133:A:SER:HB2	10	1.44
(2,221)	1:71:A:LYS:HG3	1:67:A:LYS:HA	5	1.44
(2,1506)	1:66:A:GLU:HB2	1:70:A:SER:HB2	9	1.43
(2,1470)	1:86:A:ILE:HD12	1:122:A:ILE:HG13	6	1.43
(2,1421)	1:125:A:ALA:HB2	1:122:A:ILE:HD13	10	1.43
(2,88)	1:63:A:MET:HB2	1:132:A:ASP:HB2	5	1.43
(2,1933)	1:92:A:SER:H	1:104:A:ILE:HG12	1	1.42
(2,1554)	1:86:A:ILE:HA	1:88:A:GLU:HB3	2	1.42
(2,1177)	1:58:A:GLU:HG2	1:107:A:PRO:HD3	10	1.42
(2,1174)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	3	1.42
(2,1426)	1:124:A:ALA:HB3	1:117:A:GLN:HB3	9	1.41
(2,597)	1:61:A:ARG:HA	1:103:A:MET:HG3	6	1.41
(2,1933)	1:92:A:SER:H	1:104:A:ILE:HG12	6	1.4
(2,1585)	1:104:A:ILE:HA	1:122:A:ILE:HG23	8	1.4
(2,1579)	1:104:A:ILE:HA	1:105:A:GLU:HG2	2	1.4
(2,1579)	1:104:A:ILE:HA	1:105:A:GLU:HG2	3	1.4
(2,1554)	1:86:A:ILE:HA	1:88:A:GLU:HB3	4	1.4
(2,1387)	1:84:A:THR:HG23	1:86:A:ILE:HA	4	1.4
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD12	8	1.4
(2,139)	1:71:A:LYS:HD3	1:74:A:SER:HA	5	1.4
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG21	10	1.4
(1,7)	1:107:A:PRO:HB2	1:59:A:MET:HG3	3	1.4
(2,1933)	1:92:A:SER:H	1:104:A:ILE:HG12	2	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1933)	1:92:A:SER:H	1:104:A:ILE:HG12	4	1.39
(2,1470)	1:86:A:ILE:HD11	1:122:A:ILE:HG13	1	1.39
(2,1435)	1:104:A:ILE:HG23	1:91:A:GLY:HA2	2	1.39
(2,1435)	1:104:A:ILE:HG21	1:91:A:GLY:HA2	3	1.39
(2,1426)	1:124:A:ALA:HB2	1:117:A:GLN:HB3	3	1.39
(2,1426)	1:124:A:ALA:HB2	1:117:A:GLN:HB3	6	1.39
(2,403)	1:84:A:THR:HA	1:87:A:GLU:HB3	4	1.39
(2,139)	1:71:A:LYS:HD3	1:74:A:SER:HA	7	1.39
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB3	5	1.39
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB3	7	1.39
(2,1933)	1:92:A:SER:H	1:104:A:ILE:HG12	7	1.38
(2,1805)	1:61:A:ARG:H	1:137:A:LEU:HD22	9	1.38
(2,1579)	1:104:A:ILE:HA	1:105:A:GLU:HG2	1	1.38
(2,1554)	1:86:A:ILE:HA	1:88:A:GLU:HB3	3	1.38
(2,1421)	1:125:A:ALA:HB2	1:122:A:ILE:HD13	9	1.38
(2,86)	1:63:A:MET:HB2	1:132:A:ASP:HB3	8	1.38
(2,1579)	1:104:A:ILE:HA	1:105:A:GLU:HG2	10	1.37
(2,1470)	1:86:A:ILE:HD11	1:122:A:ILE:HG13	4	1.37
(2,1470)	1:86:A:ILE:HD13	1:122:A:ILE:HG13	9	1.37
(2,1425)	1:138:A:ALA:HB2	1:108:A:LYS:HG3	8	1.37
(2,1421)	1:125:A:ALA:HB1	1:122:A:ILE:HD12	3	1.37
(2,1369)	1:110:A:VAL:HG21	1:86:A:ILE:HA	5	1.37
(2,946)	1:58:A:GLU:H	1:58:A:GLU:HB2	8	1.37
(2,528)	1:78:A:LYS:HG2	1:75:A:LYS:HA	7	1.37
(2,221)	1:71:A:LYS:HG3	1:67:A:LYS:HA	8	1.37
(1,15)	1:136:A:LYS:HD3	1:107:A:PRO:HB2	10	1.37
(2,1933)	1:92:A:SER:H	1:104:A:ILE:HG12	5	1.36
(2,1482)	1:118:A:LEU:HD22	1:84:A:THR:HB	7	1.36
(2,1470)	1:86:A:ILE:HD12	1:122:A:ILE:HG13	7	1.36
(2,1426)	1:124:A:ALA:HB2	1:117:A:GLN:HB3	8	1.36
(2,1371)	1:101:A:VAL:HG21	1:67:A:LYS:HE2	2	1.36
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD12	3	1.36
(2,1226)	1:66:A:GLU:HB2	1:73:A:PHE:HB3	8	1.36
(1,14)	1:69:A:GLU:HB3	1:65:A:THR:HB	7	1.36
(2,1579)	1:104:A:ILE:HA	1:105:A:GLU:HG2	4	1.35
(2,1579)	1:104:A:ILE:HA	1:105:A:GLU:HG2	6	1.35
(2,1371)	1:101:A:VAL:HG22	1:67:A:LYS:HE2	10	1.35
(2,1226)	1:71:A:LYS:HB3	1:72:A:ASN:HB2	3	1.35
(2,311)	1:135:A:VAL:HG23	1:133:A:SER:HB2	3	1.35
(2,1738)	1:75:A:LYS:HE3	1:95:A:PHE:HE1	8	1.34
(2,1579)	1:104:A:ILE:HA	1:105:A:GLU:HG2	7	1.34
(2,1579)	1:104:A:ILE:HA	1:105:A:GLU:HG2	9	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1482)	1:118:A:LEU:HD22	1:84:A:THR:HB	2	1.34
(2,1470)	1:86:A:ILE:HD11	1:122:A:ILE:HG13	3	1.34
(2,1421)	1:125:A:ALA:HB3	1:122:A:ILE:HD13	2	1.34
(2,1226)	1:66:A:GLU:HB2	1:73:A:PHE:HB3	1	1.34
(2,685)	1:69:A:GLU:HA	1:67:A:LYS:HE3	1	1.34
(2,186)	1:96:A:LEU:HG	1:103:A:MET:HG2	8	1.34
(1,15)	1:136:A:LYS:HD3	1:107:A:PRO:HB2	4	1.34
(2,1653)	1:66:A:GLU:HA	1:74:A:SER:HA	7	1.33
(2,1554)	1:86:A:ILE:HA	1:88:A:GLU:HB3	10	1.33
(2,1451)	1:125:A:ALA:HB1	1:122:A:ILE:HG21	3	1.33
(2,1435)	1:104:A:ILE:HG21	1:91:A:GLY:HA2	10	1.33
(2,1426)	1:124:A:ALA:HB1	1:117:A:GLN:HB3	5	1.33
(2,1301)	1:118:A:LEU:HG	1:117:A:GLN:HA	2	1.33
(2,1252)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	6	1.33
(2,1224)	1:115:A:MET:HB3	1:109:A:THR:HA	2	1.33
(2,72)	1:59:A:MET:HG3	1:136:A:LYS:HB3	4	1.33
(2,6)	1:72:A:ASN:HB2	1:126:A:GLY:HA2	6	1.33
(2,1933)	1:92:A:SER:H	1:104:A:ILE:HG12	3	1.32
(2,1579)	1:104:A:ILE:HA	1:105:A:GLU:HG2	5	1.32
(2,1506)	1:66:A:GLU:HB2	1:70:A:SER:HB2	7	1.32
(2,1421)	1:125:A:ALA:HB2	1:122:A:ILE:HD11	1	1.32
(2,1343)	1:137:A:LEU:HD13	1:136:A:LYS:HE3	7	1.32
(2,1309)	1:118:A:LEU:HD13	1:121:A:ASP:HB3	5	1.32
(2,1309)	1:118:A:LEU:HD11	1:121:A:ASP:HB3	7	1.32
(2,1302)	1:62:A:LEU:HG	1:122:A:ILE:HG13	9	1.32
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD11	2	1.32
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD13	5	1.32
(2,237)	1:110:A:VAL:HG11	1:107:A:PRO:HD3	10	1.32
(2,139)	1:71:A:LYS:HD3	1:74:A:SER:HA	8	1.32
(2,88)	1:63:A:MET:HB2	1:132:A:ASP:HB2	2	1.32
(1,15)	1:136:A:LYS:HD3	1:107:A:PRO:HB2	5	1.32
(2,1861)	1:77:A:ALA:H	1:78:A:LYS:HE3	6	1.31
(2,1579)	1:104:A:ILE:HA	1:105:A:GLU:HG2	8	1.31
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD12	1	1.31
(2,86)	1:63:A:MET:HB2	1:132:A:ASP:HB3	2	1.31
(2,86)	1:63:A:MET:HB2	1:132:A:ASP:HB3	10	1.31
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD23	1	1.3
(2,1500)	1:133:A:SER:HB3	1:105:A:GLU:HG3	7	1.3
(2,1331)	1:137:A:LEU:HD11	1:137:A:LEU:HA	10	1.3
(2,1309)	1:118:A:LEU:HD11	1:121:A:ASP:HB3	6	1.3
(2,1258)	1:136:A:LYS:HD3	1:59:A:MET:HA	9	1.3
(2,1226)	1:66:A:GLU:HB2	1:73:A:PHE:HB3	9	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG23	2	1.3
(2,6)	1:72:A:ASN:HB2	1:126:A:GLY:HA2	3	1.3
(2,1682)	1:62:A:LEU:HA	1:63:A:MET:HB2	8	1.29
(2,1482)	1:118:A:LEU:HD23	1:84:A:THR:HB	3	1.29
(2,1451)	1:125:A:ALA:HB1	1:122:A:ILE:HG21	10	1.29
(2,1309)	1:118:A:LEU:HD13	1:121:A:ASP:HB3	4	1.29
(2,1309)	1:118:A:LEU:HD12	1:113:A:HIS:HB2	9	1.29
(2,394)	1:99:A:THR:HB	1:98:A:GLU:HB3	5	1.29
(1,7)	1:107:A:PRO:HB2	1:59:A:MET:HG3	8	1.29
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD23	7	1.28
(2,1861)	1:77:A:ALA:H	1:78:A:LYS:HE3	9	1.28
(2,1374)	1:129:A:VAL:HG11	1:73:A:PHE:HE1	8	1.28
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD13	7	1.28
(1,7)	1:107:A:PRO:HB2	1:59:A:MET:HG3	1	1.28
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD23	4	1.27
(2,1833)	1:137:A:LEU:H	1:105:A:GLU:HG3	9	1.27
(2,1805)	1:61:A:ARG:H	1:137:A:LEU:HD21	5	1.27
(2,1738)	1:71:A:LYS:HE3	1:95:A:PHE:HE2	3	1.27
(2,1412)	1:128:A:VAL:HG13	1:126:A:GLY:HA2	7	1.27
(2,1231)	1:76:A:MET:HG2	1:82:A:PHE:HE1	8	1.27
(2,1150)	1:95:A:PHE:HB3	1:77:A:ALA:HB1	7	1.27
(2,585)	1:66:A:GLU:HG3	1:71:A:LYS:HA	10	1.27
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD21	6	1.26
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD21	8	1.26
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD21	10	1.26
(2,1712)	1:91:A:GLY:HA2	1:86:A:ILE:HB	9	1.26
(2,1682)	1:62:A:LEU:HA	1:63:A:MET:HB2	6	1.26
(2,1302)	1:62:A:LEU:HG	1:122:A:ILE:HG13	10	1.26
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG22	10	1.26
(2,237)	1:110:A:VAL:HG11	1:107:A:PRO:HD3	2	1.26
(2,1712)	1:91:A:GLY:HA2	1:86:A:ILE:HB	6	1.25
(2,1426)	1:124:A:ALA:HB3	1:117:A:GLN:HB3	4	1.25
(2,1309)	1:118:A:LEU:HD13	1:121:A:ASP:HB3	1	1.25
(2,1309)	1:118:A:LEU:HD11	1:121:A:ASP:HB3	3	1.25
(2,1301)	1:118:A:LEU:HG	1:117:A:GLN:HA	10	1.25
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD13	6	1.25
(2,86)	1:63:A:MET:HB2	1:132:A:ASP:HB3	6	1.25
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD21	2	1.24
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD23	3	1.24
(2,1482)	1:118:A:LEU:HD21	1:84:A:THR:HB	8	1.24
(2,1426)	1:124:A:ALA:HB2	1:117:A:GLN:HB3	7	1.24
(2,1387)	1:84:A:THR:HG22	1:86:A:ILE:HA	10	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1360)	1:119:A:LEU:HD22	1:115:A:MET:HG3	7	1.24
(2,1309)	1:118:A:LEU:HD13	1:121:A:ASP:HB3	8	1.24
(2,1176)	1:66:A:GLU:HG3	1:128:A:VAL:HG22	6	1.24
(2,528)	1:78:A:LYS:HG2	1:75:A:LYS:HA	5	1.24
(2,333)	1:124:A:ALA:HB1	1:76:A:MET:HG3	6	1.24
(2,34)	1:58:A:GLU:HG2	1:135:A:VAL:HG12	3	1.24
(1,7)	1:107:A:PRO:HB2	1:59:A:MET:HG3	9	1.24
(2,1933)	1:92:A:SER:H	1:93:A:ILE:HD13	8	1.23
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD23	9	1.23
(2,1833)	1:137:A:LEU:H	1:105:A:GLU:HG3	5	1.23
(2,1738)	1:75:A:LYS:HE3	1:95:A:PHE:HE2	6	1.23
(2,1451)	1:125:A:ALA:HB2	1:122:A:ILE:HG21	8	1.23
(2,1425)	1:138:A:ALA:HB1	1:108:A:LYS:HG3	2	1.23
(2,1374)	1:129:A:VAL:HG13	1:73:A:PHE:HE2	6	1.23
(2,1301)	1:118:A:LEU:HG	1:117:A:GLN:HA	3	1.23
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD12	4	1.23
(2,1231)	1:76:A:MET:HG2	1:82:A:PHE:HE1	4	1.23
(2,88)	1:63:A:MET:HB2	1:132:A:ASP:HB2	3	1.23
(2,59)	1:105:A:GLU:HG3	1:59:A:MET:HG3	4	1.23
(2,1933)	1:92:A:SER:H	1:104:A:ILE:HG12	10	1.22
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD12	2	1.22
(2,1805)	1:61:A:ARG:H	1:131:A:LEU:HD13	3	1.22
(2,1387)	1:84:A:THR:HG22	1:86:A:ILE:HA	3	1.22
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD11	10	1.22
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG22	2	1.22
(2,1226)	1:66:A:GLU:HB2	1:73:A:PHE:HB3	4	1.22
(2,1177)	1:58:A:GLU:HG2	1:107:A:PRO:HD3	3	1.22
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD11	10	1.21
(2,1712)	1:91:A:GLY:HA2	1:86:A:ILE:HB	3	1.21
(2,1524)	1:110:A:VAL:HA	1:89:A:LEU:HB2	2	1.21
(2,1500)	1:66:A:GLU:HB2	1:70:A:SER:HB2	4	1.21
(2,1387)	1:84:A:THR:HG22	1:86:A:ILE:HA	2	1.21
(2,1355)	1:123:A:LEU:HD13	1:104:A:ILE:HD12	1	1.21
(2,1355)	1:123:A:LEU:HD12	1:104:A:ILE:HD12	10	1.21
(2,1343)	1:137:A:LEU:HD12	1:136:A:LYS:HE3	5	1.21
(2,1301)	1:118:A:LEU:HG	1:117:A:GLN:HA	9	1.21
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG22	9	1.21
(2,1226)	1:66:A:GLU:HB2	1:73:A:PHE:HB3	5	1.21
(2,1226)	1:71:A:LYS:HB3	1:72:A:ASN:HB2	6	1.21
(2,394)	1:99:A:THR:HB	1:98:A:GLU:HB3	7	1.21
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB3	8	1.21
(2,1470)	1:86:A:ILE:HD12	1:122:A:ILE:HG13	5	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1421)	1:125:A:ALA:HB3	1:122:A:ILE:HD12	6	1.2
(2,1355)	1:123:A:LEU:HD12	1:104:A:ILE:HD13	5	1.2
(2,394)	1:99:A:THR:HB	1:98:A:GLU:HB3	3	1.2
(2,134)	1:120:A:HIS:HB3	1:119:A:LEU:HB3	9	1.2
(1,15)	1:136:A:LYS:HD3	1:107:A:PRO:HB2	9	1.2
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD12	9	1.19
(2,1741)	1:71:A:LYS:HE2	1:72:A:ASN:HA	6	1.19
(2,1444)	1:86:A:ILE:HG22	1:92:A:SER:HB3	10	1.19
(2,1301)	1:118:A:LEU:HG	1:117:A:GLN:HA	4	1.19
(2,1258)	1:136:A:LYS:HD3	1:59:A:MET:HA	7	1.19
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG22	5	1.19
(2,1226)	1:66:A:GLU:HB2	1:73:A:PHE:HB3	7	1.19
(2,311)	1:135:A:VAL:HG21	1:133:A:SER:HB2	2	1.19
(2,237)	1:110:A:VAL:HG13	1:107:A:PRO:HD3	1	1.19
(2,134)	1:120:A:HIS:HB3	1:119:A:LEU:HB3	7	1.19
(1,7)	1:107:A:PRO:HB2	1:59:A:MET:HG3	7	1.19
(2,1712)	1:91:A:GLY:HA2	1:86:A:ILE:HB	1	1.18
(2,1712)	1:91:A:GLY:HA2	1:86:A:ILE:HB	8	1.18
(2,1701)	1:107:A:PRO:HG3	1:106:A:LEU:HB2	5	1.18
(2,1524)	1:110:A:VAL:HA	1:89:A:LEU:HB2	10	1.18
(2,1433)	1:77:A:ALA:HB1	1:78:A:LYS:HB2	3	1.18
(2,1374)	1:129:A:VAL:HG12	1:73:A:PHE:HE2	10	1.18
(2,1355)	1:123:A:LEU:HD13	1:104:A:ILE:HD13	3	1.18
(2,1302)	1:62:A:LEU:HG	1:122:A:ILE:HG13	2	1.18
(2,1257)	1:75:A:LYS:HD3	1:78:A:LYS:HE2	1	1.18
(2,1056)	1:113:A:HIS:H	1:114:A:ASP:HB3	8	1.18
(2,134)	1:120:A:HIS:HB3	1:119:A:LEU:HB3	8	1.18
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG21	3	1.18
(2,1896)	1:125:A:ALA:H	1:123:A:LEU:HD22	5	1.17
(2,1833)	1:137:A:LEU:H	1:105:A:GLU:HG3	4	1.17
(2,1738)	1:71:A:LYS:HE3	1:95:A:PHE:HE2	4	1.17
(2,1708)	1:91:A:GLY:HA3	1:60:A:THR:HB	2	1.17
(2,1701)	1:107:A:PRO:HG3	1:106:A:LEU:HB2	2	1.17
(2,1701)	1:107:A:PRO:HG3	1:106:A:LEU:HB2	3	1.17
(2,1682)	1:62:A:LEU:HA	1:103:A:MET:HG3	5	1.17
(2,1421)	1:125:A:ALA:HB1	1:122:A:ILE:HD13	5	1.17
(2,1401)	1:84:A:THR:HG22	1:89:A:LEU:HD22	3	1.17
(2,1355)	1:123:A:LEU:HD13	1:104:A:ILE:HD13	7	1.17
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG23	1	1.17
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG23	3	1.17
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG23	7	1.17
(2,394)	1:99:A:THR:HB	1:98:A:GLU:HB3	10	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,237)	1:110:A:VAL:HG12	1:107:A:PRO:HD3	4	1.17
(2,134)	1:120:A:HIS:HB3	1:119:A:LEU:HB3	6	1.17
(1,29)	1:82:A:PHE:HA	1:86:A:ILE:HG13	9	1.17
(1,7)	1:107:A:PRO:HB2	1:59:A:MET:HG3	6	1.17
(2,1908)	1:84:A:THR:H	1:88:A:GLU:HG3	8	1.16
(2,1708)	1:91:A:GLY:HA3	1:89:A:LEU:HA	3	1.16
(2,1708)	1:91:A:GLY:HA3	1:60:A:THR:HB	5	1.16
(2,1701)	1:107:A:PRO:HG3	1:106:A:LEU:HB2	6	1.16
(2,1653)	1:66:A:GLU:HA	1:74:A:SER:HA	10	1.16
(2,1451)	1:125:A:ALA:HB1	1:122:A:ILE:HG23	7	1.16
(2,1444)	1:93:A:ILE:HG23	1:94:A:SER:HB3	2	1.16
(2,1355)	1:123:A:LEU:HD13	1:104:A:ILE:HD13	4	1.16
(2,1302)	1:62:A:LEU:HG	1:122:A:ILE:HG13	3	1.16
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB1	4	1.16
(2,1256)	1:75:A:LYS:HD3	1:78:A:LYS:HE3	10	1.16
(2,1208)	1:66:A:GLU:HB3	1:74:A:SER:HA	7	1.16
(2,1176)	1:87:A:GLU:HG2	1:86:A:ILE:HG12	3	1.16
(2,237)	1:110:A:VAL:HG12	1:107:A:PRO:HD3	3	1.16
(2,237)	1:110:A:VAL:HG12	1:107:A:PRO:HD3	6	1.16
(2,167)	1:61:A:ARG:HG2	1:105:A:GLU:HA	7	1.16
(2,134)	1:120:A:HIS:HB3	1:119:A:LEU:HB3	1	1.16
(2,134)	1:120:A:HIS:HB3	1:119:A:LEU:HB3	4	1.16
(2,1774)	1:104:A:ILE:HB	1:103:A:MET:HG3	5	1.15
(2,1701)	1:107:A:PRO:HG3	1:106:A:LEU:HB2	4	1.15
(2,1701)	1:107:A:PRO:HG3	1:106:A:LEU:HB2	10	1.15
(2,1554)	1:86:A:ILE:HA	1:88:A:GLU:HB3	9	1.15
(2,1444)	1:86:A:ILE:HG23	1:92:A:SER:HB3	7	1.15
(2,1412)	1:128:A:VAL:HG11	1:126:A:GLY:HA2	5	1.15
(2,1388)	1:84:A:THR:HG21	1:85:A:ARG:HD2	8	1.15
(2,1388)	1:84:A:THR:HG22	1:85:A:ARG:HD2	9	1.15
(2,1386)	1:109:A:THR:HG22	1:58:A:GLU:HG2	9	1.15
(2,1301)	1:118:A:LEU:HG	1:117:A:GLN:HA	8	1.15
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG23	7	1.15
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG23	4	1.15
(2,1177)	1:58:A:GLU:HG2	1:107:A:PRO:HD3	2	1.15
(2,1149)	1:58:A:GLU:H	1:58:A:GLU:HG2	9	1.15
(2,1861)	1:77:A:ALA:H	1:78:A:LYS:HE3	8	1.14
(2,1833)	1:137:A:LEU:H	1:135:A:VAL:HB	6	1.14
(2,1833)	1:137:A:LEU:H	1:105:A:GLU:HG3	7	1.14
(2,1701)	1:107:A:PRO:HG3	1:106:A:LEU:HB2	1	1.14
(2,1455)	1:93:A:ILE:HD11	1:78:A:LYS:HD3	4	1.14
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG21	1	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,394)	1:99:A:THR:HB	1:98:A:GLU:HB3	4	1.14
(2,394)	1:99:A:THR:HB	1:98:A:GLU:HB3	9	1.14
(2,264)	1:65:A:THR:HG23	1:64:A:VAL:HG13	10	1.14
(2,237)	1:110:A:VAL:HG12	1:107:A:PRO:HD3	8	1.14
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB3	9	1.14
(2,1908)	1:84:A:THR:H	1:88:A:GLU:HG3	2	1.13
(2,1904)	1:66:A:GLU:H	1:71:A:LYS:HD3	2	1.13
(2,1833)	1:137:A:LEU:H	1:105:A:GLU:HG3	2	1.13
(2,1774)	1:104:A:ILE:HB	1:103:A:MET:HG3	6	1.13
(2,1712)	1:91:A:GLY:HA2	1:86:A:ILE:HB	4	1.13
(2,1444)	1:86:A:ILE:HG22	1:92:A:SER:HB3	5	1.13
(2,1360)	1:119:A:LEU:HD22	1:115:A:MET:HG3	3	1.13
(2,1355)	1:123:A:LEU:HD13	1:104:A:ILE:HD12	6	1.13
(2,1301)	1:118:A:LEU:HG	1:117:A:GLN:HA	1	1.13
(2,1280)	1:93:A:ILE:HG13	1:86:A:ILE:HD11	9	1.13
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG21	10	1.13
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB3	9	1.13
(2,1056)	1:113:A:HIS:H	1:114:A:ASP:HB3	5	1.13
(2,586)	1:71:A:LYS:HA	1:66:A:GLU:HB2	2	1.13
(2,237)	1:110:A:VAL:HG13	1:107:A:PRO:HD3	7	1.13
(2,134)	1:120:A:HIS:HB3	1:119:A:LEU:HB3	3	1.13
(2,134)	1:120:A:HIS:HB3	1:119:A:LEU:HB3	5	1.13
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB3	6	1.13
(2,1861)	1:77:A:ALA:H	1:78:A:LYS:HE3	1	1.12
(2,1712)	1:91:A:GLY:HA2	1:86:A:ILE:HB	7	1.12
(2,1701)	1:107:A:PRO:HG3	1:106:A:LEU:HB2	7	1.12
(2,1455)	1:93:A:ILE:HD11	1:78:A:LYS:HD3	5	1.12
(2,1426)	1:124:A:ALA:HB3	1:117:A:GLN:HB3	1	1.12
(2,1355)	1:123:A:LEU:HD12	1:104:A:ILE:HD13	9	1.12
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG23	5	1.12
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG23	6	1.12
(2,1226)	1:71:A:LYS:HB3	1:72:A:ASN:HB2	2	1.12
(2,1056)	1:113:A:HIS:H	1:114:A:ASP:HB3	9	1.12
(2,360)	1:122:A:ILE:HG22	1:127:A:GLY:HA2	10	1.12
(2,86)	1:63:A:MET:HB2	1:132:A:ASP:HB3	4	1.12
(2,59)	1:105:A:GLU:HG3	1:59:A:MET:HG3	7	1.12
(2,6)	1:72:A:ASN:HB2	1:126:A:GLY:HA2	2	1.12
(2,1908)	1:84:A:THR:H	1:88:A:GLU:HG3	3	1.11
(2,1738)	1:75:A:LYS:HE3	1:95:A:PHE:HE2	7	1.11
(2,1701)	1:107:A:PRO:HG3	1:106:A:LEU:HB2	8	1.11
(2,1500)	1:66:A:GLU:HB2	1:70:A:SER:HB2	10	1.11
(2,1360)	1:63:A:MET:HB2	1:96:A:LEU:HD21	10	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1304)	1:118:A:LEU:HD11	1:82:A:PHE:HE1	9	1.11
(2,1302)	1:62:A:LEU:HG	1:122:A:ILE:HG13	8	1.11
(2,1231)	1:76:A:MET:HG2	1:82:A:PHE:HE1	1	1.11
(2,1149)	1:58:A:GLU:H	1:58:A:GLU:HG2	7	1.11
(2,131)	1:136:A:LYS:HD3	1:58:A:GLU:HG3	6	1.11
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB2	10	1.11
(2,1701)	1:107:A:PRO:HG3	1:106:A:LEU:HB2	9	1.1
(2,1451)	1:125:A:ALA:HB1	1:122:A:ILE:HG23	4	1.1
(2,1378)	1:64:A:VAL:HG13	1:101:A:VAL:HA	6	1.1
(2,1374)	1:129:A:VAL:HG13	1:73:A:PHE:HE2	4	1.1
(2,1360)	1:63:A:MET:HB2	1:96:A:LEU:HD22	8	1.1
(2,1248)	1:67:A:LYS:HD3	1:69:A:GLU:HB3	7	1.1
(2,1245)	1:87:A:GLU:HB3	1:86:A:ILE:HG21	8	1.1
(2,1231)	1:76:A:MET:HG2	1:82:A:PHE:HE1	9	1.1
(2,597)	1:61:A:ARG:HA	1:103:A:MET:HG3	5	1.1
(1,29)	1:82:A:PHE:HA	1:86:A:ILE:HG13	5	1.1
(1,7)	1:107:A:PRO:HB2	1:59:A:MET:HG3	5	1.1
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG22	6	1.09
(2,1774)	1:104:A:ILE:HB	1:103:A:MET:HG3	8	1.09
(2,1554)	1:86:A:ILE:HA	1:88:A:GLU:HB3	7	1.09
(2,1451)	1:125:A:ALA:HB2	1:122:A:ILE:HG22	9	1.09
(2,1433)	1:77:A:ALA:HB3	1:78:A:LYS:HB2	4	1.09
(2,1360)	1:63:A:MET:HB2	1:96:A:LEU:HD21	4	1.09
(2,1348)	1:62:A:LEU:HD21	1:115:A:MET:HG3	1	1.09
(2,1343)	1:137:A:LEU:HD11	1:136:A:LYS:HE2	3	1.09
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG23	4	1.09
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG22	9	1.09
(2,1256)	1:75:A:LYS:HD3	1:78:A:LYS:HE3	3	1.09
(2,1231)	1:76:A:MET:HG2	1:82:A:PHE:HE1	7	1.09
(2,1157)	1:96:A:LEU:HB2	1:96:A:LEU:HD21	7	1.09
(2,1149)	1:58:A:GLU:H	1:58:A:GLU:HG2	4	1.09
(2,1056)	1:113:A:HIS:H	1:114:A:ASP:HB3	4	1.09
(2,237)	1:110:A:VAL:HG11	1:107:A:PRO:HD3	9	1.09
(2,131)	1:136:A:LYS:HD3	1:58:A:GLU:HG3	8	1.09
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB3	3	1.09
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB3	4	1.09
(2,88)	1:63:A:MET:HB2	1:132:A:ASP:HB2	10	1.09
(2,59)	1:105:A:GLU:HG3	1:59:A:MET:HG3	8	1.09
(2,59)	1:105:A:GLU:HG3	1:59:A:MET:HG3	9	1.09
(1,29)	1:82:A:PHE:HA	1:86:A:ILE:HG13	10	1.09
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD11	4	1.08
(2,1506)	1:66:A:GLU:HB2	1:70:A:SER:HB2	5	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1500)	1:66:A:GLU:HB2	1:70:A:SER:HB2	2	1.08
(2,1451)	1:125:A:ALA:HB3	1:122:A:ILE:HG22	2	1.08
(2,1444)	1:86:A:ILE:HG23	1:92:A:SER:HB3	3	1.08
(2,1433)	1:77:A:ALA:HB3	1:78:A:LYS:HB2	8	1.08
(2,1360)	1:119:A:LEU:HD21	1:115:A:MET:HG3	1	1.08
(2,1304)	1:118:A:LEU:HD13	1:82:A:PHE:HE1	4	1.08
(2,1301)	1:118:A:LEU:HG	1:117:A:GLN:HA	6	1.08
(2,1056)	1:113:A:HIS:H	1:114:A:ASP:HB3	7	1.08
(2,679)	1:89:A:LEU:HB3	1:114:A:ASP:HB2	8	1.08
(2,394)	1:99:A:THR:HB	1:98:A:GLU:HB3	1	1.08
(1,24)	1:75:A:LYS:HG3	1:78:A:LYS:HE3	4	1.08
(2,1908)	1:84:A:THR:H	1:88:A:GLU:HG3	1	1.07
(2,1738)	1:75:A:LYS:HE3	1:95:A:PHE:HE2	2	1.07
(2,1712)	1:91:A:GLY:HA2	1:86:A:ILE:HB	5	1.07
(2,1451)	1:125:A:ALA:HB3	1:122:A:ILE:HG22	6	1.07
(2,1418)	1:64:A:VAL:HG22	1:127:A:GLY:HA2	10	1.07
(2,1387)	1:84:A:THR:HG22	1:86:A:ILE:HA	6	1.07
(2,1374)	1:129:A:VAL:HG13	1:73:A:PHE:HE2	7	1.07
(2,1360)	1:63:A:MET:HB2	1:96:A:LEU:HD23	2	1.07
(2,1358)	1:119:A:LEU:HD21	1:121:A:ASP:HB3	2	1.07
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG13	5	1.06
(2,1544)	1:74:A:SER:HB3	1:71:A:LYS:HG2	5	1.06
(2,1500)	1:66:A:GLU:HB2	1:70:A:SER:HB2	8	1.06
(2,1386)	1:84:A:THR:HG22	1:88:A:GLU:HB3	10	1.06
(2,1380)	1:64:A:VAL:HG13	1:128:A:VAL:HG23	4	1.06
(2,1324)	1:115:A:MET:HG3	1:108:A:LYS:HG3	8	1.06
(2,1302)	1:62:A:LEU:HG	1:122:A:ILE:HG13	4	1.06
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB3	8	1.06
(2,586)	1:71:A:LYS:HA	1:66:A:GLU:HB2	1	1.06
(2,1904)	1:66:A:GLU:H	1:71:A:LYS:HD3	6	1.05
(2,1653)	1:66:A:GLU:HA	1:74:A:SER:HA	8	1.05
(2,1524)	1:110:A:VAL:HA	1:89:A:LEU:HB2	4	1.05
(2,1444)	1:86:A:ILE:HG21	1:92:A:SER:HB3	8	1.05
(2,1387)	1:84:A:THR:HG21	1:86:A:ILE:HA	8	1.05
(2,1374)	1:129:A:VAL:HG13	1:73:A:PHE:HE1	2	1.05
(2,1355)	1:123:A:LEU:HD13	1:104:A:ILE:HD12	2	1.05
(2,1345)	1:107:A:PRO:HB3	1:110:A:VAL:HG11	10	1.05
(2,1258)	1:136:A:LYS:HD3	1:59:A:MET:HA	4	1.05
(2,1056)	1:113:A:HIS:H	1:114:A:ASP:HB3	1	1.05
(2,679)	1:89:A:LEU:HB3	1:114:A:ASP:HB2	6	1.05
(2,240)	1:110:A:VAL:HG13	1:89:A:LEU:HB2	10	1.05
(2,134)	1:120:A:HIS:HB3	1:119:A:LEU:HB3	2	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1833)	1:137:A:LEU:H	1:135:A:VAL:HB	1	1.04
(2,1833)	1:137:A:LEU:H	1:105:A:GLU:HG3	10	1.04
(2,1506)	1:66:A:GLU:HB2	1:70:A:SER:HB2	3	1.04
(2,1506)	1:66:A:GLU:HB2	1:70:A:SER:HB2	4	1.04
(2,1451)	1:125:A:ALA:HB2	1:122:A:ILE:HG21	1	1.04
(2,1386)	1:109:A:THR:HG23	1:58:A:GLU:HG2	7	1.04
(2,1378)	1:64:A:VAL:HG13	1:129:A:VAL:HA	4	1.04
(2,1360)	1:63:A:MET:HB2	1:96:A:LEU:HD23	6	1.04
(2,1360)	1:63:A:MET:HB2	1:96:A:LEU:HD22	9	1.04
(2,1301)	1:118:A:LEU:HG	1:117:A:GLN:HA	5	1.04
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG21	3	1.04
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG22	6	1.04
(2,1190)	1:107:A:PRO:HB3	1:90:A:GLY:HA2	3	1.04
(2,446)	1:118:A:LEU:HD21	1:81:A:SER:HA	5	1.04
(2,394)	1:99:A:THR:HB	1:98:A:GLU:HB3	6	1.04
(2,237)	1:110:A:VAL:HG11	1:107:A:PRO:HD3	5	1.04
(2,59)	1:105:A:GLU:HG3	1:59:A:MET:HG3	5	1.04
(1,29)	1:82:A:PHE:HA	1:86:A:ILE:HG13	3	1.04
(1,29)	1:82:A:PHE:HA	1:86:A:ILE:HG13	8	1.04
(2,1708)	1:91:A:GLY:HA3	1:60:A:THR:HB	7	1.03
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG11	6	1.03
(2,1500)	1:133:A:SER:HB3	1:105:A:GLU:HG3	5	1.03
(2,1500)	1:128:A:VAL:HB	1:70:A:SER:HB2	6	1.03
(2,1446)	1:86:A:ILE:HG22	1:107:A:PRO:HG3	3	1.03
(2,1378)	1:64:A:VAL:HG11	1:129:A:VAL:HA	3	1.03
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB2	7	1.03
(2,1056)	1:113:A:HIS:H	1:114:A:ASP:HB3	3	1.03
(2,86)	1:63:A:MET:HB2	1:132:A:ASP:HB3	5	1.03
(1,46)	1:108:A:LYS:HE3	1:59:A:MET:HA	9	1.03
(1,29)	1:82:A:PHE:HA	1:86:A:ILE:HG13	4	1.03
(1,29)	1:82:A:PHE:HA	1:86:A:ILE:HG13	6	1.03
(2,1446)	1:86:A:ILE:HG22	1:107:A:PRO:HG3	10	1.02
(2,1444)	1:86:A:ILE:HG23	1:92:A:SER:HB3	1	1.02
(2,1433)	1:77:A:ALA:HB1	1:78:A:LYS:HB2	2	1.02
(2,1425)	1:138:A:ALA:HB3	1:61:A:ARG:HG3	3	1.02
(2,1374)	1:129:A:VAL:HG11	1:73:A:PHE:HE1	1	1.02
(2,1374)	1:129:A:VAL:HG12	1:73:A:PHE:HE1	5	1.02
(2,1304)	1:118:A:LEU:HD13	1:82:A:PHE:HE1	5	1.02
(2,1301)	1:118:A:LEU:HG	1:117:A:GLN:HA	7	1.02
(2,1231)	1:76:A:MET:HG2	1:82:A:PHE:HE2	3	1.02
(2,1190)	1:107:A:PRO:HB3	1:90:A:GLY:HA2	5	1.02
(2,1176)	1:66:A:GLU:HG3	1:128:A:VAL:HG23	1	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:82:A:PHE:HA	1:86:A:ILE:HG13	2	1.02
(2,1740)	1:128:A:VAL:HG21	1:67:A:LYS:HE3	1	1.01
(2,1478)	1:97:A:THR:HB	1:78:A:LYS:HE2	2	1.01
(2,1451)	1:125:A:ALA:HB1	1:122:A:ILE:HG23	5	1.01
(2,1386)	1:109:A:THR:HG22	1:58:A:GLU:HG2	1	1.01
(2,1374)	1:129:A:VAL:HG12	1:73:A:PHE:HE1	3	1.01
(2,1358)	1:119:A:LEU:HD21	1:121:A:ASP:HB3	9	1.01
(2,1304)	1:118:A:LEU:HD13	1:82:A:PHE:HE1	8	1.01
(2,1190)	1:107:A:PRO:HB3	1:90:A:GLY:HA2	10	1.01
(2,1176)	1:87:A:GLU:HG2	1:86:A:ILE:HG12	4	1.01
(2,586)	1:71:A:LYS:HA	1:66:A:GLU:HB2	6	1.01
(2,375)	1:64:A:VAL:HG11	1:122:A:ILE:HD12	6	1.01
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD12	7	1.0
(2,1867)	1:88:A:GLU:H	1:86:A:ILE:HB	5	1.0
(2,1738)	1:71:A:LYS:HE2	1:95:A:PHE:HE2	10	1.0
(2,1708)	1:91:A:GLY:HA3	1:60:A:THR:HB	9	1.0
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD21	9	1.0
(2,1500)	1:66:A:GLU:HB2	1:70:A:SER:HB2	1	1.0
(2,1482)	1:118:A:LEU:HD22	1:84:A:THR:HB	9	1.0
(2,1446)	1:86:A:ILE:HG22	1:107:A:PRO:HG3	2	1.0
(2,1401)	1:84:A:THR:HG23	1:89:A:LEU:HD22	4	1.0
(2,1387)	1:84:A:THR:HG23	1:86:A:ILE:HA	5	1.0
(2,1387)	1:84:A:THR:HG22	1:86:A:ILE:HA	9	1.0
(2,1258)	1:136:A:LYS:HD3	1:59:A:MET:HA	6	1.0
(2,1190)	1:107:A:PRO:HB3	1:90:A:GLY:HA2	7	1.0
(2,943)	1:58:A:GLU:H	1:59:A:MET:H	6	1.0
(2,679)	1:89:A:LEU:HB3	1:114:A:ASP:HB2	3	1.0
(2,623)	1:59:A:MET:HA	1:107:A:PRO:HB2	2	1.0
(2,446)	1:118:A:LEU:HD23	1:81:A:SER:HA	3	1.0
(2,446)	1:118:A:LEU:HD21	1:81:A:SER:HA	8	1.0
(2,134)	1:120:A:HIS:HB3	1:119:A:LEU:HB3	10	1.0
(2,88)	1:63:A:MET:HB2	1:132:A:ASP:HB2	4	1.0
(2,86)	1:63:A:MET:HB2	1:132:A:ASP:HB3	9	1.0
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG21	7	1.0
(1,29)	1:82:A:PHE:HA	1:86:A:ILE:HG13	7	1.0
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG12	10	0.99
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD11	5	0.99
(2,1861)	1:77:A:ALA:H	1:78:A:LYS:HE3	2	0.99
(2,1805)	1:61:A:ARG:H	1:131:A:LEU:HD13	7	0.99
(2,1738)	1:71:A:LYS:HE3	1:95:A:PHE:HE2	5	0.99
(2,1708)	1:91:A:GLY:HA3	1:60:A:THR:HB	10	0.99
(2,1502)	1:133:A:SER:HB3	1:136:A:LYS:HB2	2	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1455)	1:93:A:ILE:HD11	1:78:A:LYS:HD3	7	0.99
(2,1444)	1:86:A:ILE:HG23	1:92:A:SER:HB3	4	0.99
(2,1379)	1:64:A:VAL:HG12	1:102:A:THR:HG22	5	0.99
(2,1378)	1:64:A:VAL:HG11	1:101:A:VAL:HA	9	0.99
(2,1304)	1:118:A:LEU:HD11	1:82:A:PHE:HE1	7	0.99
(2,1190)	1:107:A:PRO:HB3	1:90:A:GLY:HA2	2	0.99
(2,1190)	1:107:A:PRO:HB3	1:90:A:GLY:HA2	9	0.99
(2,1174)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	7	0.99
(2,943)	1:58:A:GLU:H	1:59:A:MET:H	5	0.99
(2,623)	1:59:A:MET:HA	1:107:A:PRO:HB2	10	0.99
(2,528)	1:78:A:LYS:HG2	1:75:A:LYS:HA	9	0.99
(2,446)	1:118:A:LEU:HD23	1:81:A:SER:HA	1	0.99
(2,59)	1:105:A:GLU:HG3	1:59:A:MET:HG3	6	0.99
(1,15)	1:136:A:LYS:HD3	1:107:A:PRO:HB2	7	0.99
(2,1708)	1:91:A:GLY:HA3	1:60:A:THR:HB	1	0.98
(2,1355)	1:123:A:LEU:HD11	1:104:A:ILE:HD11	8	0.98
(2,1302)	1:62:A:LEU:HG	1:122:A:ILE:HG13	1	0.98
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG22	2	0.98
(2,1174)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	8	0.98
(2,727)	1:111:A:SER:HB3	1:114:A:ASP:HB3	4	0.98
(2,727)	1:111:A:SER:HB3	1:114:A:ASP:HB3	9	0.98
(2,679)	1:89:A:LEU:HB3	1:114:A:ASP:HB2	7	0.98
(2,446)	1:118:A:LEU:HD23	1:81:A:SER:HA	2	0.98
(2,329)	1:125:A:ALA:HB1	1:122:A:ILE:HG21	3	0.98
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB3	1	0.98
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG22	1	0.98
(2,1867)	1:88:A:GLU:H	1:86:A:ILE:HB	7	0.97
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG11	3	0.97
(2,1558)	1:95:A:PHE:HE1	1:100:A:GLY:HA2	8	0.97
(2,1532)	1:87:A:GLU:HB3	1:83:A:SER:HA	2	0.97
(2,1532)	1:87:A:GLU:HB3	1:83:A:SER:HA	7	0.97
(2,1406)	1:135:A:VAL:HG13	1:107:A:PRO:HD3	7	0.97
(2,1388)	1:84:A:THR:HG22	1:85:A:ARG:HD2	7	0.97
(2,1378)	1:64:A:VAL:HG11	1:101:A:VAL:HA	5	0.97
(2,1332)	1:119:A:LEU:HD11	1:119:A:LEU:HA	4	0.97
(2,1309)	1:118:A:LEU:HD13	1:121:A:ASP:HB3	10	0.97
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB2	1	0.97
(2,1231)	1:76:A:MET:HG2	1:82:A:PHE:HE1	10	0.97
(2,727)	1:111:A:SER:HB3	1:114:A:ASP:HB3	1	0.97
(2,679)	1:89:A:LEU:HB3	1:114:A:ASP:HB2	5	0.97
(1,60)	1:119:A:LEU:H	1:114:A:ASP:HB2	6	0.97
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG23	4	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG11	5	0.96
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD11	8	0.96
(2,1532)	1:87:A:GLU:HB3	1:83:A:SER:HA	1	0.96
(2,1412)	1:128:A:VAL:HG12	1:126:A:GLY:HA2	3	0.96
(2,1378)	1:64:A:VAL:HG13	1:101:A:VAL:HA	7	0.96
(2,1056)	1:113:A:HIS:H	1:114:A:ASP:HB3	6	0.96
(2,1032)	1:84:A:THR:H	1:84:A:THR:HG22	3	0.96
(2,727)	1:111:A:SER:HB3	1:114:A:ASP:HB3	8	0.96
(2,360)	1:122:A:ILE:HG21	1:127:A:GLY:HA2	7	0.96
(1,29)	1:82:A:PHE:HA	1:86:A:ILE:HG13	1	0.96
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD12	3	0.95
(2,1867)	1:88:A:GLU:H	1:86:A:ILE:HB	1	0.95
(2,1867)	1:88:A:GLU:H	1:86:A:ILE:HB	6	0.95
(2,1741)	1:136:A:LYS:HE2	1:136:A:LYS:HA	7	0.95
(2,1708)	1:91:A:GLY:HA3	1:60:A:THR:HB	8	0.95
(2,1705)	1:126:A:GLY:HA3	1:73:A:PHE:HA	5	0.95
(2,1483)	1:84:A:THR:HA	1:87:A:GLU:HG2	7	0.95
(2,1444)	1:86:A:ILE:HG23	1:92:A:SER:HB3	6	0.95
(2,1433)	1:77:A:ALA:HB1	1:78:A:LYS:HB2	10	0.95
(2,1379)	1:64:A:VAL:HG12	1:102:A:THR:HG21	9	0.95
(2,1258)	1:136:A:LYS:HD3	1:59:A:MET:HA	8	0.95
(2,1176)	1:87:A:GLU:HG2	1:86:A:ILE:HG12	2	0.95
(2,623)	1:59:A:MET:HA	1:107:A:PRO:HB2	1	0.95
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD13	3	0.94
(2,1712)	1:91:A:GLY:HA2	1:86:A:ILE:HB	10	0.94
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG12	7	0.94
(2,1506)	1:66:A:GLU:HB2	1:70:A:SER:HB2	10	0.94
(2,1455)	1:93:A:ILE:HD12	1:78:A:LYS:HD3	3	0.94
(2,1446)	1:86:A:ILE:HG23	1:107:A:PRO:HG3	4	0.94
(2,1446)	1:86:A:ILE:HG22	1:107:A:PRO:HG3	7	0.94
(2,1388)	1:84:A:THR:HG23	1:85:A:ARG:HD2	1	0.94
(2,1387)	1:84:A:THR:HG23	1:86:A:ILE:HA	1	0.94
(2,1379)	1:64:A:VAL:HG13	1:102:A:THR:HG23	1	0.94
(2,1378)	1:64:A:VAL:HG12	1:129:A:VAL:HA	10	0.94
(2,1304)	1:118:A:LEU:HD11	1:82:A:PHE:HE1	2	0.94
(2,1304)	1:118:A:LEU:HD13	1:82:A:PHE:HE1	10	0.94
(2,1265)	1:78:A:LYS:HD3	1:78:A:LYS:HA	9	0.94
(2,1032)	1:84:A:THR:H	1:84:A:THR:HG22	2	0.94
(2,679)	1:89:A:LEU:HB3	1:114:A:ASP:HB2	1	0.94
(2,446)	1:118:A:LEU:HD21	1:81:A:SER:HA	6	0.94
(2,329)	1:125:A:ALA:HB1	1:122:A:ILE:HG21	10	0.94
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG23	9	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD11	1	0.93
(2,1712)	1:91:A:GLY:HA2	1:86:A:ILE:HB	2	0.93
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG11	4	0.93
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD22	3	0.93
(2,1578)	1:102:A:THR:HG23	1:93:A:ILE:HA	8	0.93
(2,1532)	1:87:A:GLU:HB3	1:83:A:SER:HA	3	0.93
(2,1455)	1:93:A:ILE:HD11	1:85:A:ARG:HG2	9	0.93
(2,1446)	1:86:A:ILE:HG21	1:107:A:PRO:HG3	9	0.93
(2,1406)	1:135:A:VAL:HG13	1:107:A:PRO:HD3	5	0.93
(2,1393)	1:110:A:VAL:HG23	1:119:A:LEU:HG	1	0.93
(2,1348)	1:62:A:LEU:HD23	1:115:A:MET:HG3	7	0.93
(2,1345)	1:110:A:VAL:HG13	1:114:A:ASP:HB2	2	0.93
(2,1309)	1:118:A:LEU:HD12	1:113:A:HIS:HB2	2	0.93
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB3	2	0.93
(2,689)	1:108:A:LYS:HG3	1:108:A:LYS:HE3	9	0.93
(2,679)	1:89:A:LEU:HB3	1:114:A:ASP:HB2	4	0.93
(2,623)	1:59:A:MET:HA	1:107:A:PRO:HB2	8	0.93
(2,360)	1:122:A:ILE:HG21	1:127:A:GLY:HA2	4	0.93
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG22	5	0.93
(1,60)	1:119:A:LEU:H	1:114:A:ASP:HB2	1	0.93
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD13	6	0.92
(2,1867)	1:88:A:GLU:H	1:86:A:ILE:HB	8	0.92
(2,1866)	1:88:A:GLU:H	1:88:A:GLU:HB3	1	0.92
(2,1544)	1:74:A:SER:HB3	1:71:A:LYS:HG2	7	0.92
(2,1406)	1:135:A:VAL:HG12	1:107:A:PRO:HD3	8	0.92
(2,1406)	1:135:A:VAL:HG12	1:107:A:PRO:HD3	9	0.92
(2,1379)	1:64:A:VAL:HG13	1:102:A:THR:HG23	3	0.92
(2,1357)	1:96:A:LEU:HD22	1:61:A:ARG:HD3	5	0.92
(2,1190)	1:107:A:PRO:HB3	1:90:A:GLY:HA2	6	0.92
(2,1173)	1:66:A:GLU:HG3	1:70:A:SER:HB2	10	0.92
(2,1867)	1:88:A:GLU:H	1:86:A:ILE:HB	2	0.91
(2,1866)	1:88:A:GLU:H	1:88:A:GLU:HB3	6	0.91
(2,1657)	1:105:A:GLU:HA	1:106:A:LEU:HB3	7	0.91
(2,1608)	1:76:A:MET:HA	1:77:A:ALA:HB1	1	0.91
(2,1608)	1:76:A:MET:HA	1:77:A:ALA:HB2	10	0.91
(2,1506)	1:66:A:GLU:HB2	1:70:A:SER:HB2	2	0.91
(2,1433)	1:77:A:ALA:HB3	1:78:A:LYS:HB2	1	0.91
(2,1418)	1:64:A:VAL:HG22	1:127:A:GLY:HA2	4	0.91
(2,1412)	1:128:A:VAL:HG12	1:126:A:GLY:HA2	8	0.91
(2,1406)	1:135:A:VAL:HG13	1:107:A:PRO:HD3	10	0.91
(2,1358)	1:119:A:LEU:HD22	1:121:A:ASP:HB3	1	0.91
(2,1304)	1:118:A:LEU:HD13	1:82:A:PHE:HE1	1	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1278)	1:104:A:ILE:HG13	1:122:A:ILE:HG21	8	0.91
(2,1257)	1:136:A:LYS:HD2	1:59:A:MET:HG2	3	0.91
(2,727)	1:111:A:SER:HB3	1:114:A:ASP:HB3	7	0.91
(2,586)	1:71:A:LYS:HA	1:66:A:GLU:HB2	5	0.91
(2,586)	1:71:A:LYS:HA	1:66:A:GLU:HB2	10	0.91
(2,282)	1:97:A:THR:HG23	1:78:A:LYS:HE2	2	0.91
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG12	10	0.9
(2,1907)	1:117:A:GLN:H	1:118:A:LEU:HD12	6	0.9
(2,1867)	1:88:A:GLU:H	1:86:A:ILE:HB	3	0.9
(2,1866)	1:88:A:GLU:H	1:88:A:GLU:HB3	3	0.9
(2,1705)	1:126:A:GLY:HA3	1:69:A:GLU:HA	6	0.9
(2,1653)	1:66:A:GLU:HA	1:74:A:SER:HA	5	0.9
(2,1608)	1:76:A:MET:HA	1:77:A:ALA:HB1	4	0.9
(2,1599)	1:75:A:LYS:HG2	1:75:A:LYS:HA	9	0.9
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD21	10	0.9
(2,1578)	1:102:A:THR:HG22	1:93:A:ILE:HA	1	0.9
(2,1412)	1:128:A:VAL:HG11	1:126:A:GLY:HA2	2	0.9
(2,1406)	1:135:A:VAL:HG12	1:107:A:PRO:HD3	4	0.9
(2,1358)	1:119:A:LEU:HD23	1:121:A:ASP:HB3	3	0.9
(2,1242)	1:120:A:HIS:HB2	1:122:A:ILE:HB	2	0.9
(2,943)	1:58:A:GLU:H	1:59:A:MET:H	1	0.9
(2,240)	1:110:A:VAL:HG13	1:89:A:LEU:HB2	5	0.9
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD13	2	0.89
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD11	9	0.89
(2,1867)	1:88:A:GLU:H	1:86:A:ILE:HB	4	0.89
(2,1866)	1:88:A:GLU:H	1:88:A:GLU:HB3	4	0.89
(2,1866)	1:88:A:GLU:H	1:88:A:GLU:HB3	9	0.89
(2,1705)	1:126:A:GLY:HA3	1:73:A:PHE:HA	4	0.89
(2,1653)	1:66:A:GLU:HA	1:74:A:SER:HA	9	0.89
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG11	8	0.89
(2,1608)	1:76:A:MET:HA	1:77:A:ALA:HB1	8	0.89
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD22	5	0.89
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD23	8	0.89
(2,1506)	1:66:A:GLU:HB2	1:70:A:SER:HB2	8	0.89
(2,1446)	1:86:A:ILE:HG22	1:107:A:PRO:HG3	5	0.89
(2,1387)	1:84:A:THR:HG22	1:86:A:ILE:HA	7	0.89
(2,1360)	1:63:A:MET:HB2	1:96:A:LEU:HD23	5	0.89
(2,1358)	1:119:A:LEU:HD22	1:121:A:ASP:HB3	6	0.89
(2,1358)	1:119:A:LEU:HD21	1:121:A:ASP:HB3	8	0.89
(2,1348)	1:62:A:LEU:HD22	1:115:A:MET:HG3	6	0.89
(2,1332)	1:119:A:LEU:HD13	1:119:A:LEU:HA	6	0.89
(2,1325)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	4	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1304)	1:118:A:LEU:HD11	1:82:A:PHE:HE1	3	0.89
(2,1302)	1:62:A:LEU:HG	1:122:A:ILE:HG13	6	0.89
(2,1258)	1:136:A:LYS:HD2	1:59:A:MET:HA	10	0.89
(2,1252)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	7	0.89
(2,1242)	1:120:A:HIS:HB2	1:122:A:ILE:HB	5	0.89
(2,1176)	1:66:A:GLU:HG3	1:128:A:VAL:HG22	7	0.89
(2,946)	1:58:A:GLU:H	1:58:A:GLU:HB2	4	0.89
(2,867)	1:87:A:GLU:H	1:86:A:ILE:HG13	3	0.89
(2,727)	1:111:A:SER:HB3	1:114:A:ASP:HB3	5	0.89
(2,687)	1:108:A:LYS:HE3	1:60:A:THR:HA	8	0.89
(2,623)	1:59:A:MET:HA	1:107:A:PRO:HB2	3	0.89
(2,216)	1:96:A:LEU:HD12	1:103:A:MET:HA	8	0.89
(1,60)	1:119:A:LEU:H	1:114:A:ASP:HB2	3	0.89
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG13	7	0.88
(2,1908)	1:84:A:THR:H	1:88:A:GLU:HG3	6	0.88
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD11	5	0.88
(2,1866)	1:88:A:GLU:H	1:88:A:GLU:HB3	2	0.88
(2,1866)	1:88:A:GLU:H	1:88:A:GLU:HB3	8	0.88
(2,1805)	1:61:A:ARG:H	1:137:A:LEU:HD11	8	0.88
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG12	1	0.88
(2,1608)	1:117:A:GLN:HA	1:118:A:LEU:HD23	6	0.88
(2,1608)	1:117:A:GLN:HA	1:118:A:LEU:HD21	7	0.88
(2,1608)	1:76:A:MET:HA	1:77:A:ALA:HB2	9	0.88
(2,1578)	1:102:A:THR:HG21	1:93:A:ILE:HA	5	0.88
(2,1445)	1:87:A:GLU:HG3	1:86:A:ILE:HG22	5	0.88
(2,1432)	1:124:A:ALA:HB2	1:123:A:LEU:HB3	2	0.88
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG22	7	0.88
(2,1379)	1:64:A:VAL:HG11	1:102:A:THR:HG23	7	0.88
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB3	6	0.88
(2,1252)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	8	0.88
(2,1242)	1:120:A:HIS:HB2	1:122:A:ILE:HB	4	0.88
(2,727)	1:111:A:SER:HB3	1:114:A:ASP:HB3	3	0.88
(2,446)	1:118:A:LEU:HD23	1:81:A:SER:HA	9	0.88
(2,375)	1:64:A:VAL:HG12	1:122:A:ILE:HD13	5	0.88
(2,331)	1:125:A:ALA:HB1	1:121:A:ASP:HB3	5	0.88
(2,329)	1:125:A:ALA:HB2	1:122:A:ILE:HG21	8	0.88
(2,131)	1:136:A:LYS:HD3	1:58:A:GLU:HG3	1	0.88
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG12	3	0.87
(2,1866)	1:88:A:GLU:H	1:88:A:GLU:HB3	10	0.87
(2,1741)	1:136:A:LYS:HE2	1:136:A:LYS:HA	9	0.87
(2,1578)	1:102:A:THR:HG23	1:93:A:ILE:HA	9	0.87
(2,1524)	1:110:A:VAL:HA	1:89:A:LEU:HB2	7	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1509)	1:110:A:VAL:HA	1:114:A:ASP:HB2	2	0.87
(2,1507)	1:133:A:SER:HB3	1:61:A:ARG:HB3	1	0.87
(2,1446)	1:86:A:ILE:HG22	1:107:A:PRO:HG3	6	0.87
(2,1433)	1:77:A:ALA:HB3	1:76:A:MET:HG2	6	0.87
(2,1348)	1:62:A:LEU:HD22	1:115:A:MET:HG3	5	0.87
(2,1344)	1:106:A:LEU:HD21	1:62:A:LEU:HD21	3	0.87
(2,1311)	1:89:A:LEU:HD13	1:107:A:PRO:HG3	10	0.87
(2,1242)	1:120:A:HIS:HB2	1:122:A:ILE:HB	6	0.87
(2,1204)	1:59:A:MET:HG3	1:58:A:GLU:HA	4	0.87
(2,867)	1:87:A:GLU:H	1:86:A:ILE:HG13	9	0.87
(2,689)	1:108:A:LYS:HG3	1:108:A:LYS:HE3	10	0.87
(2,375)	1:64:A:VAL:HG13	1:122:A:ILE:HD11	4	0.87
(2,360)	1:122:A:ILE:HG22	1:127:A:GLY:HA2	1	0.87
(2,360)	1:122:A:ILE:HG23	1:127:A:GLY:HA2	9	0.87
(2,216)	1:96:A:LEU:HD11	1:103:A:MET:HA	3	0.87
(2,1866)	1:88:A:GLU:H	1:87:A:GLU:HB3	5	0.86
(2,1861)	1:77:A:ALA:H	1:78:A:LYS:HE3	10	0.86
(2,1736)	1:71:A:LYS:HE2	1:73:A:PHE:HD1	10	0.86
(2,1714)	1:106:A:LEU:HB2	1:91:A:GLY:HA2	8	0.86
(2,1608)	1:76:A:MET:HA	1:77:A:ALA:HB2	2	0.86
(2,1578)	1:102:A:THR:HG22	1:93:A:ILE:HA	7	0.86
(2,1506)	1:128:A:VAL:HB	1:70:A:SER:HB2	6	0.86
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG22	10	0.86
(2,1432)	1:124:A:ALA:HB3	1:123:A:LEU:HB3	1	0.86
(2,1258)	1:136:A:LYS:HD3	1:59:A:MET:HA	5	0.86
(2,1242)	1:120:A:HIS:HB2	1:122:A:ILE:HB	3	0.86
(2,1242)	1:120:A:HIS:HB2	1:122:A:ILE:HB	7	0.86
(2,1242)	1:120:A:HIS:HB2	1:122:A:ILE:HB	8	0.86
(2,1242)	1:120:A:HIS:HB2	1:123:A:LEU:HB3	10	0.86
(2,867)	1:87:A:GLU:H	1:86:A:ILE:HG13	4	0.86
(2,772)	1:62:A:LEU:H	1:103:A:MET:HG3	8	0.86
(2,360)	1:122:A:ILE:HG22	1:127:A:GLY:HA2	3	0.86
(2,258)	1:89:A:LEU:HD22	1:114:A:ASP:HB2	9	0.86
(2,216)	1:96:A:LEU:HD13	1:103:A:MET:HA	5	0.86
(2,216)	1:96:A:LEU:HD12	1:103:A:MET:HA	10	0.86
(2,44)	1:103:A:MET:HB2	1:96:A:LEU:HD23	7	0.86
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD13	8	0.85
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD11	10	0.85
(2,1714)	1:106:A:LEU:HB2	1:91:A:GLY:HA2	7	0.85
(2,1708)	1:91:A:GLY:HA3	1:60:A:THR:HB	6	0.85
(2,1657)	1:61:A:ARG:HG2	1:105:A:GLU:HA	9	0.85
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG13	10	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD22	1	0.85
(2,1432)	1:124:A:ALA:HB2	1:123:A:LEU:HB3	3	0.85
(2,1432)	1:124:A:ALA:HB2	1:123:A:LEU:HB3	8	0.85
(2,1386)	1:109:A:THR:HG21	1:58:A:GLU:HG2	4	0.85
(2,1379)	1:64:A:VAL:HG11	1:122:A:ILE:HG12	10	0.85
(2,1378)	1:64:A:VAL:HG13	1:129:A:VAL:HA	2	0.85
(2,1348)	1:62:A:LEU:HD22	1:115:A:MET:HG3	9	0.85
(2,1332)	1:119:A:LEU:HD12	1:119:A:LEU:HA	3	0.85
(2,1311)	1:89:A:LEU:HD11	1:107:A:PRO:HG3	5	0.85
(2,1298)	1:86:A:ILE:HG13	1:85:A:ARG:HA	2	0.85
(2,1242)	1:120:A:HIS:HB2	1:122:A:ILE:HB	1	0.85
(2,1242)	1:120:A:HIS:HB2	1:122:A:ILE:HB	9	0.85
(2,1071)	1:86:A:ILE:H	1:86:A:ILE:HG13	3	0.85
(2,946)	1:58:A:GLU:H	1:58:A:GLU:HB2	9	0.85
(2,943)	1:58:A:GLU:H	1:59:A:MET:H	10	0.85
(2,867)	1:87:A:GLU:H	1:86:A:ILE:HG13	8	0.85
(2,623)	1:59:A:MET:HA	1:107:A:PRO:HB2	4	0.85
(2,612)	1:77:A:ALA:HA	1:76:A:MET:HB2	2	0.85
(2,612)	1:77:A:ALA:HA	1:76:A:MET:HB2	3	0.85
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG12	7	0.85
(2,360)	1:122:A:ILE:HG22	1:127:A:GLY:HA2	8	0.85
(2,129)	1:120:A:HIS:HB2	1:117:A:GLN:HB2	2	0.85
(1,60)	1:119:A:LEU:H	1:114:A:ASP:HB2	8	0.85
(1,8)	1:107:A:PRO:HB2	1:90:A:GLY:HA2	3	0.85
(2,1714)	1:106:A:LEU:HB2	1:91:A:GLY:HA2	5	0.84
(2,1657)	1:61:A:ARG:HG2	1:105:A:GLU:HA	4	0.84
(2,1608)	1:117:A:GLN:HA	1:118:A:LEU:HD22	5	0.84
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD22	4	0.84
(2,1578)	1:102:A:THR:HG23	1:93:A:ILE:HA	4	0.84
(2,1578)	1:102:A:THR:HG22	1:93:A:ILE:HA	6	0.84
(2,1455)	1:93:A:ILE:HD13	1:78:A:LYS:HD3	2	0.84
(2,1432)	1:124:A:ALA:HB2	1:123:A:LEU:HB3	7	0.84
(2,1406)	1:135:A:VAL:HG11	1:107:A:PRO:HD3	6	0.84
(2,1379)	1:64:A:VAL:HG13	1:102:A:THR:HG21	8	0.84
(2,1332)	1:119:A:LEU:HD12	1:119:A:LEU:HA	2	0.84
(2,1311)	1:89:A:LEU:HD13	1:107:A:PRO:HG3	6	0.84
(2,1208)	1:66:A:GLU:HB3	1:74:A:SER:HA	10	0.84
(2,1071)	1:86:A:ILE:H	1:86:A:ILE:HG13	6	0.84
(2,1032)	1:84:A:THR:H	1:84:A:THR:HG21	8	0.84
(2,946)	1:58:A:GLU:H	1:58:A:GLU:HB2	1	0.84
(2,946)	1:58:A:GLU:H	1:58:A:GLU:HB2	7	0.84
(2,946)	1:58:A:GLU:H	1:58:A:GLU:HB2	10	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,911)	1:88:A:GLU:H	1:88:A:GLU:HG3	7	0.84
(2,867)	1:87:A:GLU:H	1:86:A:ILE:HG13	2	0.84
(2,623)	1:59:A:MET:HA	1:107:A:PRO:HB2	6	0.84
(2,586)	1:71:A:LYS:HA	1:66:A:GLU:HB2	3	0.84
(2,472)	1:82:A:PHE:HA	1:84:A:THR:HG22	3	0.84
(2,294)	1:64:A:VAL:HG12	1:102:A:THR:HG22	5	0.84
(2,33)	1:88:A:GLU:HG2	1:88:A:GLU:HA	7	0.84
(1,60)	1:119:A:LEU:H	1:114:A:ASP:HB2	7	0.84
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD12	5	0.83
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD11	8	0.83
(2,1867)	1:88:A:GLU:H	1:86:A:ILE:HB	10	0.83
(2,1805)	1:61:A:ARG:H	1:131:A:LEU:HD12	6	0.83
(2,1763)	1:82:A:PHE:HB2	1:85:A:ARG:HB3	6	0.83
(2,1657)	1:61:A:ARG:HG2	1:105:A:GLU:HA	6	0.83
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG13	9	0.83
(2,1599)	1:75:A:LYS:HG2	1:75:A:LYS:HA	5	0.83
(2,1506)	1:66:A:GLU:HB2	1:70:A:SER:HB2	1	0.83
(2,1432)	1:124:A:ALA:HB3	1:123:A:LEU:HB3	4	0.83
(2,1419)	1:64:A:VAL:HG21	1:122:A:ILE:HG13	6	0.83
(2,1401)	1:84:A:THR:HG21	1:89:A:LEU:HD22	8	0.83
(2,1379)	1:64:A:VAL:HG12	1:102:A:THR:HG22	2	0.83
(2,1348)	1:62:A:LEU:HD23	1:115:A:MET:HG3	8	0.83
(2,1332)	1:137:A:LEU:HD11	1:133:A:SER:HB3	9	0.83
(2,1071)	1:86:A:ILE:H	1:86:A:ILE:HG13	7	0.83
(2,1071)	1:86:A:ILE:H	1:86:A:ILE:HG13	8	0.83
(2,1071)	1:86:A:ILE:H	1:86:A:ILE:HG13	9	0.83
(2,946)	1:58:A:GLU:H	1:58:A:GLU:HB2	5	0.83
(2,946)	1:58:A:GLU:H	1:58:A:GLU:HB2	6	0.83
(2,446)	1:118:A:LEU:HD22	1:81:A:SER:HA	10	0.83
(2,282)	1:97:A:THR:HG23	1:78:A:LYS:HE2	5	0.83
(2,131)	1:136:A:LYS:HD3	1:58:A:GLU:HG3	5	0.83
(1,60)	1:119:A:LEU:H	1:114:A:ASP:HB2	5	0.83
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD13	3	0.82
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD12	1	0.82
(2,1846)	1:106:A:LEU:H	1:105:A:GLU:HG3	5	0.82
(2,1738)	1:75:A:LYS:HE3	1:95:A:PHE:HE2	1	0.82
(2,1714)	1:106:A:LEU:HB2	1:91:A:GLY:HA2	9	0.82
(2,1657)	1:61:A:ARG:HG2	1:105:A:GLU:HA	1	0.82
(2,1608)	1:76:A:MET:HA	1:77:A:ALA:HB2	3	0.82
(2,1599)	1:75:A:LYS:HG2	1:75:A:LYS:HA	7	0.82
(2,1578)	1:102:A:THR:HG21	1:93:A:ILE:HA	2	0.82
(2,1432)	1:124:A:ALA:HB3	1:123:A:LEU:HB3	9	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1379)	1:64:A:VAL:HG12	1:102:A:THR:HG21	4	0.82
(2,1358)	1:119:A:LEU:HD23	1:121:A:ASP:HB3	5	0.82
(2,1311)	1:89:A:LEU:HD11	1:107:A:PRO:HG3	1	0.82
(2,1304)	1:118:A:LEU:HD11	1:82:A:PHE:HE1	6	0.82
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB1	3	0.82
(2,1071)	1:86:A:ILE:H	1:86:A:ILE:HG13	1	0.82
(2,1071)	1:86:A:ILE:H	1:86:A:ILE:HG13	4	0.82
(2,689)	1:108:A:LYS:HG3	1:108:A:LYS:HE3	8	0.82
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG12	2	0.82
(2,375)	1:64:A:VAL:HG12	1:122:A:ILE:HD13	2	0.82
(2,375)	1:64:A:VAL:HG13	1:122:A:ILE:HD12	8	0.82
(2,375)	1:64:A:VAL:HG12	1:122:A:ILE:HD13	9	0.82
(2,296)	1:101:A:VAL:HG12	1:94:A:SER:HB2	10	0.82
(2,263)	1:65:A:THR:HG22	1:67:A:LYS:HE2	1	0.82
(2,133)	1:67:A:LYS:HD3	1:69:A:GLU:HB3	4	0.82
(1,24)	1:75:A:LYS:HG3	1:78:A:LYS:HE3	10	0.82
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD13	1	0.81
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD11	2	0.81
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD12	4	0.81
(2,1867)	1:88:A:GLU:H	1:86:A:ILE:HB	9	0.81
(2,1714)	1:106:A:LEU:HB2	1:91:A:GLY:HA2	6	0.81
(2,1657)	1:61:A:ARG:HG2	1:105:A:GLU:HA	5	0.81
(2,1509)	1:110:A:VAL:HA	1:114:A:ASP:HB2	10	0.81
(2,1444)	1:86:A:ILE:HG22	1:92:A:SER:HB3	9	0.81
(2,1406)	1:135:A:VAL:HG12	1:107:A:PRO:HD3	3	0.81
(2,1357)	1:96:A:LEU:HD22	1:61:A:ARG:HD3	6	0.81
(2,1348)	1:62:A:LEU:HD21	1:115:A:MET:HG3	3	0.81
(2,1348)	1:62:A:LEU:HD22	1:115:A:MET:HG3	4	0.81
(2,1348)	1:62:A:LEU:HD21	1:115:A:MET:HG3	10	0.81
(2,1332)	1:119:A:LEU:HD11	1:119:A:LEU:HA	5	0.81
(2,1311)	1:89:A:LEU:HD12	1:107:A:PRO:HG3	7	0.81
(2,1311)	1:89:A:LEU:HD13	1:107:A:PRO:HG3	9	0.81
(2,1298)	1:86:A:ILE:HG13	1:85:A:ARG:HA	10	0.81
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB2	10	0.81
(2,1212)	1:108:A:LYS:HB3	1:109:A:THR:HG22	1	0.81
(2,1190)	1:107:A:PRO:HB3	1:90:A:GLY:HA2	8	0.81
(2,1071)	1:86:A:ILE:H	1:86:A:ILE:HG13	5	0.81
(2,946)	1:58:A:GLU:H	1:58:A:GLU:HB2	2	0.81
(2,867)	1:87:A:GLU:H	1:86:A:ILE:HG13	1	0.81
(2,679)	1:89:A:LEU:HB3	1:114:A:ASP:HB2	9	0.81
(2,612)	1:77:A:ALA:HA	1:76:A:MET:HB2	5	0.81
(2,612)	1:77:A:ALA:HA	1:76:A:MET:HB2	6	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,612)	1:77:A:ALA:HA	1:76:A:MET:HB2	9	0.81
(2,375)	1:64:A:VAL:HG13	1:122:A:ILE:HD12	3	0.81
(2,329)	1:125:A:ALA:HB1	1:122:A:ILE:HG23	7	0.81
(2,216)	1:96:A:LEU:HD11	1:103:A:MET:HA	2	0.81
(2,88)	1:63:A:MET:HB2	1:132:A:ASP:HB2	6	0.81
(2,59)	1:105:A:GLU:HG3	1:59:A:MET:HG3	3	0.81
(1,60)	1:119:A:LEU:H	1:114:A:ASP:HB2	4	0.81
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG11	2	0.8
(2,1870)	1:121:A:ASP:H	1:122:A:ILE:HD13	7	0.8
(2,1861)	1:77:A:ALA:H	1:78:A:LYS:HE3	3	0.8
(2,1805)	1:61:A:ARG:H	1:131:A:LEU:HD11	1	0.8
(2,1714)	1:106:A:LEU:HB2	1:91:A:GLY:HA2	1	0.8
(2,1708)	1:91:A:GLY:HA3	1:60:A:THR:HB	4	0.8
(2,1657)	1:61:A:ARG:HG2	1:105:A:GLU:HA	8	0.8
(2,1624)	1:118:A:LEU:HA	1:114:A:ASP:HB2	2	0.8
(2,1478)	1:97:A:THR:HB	1:78:A:LYS:HE2	8	0.8
(2,1432)	1:124:A:ALA:HB1	1:123:A:LEU:HB3	5	0.8
(2,1431)	1:124:A:ALA:HB1	1:76:A:MET:HG3	2	0.8
(2,1425)	1:138:A:ALA:HB1	1:61:A:ARG:HG3	4	0.8
(2,1425)	1:138:A:ALA:HB2	1:61:A:ARG:HG3	10	0.8
(2,1386)	1:109:A:THR:HG22	1:58:A:GLU:HG2	6	0.8
(2,1380)	1:64:A:VAL:HG12	1:128:A:VAL:HG22	6	0.8
(2,1379)	1:64:A:VAL:HG11	1:102:A:THR:HG23	6	0.8
(2,1298)	1:86:A:ILE:HG13	1:85:A:ARG:HA	4	0.8
(2,1273)	1:122:A:ILE:HG12	1:125:A:ALA:HB1	5	0.8
(2,1032)	1:84:A:THR:H	1:84:A:THR:HG22	9	0.8
(2,943)	1:58:A:GLU:H	1:59:A:MET:H	2	0.8
(2,867)	1:87:A:GLU:H	1:86:A:ILE:HG13	7	0.8
(2,612)	1:77:A:ALA:HA	1:76:A:MET:HB2	8	0.8
(2,612)	1:77:A:ALA:HA	1:76:A:MET:HB2	10	0.8
(2,586)	1:71:A:LYS:HA	1:66:A:GLU:HB2	4	0.8
(2,360)	1:122:A:ILE:HG23	1:127:A:GLY:HA2	6	0.8
(2,331)	1:125:A:ALA:HB1	1:121:A:ASP:HB3	2	0.8
(2,294)	1:64:A:VAL:HG12	1:102:A:THR:HG21	9	0.8
(2,258)	1:89:A:LEU:HD21	1:114:A:ASP:HB2	8	0.8
(2,216)	1:96:A:LEU:HD12	1:103:A:MET:HA	4	0.8
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD13	4	0.79
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD12	9	0.79
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG12	1	0.79
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG12	8	0.79
(2,1657)	1:105:A:GLU:HA	1:106:A:LEU:HB3	2	0.79
(2,1657)	1:61:A:ARG:HG2	1:105:A:GLU:HA	10	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1624)	1:118:A:LEU:HA	1:114:A:ASP:HB2	10	0.79
(2,1446)	1:86:A:ILE:HG23	1:107:A:PRO:HG3	8	0.79
(2,1418)	1:64:A:VAL:HG22	1:127:A:GLY:HA2	7	0.79
(2,1412)	1:128:A:VAL:HG12	1:126:A:GLY:HA2	1	0.79
(2,1386)	1:84:A:THR:HG22	1:88:A:GLU:HB3	5	0.79
(2,1378)	1:64:A:VAL:HG11	1:129:A:VAL:HA	1	0.79
(2,1298)	1:86:A:ILE:HG13	1:85:A:ARG:HA	1	0.79
(2,1298)	1:86:A:ILE:HG13	1:85:A:ARG:HA	6	0.79
(2,1298)	1:86:A:ILE:HG13	1:85:A:ARG:HA	7	0.79
(2,1298)	1:86:A:ILE:HG13	1:85:A:ARG:HA	8	0.79
(2,1298)	1:86:A:ILE:HG13	1:85:A:ARG:HA	9	0.79
(2,1258)	1:136:A:LYS:HD3	1:59:A:MET:HA	1	0.79
(2,1071)	1:86:A:ILE:H	1:86:A:ILE:HG13	2	0.79
(2,946)	1:58:A:GLU:H	1:58:A:GLU:HB2	3	0.79
(2,612)	1:77:A:ALA:HA	1:76:A:MET:HB2	1	0.79
(2,612)	1:77:A:ALA:HA	1:76:A:MET:HB2	7	0.79
(2,446)	1:118:A:LEU:HD22	1:81:A:SER:HA	7	0.79
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG13	5	0.79
(2,294)	1:64:A:VAL:HG13	1:102:A:THR:HG23	1	0.79
(1,4)	1:58:A:GLU:HG2	1:91:A:GLY:HA3	4	0.79
(2,1904)	1:66:A:GLU:H	1:71:A:LYS:HD3	3	0.78
(2,1714)	1:106:A:LEU:HB2	1:91:A:GLY:HA2	3	0.78
(2,1657)	1:61:A:ARG:HG2	1:105:A:GLU:HA	3	0.78
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD21	7	0.78
(2,1524)	1:110:A:VAL:HA	1:89:A:LEU:HB2	9	0.78
(2,1471)	1:86:A:ILE:HD12	1:89:A:LEU:HB2	2	0.78
(2,1455)	1:93:A:ILE:HD12	1:78:A:LYS:HD3	8	0.78
(2,1450)	1:122:A:ILE:HG21	1:119:A:LEU:HA	2	0.78
(2,1298)	1:86:A:ILE:HG13	1:85:A:ARG:HA	3	0.78
(2,1258)	1:136:A:LYS:HD3	1:59:A:MET:HA	3	0.78
(2,1212)	1:108:A:LYS:HB3	1:109:A:THR:HG22	5	0.78
(2,867)	1:87:A:GLU:H	1:86:A:ILE:HG13	6	0.78
(2,623)	1:59:A:MET:HA	1:107:A:PRO:HB2	7	0.78
(2,623)	1:59:A:MET:HA	1:107:A:PRO:HB2	9	0.78
(2,296)	1:101:A:VAL:HG13	1:94:A:SER:HB2	2	0.78
(2,282)	1:97:A:THR:HG22	1:78:A:LYS:HE2	7	0.78
(2,258)	1:89:A:LEU:HD21	1:114:A:ASP:HB2	4	0.78
(2,216)	1:96:A:LEU:HD12	1:103:A:MET:HA	9	0.78
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD13	7	0.77
(2,1941)	1:127:A:GLY:H	1:128:A:VAL:HG12	9	0.77
(2,1833)	1:137:A:LEU:H	1:135:A:VAL:HB	8	0.77
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD22	2	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1578)	1:102:A:THR:HG23	1:93:A:ILE:HA	10	0.77
(2,1546)	1:95:A:PHE:HE2	1:102:A:THR:HA	1	0.77
(2,1546)	1:95:A:PHE:HE1	1:102:A:THR:HA	3	0.77
(2,1523)	1:110:A:VAL:HA	1:107:A:PRO:HG3	10	0.77
(2,1500)	1:133:A:SER:HB3	1:105:A:GLU:HG3	3	0.77
(2,1432)	1:124:A:ALA:HB2	1:123:A:LEU:HB3	6	0.77
(2,1431)	1:124:A:ALA:HB2	1:76:A:MET:HG3	1	0.77
(2,1420)	1:64:A:VAL:HG23	1:62:A:LEU:HG	1	0.77
(2,1406)	1:135:A:VAL:HG13	1:107:A:PRO:HD3	1	0.77
(2,1311)	1:89:A:LEU:HD11	1:107:A:PRO:HG3	2	0.77
(2,1311)	1:89:A:LEU:HD12	1:107:A:PRO:HG3	4	0.77
(2,1223)	1:115:A:MET:HB3	1:106:A:LEU:HD21	7	0.77
(2,1212)	1:108:A:LYS:HB3	1:109:A:THR:HG21	8	0.77
(2,772)	1:62:A:LEU:H	1:103:A:MET:HG3	6	0.77
(2,623)	1:59:A:MET:HA	1:107:A:PRO:HB2	5	0.77
(2,586)	1:71:A:LYS:HA	1:66:A:GLU:HB2	7	0.77
(2,360)	1:122:A:ILE:HG21	1:127:A:GLY:HA2	5	0.77
(2,294)	1:64:A:VAL:HG13	1:102:A:THR:HG23	3	0.77
(2,258)	1:89:A:LEU:HD22	1:114:A:ASP:HB2	3	0.77
(2,182)	1:137:A:LEU:HG	1:61:A:ARG:HD2	5	0.77
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG22	6	0.77
(1,4)	1:58:A:GLU:HG2	1:91:A:GLY:HA3	1	0.77
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD13	6	0.76
(2,1953)	1:126:A:GLY:H	1:123:A:LEU:HD12	10	0.76
(2,1910)	1:89:A:LEU:H	1:84:A:THR:HG22	5	0.76
(2,1763)	1:82:A:PHE:HB2	1:85:A:ARG:HB3	8	0.76
(2,1759)	1:82:A:PHE:HB3	1:85:A:ARG:HG3	8	0.76
(2,1705)	1:126:A:GLY:HA3	1:73:A:PHE:HA	9	0.76
(2,1705)	1:126:A:GLY:HA3	1:73:A:PHE:HA	10	0.76
(2,1653)	1:66:A:GLU:HA	1:74:A:SER:HA	3	0.76
(2,1621)	1:114:A:ASP:HA	1:110:A:VAL:HG13	2	0.76
(2,1617)	1:79:A:SER:HA	1:78:A:LYS:HB3	6	0.76
(2,1578)	1:102:A:THR:HG22	1:93:A:ILE:HA	3	0.76
(2,1546)	1:95:A:PHE:HE2	1:102:A:THR:HA	5	0.76
(2,1532)	1:87:A:GLU:HB3	1:83:A:SER:HA	4	0.76
(2,1470)	1:86:A:ILE:HD13	1:122:A:ILE:HG13	2	0.76
(2,1446)	1:86:A:ILE:HG22	1:107:A:PRO:HG3	1	0.76
(2,1424)	1:73:A:PHE:HB3	1:125:A:ALA:HB1	7	0.76
(2,1367)	1:65:A:THR:HG21	1:100:A:GLY:HA2	10	0.76
(2,1269)	1:78:A:LYS:HD2	1:75:A:LYS:HE2	6	0.76
(2,296)	1:101:A:VAL:HG13	1:94:A:SER:HB2	1	0.76
(2,65)	1:107:A:PRO:HB2	1:107:A:PRO:HD2	2	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,65)	1:107:A:PRO:HB2	1:107:A:PRO:HD2	3	0.76
(2,65)	1:107:A:PRO:HB2	1:107:A:PRO:HD2	7	0.76
(1,11)	1:66:A:GLU:HB3	1:101:A:VAL:HA	6	0.76
(2,1763)	1:82:A:PHE:HB2	1:85:A:ARG:HB3	1	0.75
(2,1705)	1:126:A:GLY:HA3	1:73:A:PHE:HA	2	0.75
(2,1705)	1:126:A:GLY:HA3	1:73:A:PHE:HA	3	0.75
(2,1589)	1:112:A:GLU:HA	1:106:A:LEU:HD23	6	0.75
(2,1546)	1:95:A:PHE:HE2	1:102:A:THR:HA	4	0.75
(2,1525)	1:86:A:ILE:HG21	1:110:A:VAL:HA	2	0.75
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD21	2	0.75
(2,1507)	1:133:A:SER:HB3	1:61:A:ARG:HB3	8	0.75
(2,1432)	1:124:A:ALA:HB3	1:123:A:LEU:HB3	10	0.75
(2,1388)	1:109:A:THR:HG21	1:108:A:LYS:HE3	3	0.75
(2,1374)	1:129:A:VAL:HG12	1:73:A:PHE:HE1	9	0.75
(2,1358)	1:119:A:LEU:HD23	1:121:A:ASP:HB3	7	0.75
(2,1298)	1:86:A:ILE:HG13	1:85:A:ARG:HA	5	0.75
(2,1231)	1:76:A:MET:HG2	1:82:A:PHE:HE1	5	0.75
(2,1223)	1:115:A:MET:HB3	1:106:A:LEU:HD22	5	0.75
(2,1212)	1:108:A:LYS:HB3	1:109:A:THR:HG21	3	0.75
(2,612)	1:77:A:ALA:HA	1:76:A:MET:HB2	4	0.75
(2,329)	1:125:A:ALA:HB1	1:122:A:ILE:HG23	4	0.75
(2,264)	1:65:A:THR:HG23	1:64:A:VAL:HG13	7	0.75
(2,258)	1:89:A:LEU:HD23	1:114:A:ASP:HB2	7	0.75
(2,216)	1:96:A:LEU:HD13	1:103:A:MET:HA	1	0.75
(2,65)	1:107:A:PRO:HB2	1:107:A:PRO:HD2	1	0.75
(2,65)	1:107:A:PRO:HB2	1:107:A:PRO:HD2	6	0.75
(2,65)	1:107:A:PRO:HB2	1:107:A:PRO:HD2	8	0.75
(2,65)	1:107:A:PRO:HB2	1:107:A:PRO:HD2	9	0.75
(2,65)	1:107:A:PRO:HB2	1:107:A:PRO:HD2	10	0.75
(2,1908)	1:84:A:THR:H	1:88:A:GLU:HG3	10	0.74
(2,1846)	1:106:A:LEU:H	1:105:A:GLU:HG3	8	0.74
(2,1649)	1:78:A:LYS:HG3	1:78:A:LYS:HA	4	0.74
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD23	5	0.74
(2,1465)	1:122:A:ILE:HD13	1:120:A:HIS:HA	3	0.74
(2,1465)	1:122:A:ILE:HD11	1:120:A:HIS:HA	9	0.74
(2,1419)	1:64:A:VAL:HG23	1:122:A:ILE:HG13	8	0.74
(2,1358)	1:137:A:LEU:HD21	1:136:A:LYS:HE2	4	0.74
(2,1358)	1:119:A:LEU:HD22	1:121:A:ASP:HB3	10	0.74
(2,1231)	1:76:A:MET:HG2	1:82:A:PHE:HE1	2	0.74
(2,1212)	1:108:A:LYS:HB3	1:109:A:THR:HG23	9	0.74
(2,867)	1:87:A:GLU:H	1:86:A:ILE:HG13	10	0.74
(2,472)	1:82:A:PHE:HA	1:84:A:THR:HG22	2	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG11	3	0.74
(2,329)	1:125:A:ALA:HB2	1:122:A:ILE:HG22	9	0.74
(2,296)	1:101:A:VAL:HG13	1:94:A:SER:HB2	4	0.74
(2,296)	1:101:A:VAL:HG11	1:94:A:SER:HB2	9	0.74
(2,294)	1:64:A:VAL:HG11	1:102:A:THR:HG21	10	0.74
(2,282)	1:97:A:THR:HG21	1:78:A:LYS:HE2	3	0.74
(2,240)	1:110:A:VAL:HG11	1:89:A:LEU:HB2	6	0.74
(2,216)	1:96:A:LEU:HD11	1:103:A:MET:HA	6	0.74
(2,65)	1:107:A:PRO:HB2	1:107:A:PRO:HD2	4	0.74
(2,65)	1:107:A:PRO:HB2	1:107:A:PRO:HD2	5	0.74
(2,1653)	1:66:A:GLU:HA	1:74:A:SER:HA	1	0.73
(2,1653)	1:66:A:GLU:HA	1:74:A:SER:HA	6	0.73
(2,1455)	1:93:A:ILE:HD11	1:78:A:LYS:HD3	6	0.73
(2,1431)	1:124:A:ALA:HB2	1:76:A:MET:HG3	4	0.73
(2,1431)	1:124:A:ALA:HB1	1:76:A:MET:HG3	7	0.73
(2,1431)	1:124:A:ALA:HB2	1:76:A:MET:HG3	9	0.73
(2,1357)	1:96:A:LEU:HD22	1:61:A:ARG:HD3	3	0.73
(2,1223)	1:115:A:MET:HB3	1:106:A:LEU:HD23	6	0.73
(2,1212)	1:108:A:LYS:HB3	1:109:A:THR:HG21	7	0.73
(2,1071)	1:86:A:ILE:H	1:86:A:ILE:HG13	10	0.73
(2,446)	1:118:A:LEU:HD23	1:81:A:SER:HA	4	0.73
(2,329)	1:125:A:ALA:HB3	1:122:A:ILE:HG22	2	0.73
(2,294)	1:64:A:VAL:HG11	1:102:A:THR:HG23	7	0.73
(2,282)	1:97:A:THR:HG21	1:78:A:LYS:HE2	10	0.73
(2,86)	1:63:A:MET:HB2	1:132:A:ASP:HB3	3	0.73
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG12	3	0.73
(1,45)	1:125:A:ALA:HA	1:127:A:GLY:HA2	7	0.73
(1,24)	1:75:A:LYS:HG3	1:78:A:LYS:HE3	3	0.73
(1,4)	1:58:A:GLU:HG2	1:91:A:GLY:HA3	6	0.73
(2,1846)	1:106:A:LEU:H	1:105:A:GLU:HG3	4	0.72
(2,1833)	1:137:A:LEU:H	1:105:A:GLU:HG3	3	0.72
(2,1714)	1:106:A:LEU:HB2	1:91:A:GLY:HA2	4	0.72
(2,1607)	1:76:A:MET:HA	1:75:A:LYS:HG2	5	0.72
(2,1546)	1:95:A:PHE:HE2	1:102:A:THR:HA	10	0.72
(2,1523)	1:110:A:VAL:HA	1:107:A:PRO:HG3	5	0.72
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD21	3	0.72
(2,1465)	1:122:A:ILE:HD11	1:120:A:HIS:HA	5	0.72
(2,1431)	1:124:A:ALA:HB3	1:76:A:MET:HG3	5	0.72
(2,1332)	1:119:A:LEU:HD11	1:119:A:LEU:HA	7	0.72
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD21	4	0.72
(2,1032)	1:84:A:THR:H	1:84:A:THR:HG23	1	0.72
(2,1032)	1:84:A:THR:H	1:84:A:THR:HG22	7	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,329)	1:125:A:ALA:HB3	1:122:A:ILE:HG22	6	0.72
(1,6)	1:101:A:VAL:HB	1:103:A:MET:HG2	5	0.72
(1,4)	1:58:A:GLU:HG2	1:91:A:GLY:HA3	5	0.72
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG13	6	0.71
(2,1866)	1:88:A:GLU:H	1:88:A:GLU:HB3	7	0.71
(2,1738)	1:71:A:LYS:HE2	1:95:A:PHE:HE2	9	0.71
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB2	4	0.71
(2,1544)	1:74:A:SER:HB3	1:71:A:LYS:HG2	3	0.71
(2,1523)	1:110:A:VAL:HA	1:107:A:PRO:HG3	2	0.71
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD22	1	0.71
(2,1478)	1:98:A:GLU:HG3	1:97:A:THR:HB	10	0.71
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG23	7	0.71
(2,1431)	1:124:A:ALA:HB1	1:76:A:MET:HG3	8	0.71
(2,1424)	1:73:A:PHE:HB3	1:125:A:ALA:HB2	9	0.71
(2,1417)	1:64:A:VAL:HG22	1:62:A:LEU:HA	5	0.71
(2,1367)	1:65:A:THR:HG23	1:100:A:GLY:HA2	2	0.71
(2,1344)	1:123:A:LEU:HD21	1:129:A:VAL:HG21	9	0.71
(2,867)	1:87:A:GLU:H	1:86:A:ILE:HG13	5	0.71
(2,586)	1:71:A:LYS:HA	1:66:A:GLU:HB2	8	0.71
(2,375)	1:64:A:VAL:HG13	1:122:A:ILE:HD11	1	0.71
(2,88)	1:63:A:MET:HB2	1:132:A:ASP:HB2	1	0.71
(2,59)	1:105:A:GLU:HG3	1:59:A:MET:HG3	10	0.71
(1,4)	1:58:A:GLU:HG2	1:91:A:GLY:HA3	7	0.71
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG13	4	0.7
(2,1705)	1:126:A:GLY:HA3	1:73:A:PHE:HA	1	0.7
(2,1462)	1:122:A:ILE:HD12	1:118:A:LEU:HB3	2	0.7
(2,1462)	1:122:A:ILE:HD11	1:118:A:LEU:HB3	6	0.7
(2,1325)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	3	0.7
(2,1190)	1:59:A:MET:HG2	1:133:A:SER:HB2	4	0.7
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG23	2	0.7
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG12	10	0.7
(2,375)	1:64:A:VAL:HG11	1:122:A:ILE:HD12	7	0.7
(2,360)	1:122:A:ILE:HG23	1:127:A:GLY:HA2	2	0.7
(2,331)	1:125:A:ALA:HB1	1:121:A:ASP:HB3	6	0.7
(2,296)	1:101:A:VAL:HG12	1:94:A:SER:HB2	7	0.7
(2,282)	1:97:A:THR:HG23	1:78:A:LYS:HE2	6	0.7
(2,258)	1:89:A:LEU:HD22	1:114:A:ASP:HB2	1	0.7
(2,59)	1:105:A:GLU:HG3	1:59:A:MET:HG3	1	0.7
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG13	3	0.7
(1,8)	1:107:A:PRO:HB2	1:90:A:GLY:HA2	9	0.7
(2,1805)	1:61:A:ARG:H	1:131:A:LEU:HD12	10	0.69
(2,1653)	1:66:A:GLU:HA	1:74:A:SER:HA	4	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1617)	1:79:A:SER:HA	1:78:A:LYS:HB3	10	0.69
(2,1607)	1:76:A:MET:HA	1:75:A:LYS:HG2	7	0.69
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD23	10	0.69
(2,1478)	1:98:A:GLU:HG3	1:97:A:THR:HB	6	0.69
(2,1475)	1:102:A:THR:HB	1:64:A:VAL:HA	8	0.69
(2,1471)	1:86:A:ILE:HD11	1:89:A:LEU:HB2	10	0.69
(2,1465)	1:122:A:ILE:HD13	1:120:A:HIS:HA	6	0.69
(2,1450)	1:122:A:ILE:HG23	1:119:A:LEU:HA	8	0.69
(2,1431)	1:124:A:ALA:HB1	1:76:A:MET:HG3	3	0.69
(2,1424)	1:73:A:PHE:HB3	1:125:A:ALA:HB1	4	0.69
(2,1420)	1:64:A:VAL:HG21	1:62:A:LEU:HG	4	0.69
(2,1412)	1:128:A:VAL:HG12	1:126:A:GLY:HA2	9	0.69
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG23	4	0.69
(2,1388)	1:84:A:THR:HG22	1:85:A:ARG:HD2	6	0.69
(2,1348)	1:62:A:LEU:HD23	1:115:A:MET:HG3	2	0.69
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD21	1	0.69
(2,1208)	1:66:A:GLU:HB3	1:74:A:SER:HA	5	0.69
(2,586)	1:71:A:LYS:HA	1:66:A:GLU:HB2	9	0.69
(2,580)	1:134:A:GLU:HA	1:62:A:LEU:HD22	3	0.69
(2,329)	1:125:A:ALA:HB2	1:122:A:ILE:HG21	1	0.69
(2,294)	1:64:A:VAL:HG13	1:102:A:THR:HG21	8	0.69
(2,240)	1:110:A:VAL:HG12	1:89:A:LEU:HB2	7	0.69
(2,37)	1:66:A:GLU:HG3	1:73:A:PHE:HB3	10	0.69
(1,45)	1:125:A:ALA:HA	1:127:A:GLY:HA2	2	0.69
(1,45)	1:125:A:ALA:HA	1:127:A:GLY:HA2	5	0.69
(1,11)	1:66:A:GLU:HB3	1:101:A:VAL:HA	8	0.69
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG11	7	0.68
(2,1846)	1:106:A:LEU:H	1:105:A:GLU:HG3	1	0.68
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG22	2	0.68
(2,1439)	1:104:A:ILE:HG22	1:105:A:GLU:HG2	3	0.68
(2,1419)	1:64:A:VAL:HG21	1:122:A:ILE:HG13	5	0.68
(2,1418)	1:64:A:VAL:HG22	1:127:A:GLY:HA2	8	0.68
(2,1401)	1:84:A:THR:HG22	1:89:A:LEU:HD23	9	0.68
(2,1393)	1:110:A:VAL:HG23	1:119:A:LEU:HG	2	0.68
(2,1378)	1:64:A:VAL:HG11	1:129:A:VAL:HA	8	0.68
(2,1269)	1:78:A:LYS:HD2	1:75:A:LYS:HE2	5	0.68
(2,1223)	1:103:A:MET:HG2	1:101:A:VAL:HG13	8	0.68
(2,1212)	1:128:A:VAL:HB	1:65:A:THR:HG21	6	0.68
(2,1174)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	5	0.68
(2,649)	1:70:A:SER:HB2	1:126:A:GLY:HA3	10	0.68
(2,294)	1:64:A:VAL:HG12	1:102:A:THR:HG22	2	0.68
(2,258)	1:89:A:LEU:HD23	1:114:A:ASP:HB2	5	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,258)	1:89:A:LEU:HD21	1:114:A:ASP:HB2	6	0.68
(2,240)	1:110:A:VAL:HG13	1:89:A:LEU:HB2	2	0.68
(1,23)	1:93:A:ILE:HG12	1:78:A:LYS:HG2	9	0.68
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG11	3	0.67
(2,1908)	1:84:A:THR:H	1:88:A:GLU:HG3	4	0.67
(2,1846)	1:106:A:LEU:H	1:105:A:GLU:HG3	7	0.67
(2,1810)	1:136:A:LYS:H	1:136:A:LYS:HD3	4	0.67
(2,1786)	1:104:A:ILE:H	1:104:A:ILE:HG23	7	0.67
(2,1770)	1:116:A:ASP:HB2	1:112:A:GLU:HB3	5	0.67
(2,1763)	1:82:A:PHE:HB2	1:85:A:ARG:HB3	3	0.67
(2,1705)	1:126:A:GLY:HA3	1:73:A:PHE:HA	7	0.67
(2,1661)	1:134:A:GLU:HB3	1:131:A:LEU:HA	5	0.67
(2,1525)	1:86:A:ILE:HG21	1:110:A:VAL:HA	10	0.67
(2,1516)	1:107:A:PRO:HA	1:59:A:MET:HB3	9	0.67
(2,1462)	1:122:A:ILE:HD11	1:118:A:LEU:HB3	8	0.67
(2,1431)	1:124:A:ALA:HB2	1:76:A:MET:HG3	10	0.67
(2,1425)	1:138:A:ALA:HB3	1:61:A:ARG:HG3	5	0.67
(2,1420)	1:64:A:VAL:HG22	1:62:A:LEU:HG	6	0.67
(2,1412)	1:128:A:VAL:HG12	1:130:A:GLY:HA2	6	0.67
(2,1393)	1:60:A:THR:HG23	1:62:A:LEU:HB3	4	0.67
(2,1386)	1:109:A:THR:HG23	1:58:A:GLU:HG2	8	0.67
(2,1364)	1:119:A:LEU:HD22	1:104:A:ILE:HG12	1	0.67
(2,1238)	1:134:A:GLU:HB3	1:131:A:LEU:HA	5	0.67
(2,1224)	1:115:A:MET:HB3	1:111:A:SER:HB2	10	0.67
(2,812)	1:137:A:LEU:H	1:60:A:THR:HG21	3	0.67
(2,436)	1:93:A:ILE:HG23	1:82:A:PHE:HD2	1	0.67
(2,436)	1:93:A:ILE:HG21	1:82:A:PHE:HD2	5	0.67
(2,296)	1:101:A:VAL:HG12	1:94:A:SER:HB2	3	0.67
(2,294)	1:64:A:VAL:HG12	1:102:A:THR:HG21	4	0.67
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG12	4	0.67
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG21	4	0.67
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG12	9	0.67
(1,60)	1:119:A:LEU:H	1:114:A:ASP:HB2	9	0.67
(1,45)	1:125:A:ALA:HA	1:127:A:GLY:HA2	8	0.67
(1,11)	1:66:A:GLU:HB3	1:101:A:VAL:HA	5	0.67
(1,8)	1:107:A:PRO:HB2	1:90:A:GLY:HA2	2	0.67
(2,1763)	1:82:A:PHE:HB2	1:85:A:ARG:HB3	7	0.66
(2,1743)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	10	0.66
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG23	4	0.66
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG23	10	0.66
(2,1546)	1:95:A:PHE:HE1	1:102:A:THR:HA	7	0.66
(2,1526)	1:95:A:PHE:HD1	1:94:A:SER:HA	4	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1475)	1:102:A:THR:HB	1:64:A:VAL:HA	1	0.66
(2,1470)	1:86:A:ILE:HD13	1:122:A:ILE:HG13	10	0.66
(2,1465)	1:122:A:ILE:HD11	1:120:A:HIS:HA	10	0.66
(2,1456)	1:104:A:ILE:HD11	1:93:A:ILE:HA	1	0.66
(2,1450)	1:122:A:ILE:HG23	1:119:A:LEU:HA	10	0.66
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG22	9	0.66
(2,1417)	1:64:A:VAL:HG22	1:102:A:THR:HA	6	0.66
(2,1388)	1:84:A:THR:HG23	1:85:A:ARG:HD2	5	0.66
(2,1212)	1:108:A:LYS:HB3	1:109:A:THR:HG23	2	0.66
(2,1208)	1:66:A:GLU:HB3	1:74:A:SER:HA	6	0.66
(2,1208)	1:66:A:GLU:HB3	1:74:A:SER:HA	8	0.66
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG21	4	0.66
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG22	9	0.66
(2,726)	1:111:A:SER:HB2	1:113:A:HIS:HB3	2	0.66
(2,523)	1:87:A:GLU:HG3	1:87:A:GLU:HA	9	0.66
(2,329)	1:125:A:ALA:HB1	1:122:A:ILE:HG23	5	0.66
(2,288)	1:110:A:VAL:HG21	1:113:A:HIS:HB2	3	0.66
(2,282)	1:97:A:THR:HG21	1:78:A:LYS:HE2	1	0.66
(2,265)	1:110:A:VAL:HG23	1:114:A:ASP:HB2	2	0.66
(2,240)	1:110:A:VAL:HG11	1:89:A:LEU:HB2	4	0.66
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG13	5	0.66
(1,45)	1:125:A:ALA:HA	1:127:A:GLY:HA2	9	0.66
(1,4)	1:58:A:GLU:HG2	1:91:A:GLY:HA3	8	0.66
(1,4)	1:58:A:GLU:HG2	1:91:A:GLY:HA3	9	0.66
(2,1846)	1:106:A:LEU:H	1:105:A:GLU:HG3	6	0.65
(2,1846)	1:106:A:LEU:H	1:105:A:GLU:HG3	9	0.65
(2,1653)	1:66:A:GLU:HA	1:74:A:SER:HA	2	0.65
(2,1627)	1:95:A:PHE:HA	1:101:A:VAL:HB	7	0.65
(2,1617)	1:79:A:SER:HA	1:78:A:LYS:HB3	4	0.65
(2,1572)	1:82:A:PHE:HE2	1:77:A:ALA:HA	6	0.65
(2,1546)	1:95:A:PHE:HE1	1:102:A:THR:HA	6	0.65
(2,1525)	1:86:A:ILE:HG22	1:110:A:VAL:HA	1	0.65
(2,1524)	1:136:A:LYS:HD2	1:135:A:VAL:HA	5	0.65
(2,1523)	1:135:A:VAL:HA	1:58:A:GLU:HG2	6	0.65
(2,1475)	1:102:A:THR:HB	1:95:A:PHE:HA	5	0.65
(2,1456)	1:104:A:ILE:HD12	1:93:A:ILE:HA	9	0.65
(2,1424)	1:73:A:PHE:HB3	1:125:A:ALA:HB1	10	0.65
(2,1420)	1:64:A:VAL:HG22	1:62:A:LEU:HG	2	0.65
(2,1418)	1:64:A:VAL:HG21	1:127:A:GLY:HA2	1	0.65
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG22	6	0.65
(2,1341)	1:136:A:LYS:HG2	1:58:A:GLU:HG2	2	0.65
(2,1222)	1:76:A:MET:HG3	1:77:A:ALA:HB3	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,943)	1:58:A:GLU:H	1:59:A:MET:H	3	0.65
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD12	4	0.65
(2,436)	1:93:A:ILE:HG22	1:82:A:PHE:HD2	6	0.65
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG11	4	0.65
(2,387)	1:86:A:ILE:HD13	1:85:A:ARG:HD2	5	0.65
(2,387)	1:86:A:ILE:HD11	1:85:A:ARG:HD2	9	0.65
(2,294)	1:64:A:VAL:HG11	1:102:A:THR:HG23	6	0.65
(2,223)	1:131:A:LEU:HD13	1:131:A:LEU:HA	2	0.65
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG13	1	0.65
(2,51)	1:103:A:MET:HB2	1:61:A:ARG:HG2	7	0.65
(1,45)	1:125:A:ALA:HA	1:127:A:GLY:HA2	1	0.65
(1,45)	1:125:A:ALA:HA	1:127:A:GLY:HA2	3	0.65
(1,45)	1:125:A:ALA:HA	1:127:A:GLY:HA2	10	0.65
(1,11)	1:66:A:GLU:HB3	1:101:A:VAL:HA	4	0.65
(1,8)	1:107:A:PRO:HB2	1:90:A:GLY:HA2	7	0.65
(2,1860)	1:77:A:ALA:H	1:76:A:MET:HG2	3	0.64
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD12	4	0.64
(2,1759)	1:82:A:PHE:HB3	1:85:A:ARG:HG3	3	0.64
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB2	7	0.64
(2,1617)	1:79:A:SER:HA	1:78:A:LYS:HB3	5	0.64
(2,1526)	1:95:A:PHE:HD1	1:94:A:SER:HA	10	0.64
(2,1516)	1:107:A:PRO:HA	1:59:A:MET:HB3	3	0.64
(2,1478)	1:98:A:GLU:HG3	1:97:A:THR:HB	7	0.64
(2,1475)	1:102:A:THR:HB	1:95:A:PHE:HA	3	0.64
(2,1460)	1:104:A:ILE:HD13	1:102:A:THR:HB	8	0.64
(2,1450)	1:122:A:ILE:HG22	1:119:A:LEU:HA	4	0.64
(2,1450)	1:122:A:ILE:HG21	1:119:A:LEU:HA	6	0.64
(2,1419)	1:64:A:VAL:HG21	1:122:A:ILE:HG13	2	0.64
(2,1419)	1:64:A:VAL:HG22	1:122:A:ILE:HG13	3	0.64
(2,1417)	1:64:A:VAL:HG21	1:102:A:THR:HA	4	0.64
(2,1393)	1:60:A:THR:HG23	1:62:A:LEU:HB3	5	0.64
(2,1388)	1:84:A:THR:HG21	1:85:A:ARG:HD2	4	0.64
(2,1212)	1:108:A:LYS:HB3	1:109:A:THR:HG21	10	0.64
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG22	3	0.64
(2,679)	1:89:A:LEU:HB3	1:114:A:ASP:HB2	2	0.64
(2,494)	1:65:A:THR:HG22	1:99:A:THR:HA	6	0.64
(2,459)	1:77:A:ALA:HB3	1:74:A:SER:HB3	4	0.64
(2,288)	1:110:A:VAL:HG21	1:113:A:HIS:HB2	1	0.64
(2,288)	1:110:A:VAL:HG22	1:113:A:HIS:HB2	6	0.64
(2,282)	1:97:A:THR:HG23	1:78:A:LYS:HE2	8	0.64
(1,24)	1:75:A:LYS:HG3	1:78:A:LYS:HE3	2	0.64
(1,6)	1:101:A:VAL:HB	1:103:A:MET:HG2	6	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG11	1	0.63
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG13	8	0.63
(2,1763)	1:82:A:PHE:HB2	1:85:A:ARG:HB3	4	0.63
(2,1752)	1:78:A:LYS:HE2	1:75:A:LYS:HA	2	0.63
(2,1675)	1:101:A:VAL:HG13	1:103:A:MET:HA	1	0.63
(2,1526)	1:95:A:PHE:HD1	1:94:A:SER:HA	3	0.63
(2,1526)	1:95:A:PHE:HD1	1:94:A:SER:HA	7	0.63
(2,1526)	1:95:A:PHE:HD1	1:94:A:SER:HA	9	0.63
(2,1525)	1:86:A:ILE:HG22	1:110:A:VAL:HA	4	0.63
(2,1525)	1:86:A:ILE:HG22	1:110:A:VAL:HA	6	0.63
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD21	6	0.63
(2,1475)	1:102:A:THR:HB	1:64:A:VAL:HA	2	0.63
(2,1462)	1:122:A:ILE:HD11	1:118:A:LEU:HB3	3	0.63
(2,1462)	1:122:A:ILE:HD13	1:118:A:LEU:HB3	4	0.63
(2,1450)	1:122:A:ILE:HG22	1:119:A:LEU:HA	5	0.63
(2,1420)	1:64:A:VAL:HG21	1:62:A:LEU:HG	7	0.63
(2,1404)	1:102:A:THR:HG21	1:77:A:ALA:HA	8	0.63
(2,1393)	1:60:A:THR:HG21	1:62:A:LEU:HB3	10	0.63
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG22	6	0.63
(2,679)	1:89:A:LEU:HB3	1:114:A:ASP:HB2	10	0.63
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD12	7	0.63
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD12	10	0.63
(2,436)	1:93:A:ILE:HG22	1:82:A:PHE:HD2	7	0.63
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG11	8	0.63
(2,387)	1:86:A:ILE:HD12	1:85:A:ARG:HD2	3	0.63
(2,387)	1:86:A:ILE:HD12	1:85:A:ARG:HD2	4	0.63
(2,387)	1:86:A:ILE:HD13	1:85:A:ARG:HD2	6	0.63
(2,353)	1:86:A:ILE:HG23	1:104:A:ILE:HG23	2	0.63
(2,286)	1:88:A:GLU:HG3	1:84:A:THR:HG21	7	0.63
(2,200)	1:118:A:LEU:HD13	1:86:A:ILE:HA	8	0.63
(1,11)	1:66:A:GLU:HB3	1:101:A:VAL:HA	7	0.63
(1,8)	1:107:A:PRO:HB2	1:90:A:GLY:HA2	10	0.63
(2,1862)	1:121:A:ASP:H	1:116:A:ASP:HA	2	0.62
(2,1759)	1:82:A:PHE:HB3	1:85:A:ARG:HG3	5	0.62
(2,1635)	1:114:A:ASP:HA	1:115:A:MET:HA	4	0.62
(2,1626)	1:118:A:LEU:HA	1:85:A:ARG:HG2	3	0.62
(2,1617)	1:79:A:SER:HA	1:78:A:LYS:HB3	3	0.62
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG22	3	0.62
(2,1526)	1:95:A:PHE:HD1	1:94:A:SER:HA	1	0.62
(2,1526)	1:95:A:PHE:HD1	1:94:A:SER:HA	2	0.62
(2,1526)	1:95:A:PHE:HD1	1:94:A:SER:HA	5	0.62
(2,1526)	1:95:A:PHE:HD1	1:94:A:SER:HA	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB1	8	0.62
(2,1450)	1:122:A:ILE:HG23	1:119:A:LEU:HA	3	0.62
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG23	3	0.62
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG21	3	0.62
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG13	5	0.62
(2,1344)	1:123:A:LEU:HD21	1:129:A:VAL:HG22	5	0.62
(2,1257)	1:75:A:LYS:HD3	1:78:A:LYS:HE2	8	0.62
(2,1208)	1:66:A:GLU:HB3	1:74:A:SER:HA	3	0.62
(2,1208)	1:66:A:GLU:HB3	1:74:A:SER:HA	9	0.62
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD13	9	0.62
(2,459)	1:77:A:ALA:HB2	1:74:A:SER:HB3	9	0.62
(2,436)	1:93:A:ILE:HG21	1:82:A:PHE:HD2	2	0.62
(2,436)	1:93:A:ILE:HG22	1:82:A:PHE:HD2	4	0.62
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG13	9	0.62
(2,387)	1:86:A:ILE:HD12	1:85:A:ARG:HD2	1	0.62
(2,387)	1:86:A:ILE:HD12	1:85:A:ARG:HD2	8	0.62
(2,296)	1:101:A:VAL:HG12	1:94:A:SER:HB2	6	0.62
(2,275)	1:64:A:VAL:HG12	1:102:A:THR:HB	1	0.62
(1,45)	1:125:A:ALA:HA	1:127:A:GLY:HA2	4	0.62
(1,8)	1:107:A:PRO:HB2	1:90:A:GLY:HA2	5	0.62
(2,1862)	1:121:A:ASP:H	1:116:A:ASP:HA	6	0.61
(2,1846)	1:106:A:LEU:H	1:105:A:GLU:HG3	10	0.61
(2,1683)	1:131:A:LEU:HD12	1:62:A:LEU:HA	5	0.61
(2,1651)	1:104:A:ILE:HG23	1:61:A:ARG:HA	7	0.61
(2,1635)	1:114:A:ASP:HA	1:115:A:MET:HA	6	0.61
(2,1635)	1:114:A:ASP:HA	1:115:A:MET:HA	7	0.61
(2,1626)	1:118:A:LEU:HA	1:85:A:ARG:HG2	4	0.61
(2,1532)	1:87:A:GLU:HB3	1:83:A:SER:HA	6	0.61
(2,1478)	1:98:A:GLU:HG3	1:97:A:THR:HB	1	0.61
(2,1478)	1:98:A:GLU:HG3	1:97:A:THR:HB	3	0.61
(2,1465)	1:122:A:ILE:HD12	1:120:A:HIS:HA	1	0.61
(2,1465)	1:122:A:ILE:HD13	1:120:A:HIS:HA	7	0.61
(2,1462)	1:122:A:ILE:HD12	1:118:A:LEU:HB3	9	0.61
(2,1424)	1:73:A:PHE:HB3	1:125:A:ALA:HB2	8	0.61
(2,1419)	1:64:A:VAL:HG23	1:122:A:ILE:HG13	4	0.61
(2,1364)	1:119:A:LEU:HD23	1:104:A:ILE:HG12	10	0.61
(2,587)	1:71:A:LYS:HD3	1:71:A:LYS:HA	3	0.61
(2,387)	1:86:A:ILE:HD13	1:85:A:ARG:HD2	7	0.61
(2,288)	1:110:A:VAL:HG23	1:113:A:HIS:HB2	7	0.61
(2,265)	1:110:A:VAL:HG22	1:114:A:ASP:HB2	10	0.61
(2,257)	1:89:A:LEU:HD21	1:114:A:ASP:HB3	10	0.61
(2,223)	1:131:A:LEU:HD12	1:131:A:LEU:HA	4	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,200)	1:118:A:LEU:HD13	1:86:A:ILE:HA	1	0.61
(2,200)	1:118:A:LEU:HD11	1:86:A:ILE:HA	6	0.61
(2,200)	1:118:A:LEU:HD11	1:86:A:ILE:HA	7	0.61
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG12	2	0.61
(1,24)	1:75:A:LYS:HG3	1:78:A:LYS:HE3	1	0.61
(2,1860)	1:77:A:ALA:H	1:76:A:MET:HG2	10	0.6
(2,1759)	1:82:A:PHE:HB3	1:85:A:ARG:HG3	9	0.6
(2,1705)	1:126:A:GLY:HA3	1:73:A:PHE:HA	8	0.6
(2,1675)	1:101:A:VAL:HG13	1:103:A:MET:HA	4	0.6
(2,1667)	1:123:A:LEU:HD23	1:124:A:ALA:HA	3	0.6
(2,1667)	1:123:A:LEU:HD22	1:124:A:ALA:HA	7	0.6
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB3	6	0.6
(2,1635)	1:114:A:ASP:HA	1:115:A:MET:HA	1	0.6
(2,1635)	1:114:A:ASP:HA	1:115:A:MET:HA	8	0.6
(2,1607)	1:76:A:MET:HA	1:75:A:LYS:HG2	6	0.6
(2,1525)	1:86:A:ILE:HG23	1:110:A:VAL:HA	8	0.6
(2,1523)	1:135:A:VAL:HA	1:58:A:GLU:HG2	7	0.6
(2,1475)	1:102:A:THR:HB	1:64:A:VAL:HA	4	0.6
(2,1465)	1:122:A:ILE:HD12	1:120:A:HIS:HA	4	0.6
(2,1462)	1:122:A:ILE:HD13	1:118:A:LEU:HB3	1	0.6
(2,1462)	1:122:A:ILE:HD12	1:118:A:LEU:HB3	10	0.6
(2,1450)	1:122:A:ILE:HG23	1:119:A:LEU:HA	1	0.6
(2,1450)	1:122:A:ILE:HG21	1:119:A:LEU:HA	9	0.6
(2,1420)	1:64:A:VAL:HG22	1:62:A:LEU:HG	5	0.6
(2,1420)	1:64:A:VAL:HG21	1:62:A:LEU:HG	8	0.6
(2,1417)	1:64:A:VAL:HG22	1:62:A:LEU:HA	9	0.6
(2,1396)	1:101:A:VAL:HG23	1:65:A:THR:HA	6	0.6
(2,1393)	1:60:A:THR:HG22	1:62:A:LEU:HB3	3	0.6
(2,1381)	1:64:A:VAL:HG12	1:125:A:ALA:HB3	2	0.6
(2,1367)	1:65:A:THR:HG21	1:100:A:GLY:HA2	7	0.6
(2,1176)	1:66:A:GLU:HG3	1:128:A:VAL:HG21	8	0.6
(2,1042)	1:89:A:LEU:H	1:88:A:GLU:HB3	5	0.6
(2,587)	1:71:A:LYS:HD3	1:71:A:LYS:HA	6	0.6
(2,560)	1:70:A:SER:HB2	1:70:A:SER:HA	1	0.6
(2,560)	1:70:A:SER:HB2	1:70:A:SER:HA	2	0.6
(2,560)	1:70:A:SER:HB2	1:70:A:SER:HA	3	0.6
(2,560)	1:70:A:SER:HB2	1:70:A:SER:HA	4	0.6
(2,560)	1:70:A:SER:HB2	1:70:A:SER:HA	5	0.6
(2,560)	1:70:A:SER:HB2	1:70:A:SER:HA	8	0.6
(2,560)	1:70:A:SER:HB2	1:70:A:SER:HA	10	0.6
(2,296)	1:101:A:VAL:HG13	1:94:A:SER:HB2	8	0.6
(2,241)	1:106:A:LEU:HD23	1:110:A:VAL:HG11	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,200)	1:118:A:LEU:HD11	1:86:A:ILE:HA	3	0.6
(2,200)	1:118:A:LEU:HD13	1:86:A:ILE:HA	4	0.6
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG13	7	0.6
(2,1915)	1:79:A:SER:H	1:78:A:LYS:HG3	6	0.59
(2,1862)	1:121:A:ASP:H	1:116:A:ASP:HA	3	0.59
(2,1763)	1:82:A:PHE:HB2	1:85:A:ARG:HB3	5	0.59
(2,1726)	1:127:A:GLY:HA2	1:128:A:VAL:HB	5	0.59
(2,1667)	1:123:A:LEU:HD23	1:124:A:ALA:HA	4	0.59
(2,1667)	1:123:A:LEU:HD22	1:124:A:ALA:HA	9	0.59
(2,1667)	1:123:A:LEU:HD23	1:124:A:ALA:HA	10	0.59
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB3	3	0.59
(2,1635)	1:114:A:ASP:HA	1:115:A:MET:HA	9	0.59
(2,1607)	1:76:A:MET:HA	1:75:A:LYS:HG2	10	0.59
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG21	1	0.59
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG21	5	0.59
(2,1546)	1:95:A:PHE:HE2	1:102:A:THR:HA	2	0.59
(2,1532)	1:87:A:GLU:HB3	1:83:A:SER:HA	8	0.59
(2,1525)	1:86:A:ILE:HG22	1:110:A:VAL:HA	3	0.59
(2,1524)	1:136:A:LYS:HD2	1:135:A:VAL:HA	6	0.59
(2,1475)	1:102:A:THR:HB	1:64:A:VAL:HA	10	0.59
(2,1465)	1:122:A:ILE:HD13	1:120:A:HIS:HA	8	0.59
(2,1460)	1:104:A:ILE:HD12	1:102:A:THR:HB	7	0.59
(2,1450)	1:122:A:ILE:HG22	1:119:A:LEU:HA	7	0.59
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG23	1	0.59
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG23	6	0.59
(2,1420)	1:64:A:VAL:HG23	1:62:A:LEU:HG	3	0.59
(2,1419)	1:64:A:VAL:HG22	1:122:A:ILE:HG13	1	0.59
(2,1419)	1:64:A:VAL:HG21	1:122:A:ILE:HG13	9	0.59
(2,1417)	1:64:A:VAL:HG23	1:62:A:LEU:HA	3	0.59
(2,1396)	1:101:A:VAL:HG13	1:63:A:MET:HA	8	0.59
(2,1332)	1:137:A:LEU:HD12	1:133:A:SER:HB3	10	0.59
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD22	8	0.59
(2,1208)	1:66:A:GLU:HB3	1:74:A:SER:HA	2	0.59
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG23	9	0.59
(2,587)	1:71:A:LYS:HD3	1:71:A:LYS:HA	2	0.59
(2,560)	1:70:A:SER:HB2	1:70:A:SER:HA	6	0.59
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD12	6	0.59
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG22	5	0.59
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG21	9	0.59
(2,494)	1:65:A:THR:HG21	1:99:A:THR:HA	5	0.59
(2,331)	1:125:A:ALA:HB3	1:121:A:ASP:HB3	1	0.59
(2,288)	1:110:A:VAL:HG23	1:113:A:HIS:HB2	4	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,288)	1:110:A:VAL:HG21	1:113:A:HIS:HB2	8	0.59
(2,282)	1:97:A:THR:HG22	1:78:A:LYS:HE2	9	0.59
(2,137)	1:69:A:GLU:HB2	1:69:A:GLU:HA	4	0.59
(2,137)	1:69:A:GLU:HB2	1:69:A:GLU:HA	7	0.59
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG12	6	0.59
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG13	8	0.59
(1,8)	1:107:A:PRO:HB2	1:90:A:GLY:HA2	4	0.59
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG13	7	0.58
(2,1908)	1:84:A:THR:H	1:88:A:GLU:HG3	5	0.58
(2,1904)	1:66:A:GLU:H	1:71:A:LYS:HD3	10	0.58
(2,1810)	1:136:A:LYS:H	1:136:A:LYS:HD2	10	0.58
(2,1769)	1:121:A:ASP:HB2	1:82:A:PHE:HA	5	0.58
(2,1763)	1:82:A:PHE:HB2	1:85:A:ARG:HB3	9	0.58
(2,1759)	1:82:A:PHE:HB3	1:85:A:ARG:HG3	1	0.58
(2,1726)	1:127:A:GLY:HA2	1:128:A:VAL:HB	1	0.58
(2,1726)	1:127:A:GLY:HA2	1:128:A:VAL:HB	3	0.58
(2,1683)	1:131:A:LEU:HD12	1:62:A:LEU:HA	3	0.58
(2,1667)	1:123:A:LEU:HD21	1:124:A:ALA:HA	8	0.58
(2,1635)	1:114:A:ASP:HA	1:115:A:MET:HA	3	0.58
(2,1635)	1:114:A:ASP:HA	1:115:A:MET:HA	5	0.58
(2,1627)	1:95:A:PHE:HA	1:101:A:VAL:HB	8	0.58
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB3	4	0.58
(2,1546)	1:95:A:PHE:HE1	1:102:A:THR:HA	9	0.58
(2,1475)	1:102:A:THR:HB	1:95:A:PHE:HA	7	0.58
(2,1475)	1:102:A:THR:HB	1:64:A:VAL:HA	9	0.58
(2,1456)	1:104:A:ILE:HD12	1:93:A:ILE:HA	5	0.58
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG23	4	0.58
(2,1420)	1:64:A:VAL:HG21	1:62:A:LEU:HG	10	0.58
(2,1404)	1:102:A:THR:HG22	1:77:A:ALA:HA	5	0.58
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD21	9	0.58
(2,1274)	1:122:A:ILE:HG13	1:119:A:LEU:HB2	2	0.58
(2,1268)	1:78:A:LYS:HD3	1:74:A:SER:HB3	8	0.58
(2,1252)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	5	0.58
(2,759)	1:111:A:SER:H	1:114:A:ASP:HB3	3	0.58
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD13	3	0.58
(2,459)	1:77:A:ALA:HB1	1:74:A:SER:HB3	2	0.58
(2,436)	1:93:A:ILE:HG22	1:82:A:PHE:HD2	10	0.58
(2,375)	1:64:A:VAL:HG11	1:122:A:ILE:HD13	10	0.58
(2,275)	1:64:A:VAL:HG11	1:102:A:THR:HB	10	0.58
(2,240)	1:110:A:VAL:HG11	1:89:A:LEU:HB2	8	0.58
(2,59)	1:105:A:GLU:HG3	1:59:A:MET:HG3	2	0.58
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG13	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:125:A:ALA:HA	1:127:A:GLY:HA2	6	0.58
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG13	2	0.57
(2,1759)	1:82:A:PHE:HB3	1:85:A:ARG:HG3	4	0.57
(2,1726)	1:127:A:GLY:HA2	1:128:A:VAL:HB	7	0.57
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB3	10	0.57
(2,1516)	1:107:A:PRO:HA	1:59:A:MET:HB3	4	0.57
(2,1516)	1:107:A:PRO:HA	1:59:A:MET:HB3	10	0.57
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD21	4	0.57
(2,1465)	1:122:A:ILE:HD11	1:120:A:HIS:HA	2	0.57
(2,1462)	1:122:A:ILE:HD12	1:118:A:LEU:HB3	5	0.57
(2,1460)	1:104:A:ILE:HD11	1:102:A:THR:HB	6	0.57
(2,1424)	1:73:A:PHE:HB3	1:125:A:ALA:HB3	3	0.57
(2,1419)	1:64:A:VAL:HG23	1:122:A:ILE:HG13	10	0.57
(2,1364)	1:119:A:LEU:HD21	1:104:A:ILE:HG12	3	0.57
(2,1254)	1:136:A:LYS:HD3	1:135:A:VAL:HA	10	0.57
(2,1212)	1:128:A:VAL:HB	1:65:A:THR:HG23	4	0.57
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB2	9	0.57
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB1	3	0.57
(2,1042)	1:89:A:LEU:H	1:88:A:GLU:HB3	3	0.57
(2,728)	1:124:A:ALA:HB2	1:120:A:HIS:HB2	3	0.57
(2,727)	1:111:A:SER:HB3	1:114:A:ASP:HB3	6	0.57
(2,646)	1:106:A:LEU:HG	1:107:A:PRO:HD3	2	0.57
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD11	1	0.57
(2,494)	1:65:A:THR:HG21	1:99:A:THR:HA	1	0.57
(2,494)	1:65:A:THR:HG22	1:99:A:THR:HA	3	0.57
(2,459)	1:77:A:ALA:HB1	1:74:A:SER:HB3	3	0.57
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG12	1	0.57
(2,353)	1:86:A:ILE:HG23	1:104:A:ILE:HG22	9	0.57
(2,340)	1:124:A:ALA:HB1	1:121:A:ASP:HB2	3	0.57
(2,288)	1:110:A:VAL:HG21	1:113:A:HIS:HB2	2	0.57
(2,200)	1:118:A:LEU:HD13	1:86:A:ILE:HA	5	0.57
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG11	1	0.57
(1,35)	1:88:A:GLU:HG3	1:85:A:ARG:HA	7	0.57
(1,8)	1:107:A:PRO:HB2	1:90:A:GLY:HA2	8	0.57
(1,5)	1:58:A:GLU:HG2	1:90:A:GLY:HA2	10	0.57
(2,1915)	1:79:A:SER:H	1:78:A:LYS:HG3	8	0.56
(2,1862)	1:121:A:ASP:H	1:116:A:ASP:HA	1	0.56
(2,1862)	1:121:A:ASP:H	1:116:A:ASP:HA	8	0.56
(2,1862)	1:121:A:ASP:H	1:116:A:ASP:HA	9	0.56
(2,1860)	1:77:A:ALA:H	1:76:A:MET:HG2	2	0.56
(2,1860)	1:77:A:ALA:H	1:76:A:MET:HG2	8	0.56
(2,1805)	1:61:A:ARG:H	1:137:A:LEU:HD12	2	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1769)	1:121:A:ASP:HB2	1:82:A:PHE:HA	7	0.56
(2,1763)	1:82:A:PHE:HB2	1:85:A:ARG:HB3	2	0.56
(2,1752)	1:74:A:SER:HA	1:78:A:LYS:HE2	3	0.56
(2,1726)	1:127:A:GLY:HA2	1:128:A:VAL:HB	2	0.56
(2,1726)	1:127:A:GLY:HA2	1:128:A:VAL:HB	8	0.56
(2,1726)	1:127:A:GLY:HA2	1:128:A:VAL:HB	10	0.56
(2,1683)	1:131:A:LEU:HD12	1:62:A:LEU:HA	9	0.56
(2,1675)	1:101:A:VAL:HG12	1:103:A:MET:HA	6	0.56
(2,1667)	1:123:A:LEU:HD22	1:124:A:ALA:HA	5	0.56
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG23	6	0.56
(2,1523)	1:135:A:VAL:HA	1:58:A:GLU:HG2	8	0.56
(2,1456)	1:104:A:ILE:HD11	1:93:A:ILE:HA	2	0.56
(2,1424)	1:125:A:ALA:HB2	1:72:A:ASN:HB3	6	0.56
(2,1419)	1:64:A:VAL:HG23	1:122:A:ILE:HG13	7	0.56
(2,1417)	1:64:A:VAL:HG21	1:62:A:LEU:HA	7	0.56
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG23	8	0.56
(2,1357)	1:96:A:LEU:HD22	1:61:A:ARG:HD3	2	0.56
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD21	8	0.56
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB2	7	0.56
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG21	1	0.56
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG21	10	0.56
(2,1042)	1:89:A:LEU:H	1:88:A:GLU:HB3	1	0.56
(2,494)	1:65:A:THR:HG21	1:99:A:THR:HA	8	0.56
(2,459)	1:77:A:ALA:HB3	1:74:A:SER:HB3	1	0.56
(2,387)	1:86:A:ILE:HD11	1:85:A:ARG:HD2	10	0.56
(2,288)	1:110:A:VAL:HG22	1:113:A:HIS:HB2	5	0.56
(2,288)	1:110:A:VAL:HG21	1:113:A:HIS:HB2	9	0.56
(2,200)	1:118:A:LEU:HD11	1:86:A:ILE:HA	9	0.56
(2,131)	1:136:A:LYS:HD3	1:58:A:GLU:HG3	2	0.56
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG11	8	0.56
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG11	6	0.56
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG13	10	0.56
(2,62)	1:107:A:PRO:HB3	1:109:A:THR:HG21	8	0.56
(1,11)	1:66:A:GLU:HB3	1:101:A:VAL:HA	2	0.56
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG11	1	0.55
(2,1910)	1:89:A:LEU:H	1:110:A:VAL:HG13	9	0.55
(2,1878)	1:58:A:GLU:H	1:90:A:GLY:HA2	7	0.55
(2,1860)	1:77:A:ALA:H	1:76:A:MET:HG2	1	0.55
(2,1860)	1:77:A:ALA:H	1:76:A:MET:HG2	4	0.55
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD12	1	0.55
(2,1714)	1:106:A:LEU:HB2	1:91:A:GLY:HA2	10	0.55
(2,1702)	1:106:A:LEU:HB2	1:86:A:ILE:HB	1	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1670)	1:82:A:PHE:HA	1:77:A:ALA:HA	1	0.55
(2,1627)	1:95:A:PHE:HA	1:101:A:VAL:HB	5	0.55
(2,1617)	1:79:A:SER:HA	1:78:A:LYS:HB3	2	0.55
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG23	7	0.55
(2,1478)	1:98:A:GLU:HG3	1:97:A:THR:HB	5	0.55
(2,1475)	1:102:A:THR:HB	1:64:A:VAL:HA	6	0.55
(2,1460)	1:104:A:ILE:HD12	1:102:A:THR:HB	4	0.55
(2,1439)	1:104:A:ILE:HG21	1:105:A:GLU:HG2	2	0.55
(2,1420)	1:64:A:VAL:HG22	1:62:A:LEU:HG	9	0.55
(2,1324)	1:115:A:MET:HG3	1:108:A:LYS:HG3	1	0.55
(2,1285)	1:93:A:ILE:HG12	1:92:A:SER:HA	8	0.55
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD22	2	0.55
(2,1171)	1:112:A:GLU:HG3	1:112:A:GLU:HB2	1	0.55
(2,1171)	1:58:A:GLU:HG2	1:58:A:GLU:HB3	4	0.55
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG23	4	0.55
(2,1148)	1:58:A:GLU:H	1:58:A:GLU:HB3	8	0.55
(2,728)	1:124:A:ALA:HB2	1:120:A:HIS:HB2	8	0.55
(2,646)	1:106:A:LEU:HG	1:107:A:PRO:HD3	3	0.55
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD12	2	0.55
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD13	4	0.55
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD12	6	0.55
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD13	9	0.55
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD13	1	0.55
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG21	8	0.55
(2,494)	1:65:A:THR:HG22	1:99:A:THR:HA	9	0.55
(2,459)	1:77:A:ALA:HB2	1:74:A:SER:HB3	6	0.55
(2,436)	1:93:A:ILE:HG21	1:82:A:PHE:HD2	3	0.55
(2,425)	1:111:A:SER:HB2	1:114:A:ASP:HB2	2	0.55
(2,353)	1:86:A:ILE:HG21	1:104:A:ILE:HG23	1	0.55
(2,353)	1:86:A:ILE:HG21	1:104:A:ILE:HG22	4	0.55
(2,353)	1:86:A:ILE:HG22	1:104:A:ILE:HG23	8	0.55
(2,340)	1:124:A:ALA:HB2	1:121:A:ASP:HB2	1	0.55
(2,275)	1:64:A:VAL:HG11	1:102:A:THR:HB	9	0.55
(2,257)	1:89:A:LEU:HD22	1:114:A:ASP:HB3	2	0.55
(2,241)	1:106:A:LEU:HD23	1:110:A:VAL:HG12	8	0.55
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG13	1	0.55
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG12	10	0.54
(2,1769)	1:121:A:ASP:HB2	1:82:A:PHE:HA	3	0.54
(2,1759)	1:82:A:PHE:HB3	1:85:A:ARG:HG3	7	0.54
(2,1752)	1:78:A:LYS:HE2	1:75:A:LYS:HA	1	0.54
(2,1726)	1:127:A:GLY:HA2	1:128:A:VAL:HB	9	0.54
(2,1711)	1:104:A:ILE:HG23	1:91:A:GLY:HA2	1	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1670)	1:77:A:ALA:HA	1:78:A:LYS:HA	10	0.54
(2,1667)	1:123:A:LEU:HD23	1:124:A:ALA:HA	6	0.54
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB3	9	0.54
(2,1627)	1:95:A:PHE:HA	1:101:A:VAL:HB	4	0.54
(2,1626)	1:118:A:LEU:HA	1:85:A:ARG:HG2	1	0.54
(2,1617)	1:79:A:SER:HA	1:78:A:LYS:HB3	7	0.54
(2,1462)	1:122:A:ILE:HD11	1:118:A:LEU:HB3	7	0.54
(2,1460)	1:104:A:ILE:HD11	1:102:A:THR:HB	10	0.54
(2,1456)	1:104:A:ILE:HD12	1:93:A:ILE:HA	3	0.54
(2,1455)	1:93:A:ILE:HD12	1:78:A:LYS:HD3	1	0.54
(2,1438)	1:104:A:ILE:HG22	1:62:A:LEU:HB2	5	0.54
(2,1434)	1:86:A:ILE:HG22	1:106:A:LEU:HD11	6	0.54
(2,1418)	1:64:A:VAL:HG23	1:127:A:GLY:HA2	6	0.54
(2,1396)	1:101:A:VAL:HG13	1:63:A:MET:HA	4	0.54
(2,1274)	1:122:A:ILE:HG13	1:119:A:LEU:HB2	10	0.54
(2,1269)	1:78:A:LYS:HD2	1:75:A:LYS:HE2	1	0.54
(2,1178)	1:85:A:ARG:H	1:86:A:ILE:HB	7	0.54
(2,1178)	1:85:A:ARG:H	1:86:A:ILE:HB	10	0.54
(2,1171)	1:58:A:GLU:HG2	1:107:A:PRO:HB2	6	0.54
(2,759)	1:111:A:SER:H	1:114:A:ASP:HB3	1	0.54
(2,387)	1:86:A:ILE:HD11	1:85:A:ARG:HD2	2	0.54
(2,353)	1:86:A:ILE:HG21	1:104:A:ILE:HG21	3	0.54
(2,296)	1:101:A:VAL:HG13	1:94:A:SER:HB2	5	0.54
(2,240)	1:110:A:VAL:HG12	1:89:A:LEU:HB2	1	0.54
(2,144)	1:78:A:LYS:HB3	1:78:A:LYS:HD2	9	0.54
(2,34)	1:58:A:GLU:HG2	1:135:A:VAL:HG12	2	0.54
(1,8)	1:107:A:PRO:HB2	1:90:A:GLY:HA2	6	0.54
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD12	9	0.53
(2,1904)	1:66:A:GLU:H	1:71:A:LYS:HD3	1	0.53
(2,1860)	1:77:A:ALA:H	1:76:A:MET:HG2	7	0.53
(2,1770)	1:116:A:ASP:HB2	1:115:A:MET:HB2	6	0.53
(2,1675)	1:101:A:VAL:HG11	1:103:A:MET:HA	9	0.53
(2,1670)	1:77:A:ALA:HA	1:78:A:LYS:HA	4	0.53
(2,1670)	1:82:A:PHE:HA	1:77:A:ALA:HA	9	0.53
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB3	1	0.53
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD1	5	0.53
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD1	8	0.53
(2,1626)	1:118:A:LEU:HA	1:85:A:ARG:HG2	8	0.53
(2,1516)	1:107:A:PRO:HA	1:59:A:MET:HB3	7	0.53
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD22	9	0.53
(2,1445)	1:87:A:GLU:HG2	1:86:A:ILE:HG21	8	0.53
(2,1417)	1:64:A:VAL:HG21	1:62:A:LEU:HA	8	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1404)	1:102:A:THR:HG21	1:77:A:ALA:HA	4	0.53
(2,1388)	1:84:A:THR:HG23	1:85:A:ARG:HD2	10	0.53
(2,1367)	1:65:A:THR:HG22	1:100:A:GLY:HA2	3	0.53
(2,1345)	1:110:A:VAL:HG11	1:114:A:ASP:HB2	6	0.53
(2,1249)	1:117:A:GLN:HB2	1:113:A:HIS:HA	7	0.53
(2,1178)	1:85:A:ARG:H	1:86:A:ILE:HB	5	0.53
(2,1171)	1:112:A:GLU:HG3	1:112:A:GLU:HB2	2	0.53
(2,1148)	1:58:A:GLU:H	1:58:A:GLU:HB3	9	0.53
(2,871)	1:87:A:GLU:H	1:92:A:SER:HB3	8	0.53
(2,871)	1:87:A:GLU:H	1:92:A:SER:HB3	9	0.53
(2,812)	1:137:A:LEU:H	1:60:A:THR:HG22	4	0.53
(2,759)	1:111:A:SER:H	1:114:A:ASP:HB3	4	0.53
(2,604)	1:131:A:LEU:HD22	1:131:A:LEU:HA	9	0.53
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD12	5	0.53
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG21	2	0.53
(2,264)	1:65:A:THR:HG21	1:64:A:VAL:HG12	3	0.53
(2,264)	1:65:A:THR:HG21	1:64:A:VAL:HG11	9	0.53
(2,200)	1:118:A:LEU:HD13	1:86:A:ILE:HA	10	0.53
(2,1940)	1:127:A:GLY:H	1:123:A:LEU:HG	5	0.52
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG11	8	0.52
(2,1862)	1:121:A:ASP:H	1:116:A:ASP:HA	10	0.52
(2,1846)	1:106:A:LEU:H	1:105:A:GLU:HG3	2	0.52
(2,1810)	1:136:A:LYS:H	1:136:A:LYS:HD3	7	0.52
(2,1741)	1:136:A:LYS:HE2	1:136:A:LYS:HA	3	0.52
(2,1711)	1:104:A:ILE:HG23	1:91:A:GLY:HA2	8	0.52
(2,1700)	1:107:A:PRO:HD2	1:106:A:LEU:HB2	5	0.52
(2,1675)	1:101:A:VAL:HG13	1:103:A:MET:HA	8	0.52
(2,1670)	1:82:A:PHE:HA	1:77:A:ALA:HA	8	0.52
(2,1667)	1:123:A:LEU:HD23	1:124:A:ALA:HA	1	0.52
(2,1667)	1:123:A:LEU:HD21	1:124:A:ALA:HA	2	0.52
(2,1651)	1:104:A:ILE:HG22	1:61:A:ARG:HA	10	0.52
(2,1648)	1:136:A:LYS:HG2	1:136:A:LYS:HA	10	0.52
(2,1618)	1:79:A:SER:HA	1:78:A:LYS:HB2	5	0.52
(2,1572)	1:82:A:PHE:HE2	1:77:A:ALA:HA	3	0.52
(2,1572)	1:82:A:PHE:HE2	1:77:A:ALA:HA	8	0.52
(2,1439)	1:104:A:ILE:HG22	1:105:A:GLU:HG2	10	0.52
(2,1434)	1:86:A:ILE:HG21	1:106:A:LEU:HD13	5	0.52
(2,1408)	1:135:A:VAL:HG21	1:134:A:GLU:HA	6	0.52
(2,1404)	1:102:A:THR:HG23	1:77:A:ALA:HA	1	0.52
(2,1393)	1:60:A:THR:HG22	1:62:A:LEU:HB3	6	0.52
(2,1393)	1:60:A:THR:HG23	1:62:A:LEU:HB3	8	0.52
(2,1367)	1:65:A:THR:HG21	1:100:A:GLY:HA2	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1331)	1:137:A:LEU:HD12	1:137:A:LEU:HA	1	0.52
(2,1331)	1:137:A:LEU:HD11	1:137:A:LEU:HA	8	0.52
(2,1311)	1:89:A:LEU:HD13	1:107:A:PRO:HG3	8	0.52
(2,1274)	1:122:A:ILE:HG13	1:119:A:LEU:HB2	1	0.52
(2,1265)	1:78:A:LYS:HD2	1:78:A:LYS:HA	7	0.52
(2,1171)	1:112:A:GLU:HG3	1:112:A:GLU:HB2	5	0.52
(2,1171)	1:112:A:GLU:HG3	1:112:A:GLU:HB2	8	0.52
(2,1148)	1:58:A:GLU:H	1:58:A:GLU:HB3	7	0.52
(2,871)	1:87:A:GLU:H	1:92:A:SER:HB3	6	0.52
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD11	2	0.52
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG21	3	0.52
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG23	4	0.52
(2,279)	1:64:A:VAL:HG11	1:122:A:ILE:HG22	6	0.52
(2,240)	1:110:A:VAL:HG11	1:89:A:LEU:HB2	3	0.52
(2,103)	1:103:A:MET:HG3	1:61:A:ARG:HD2	7	0.52
(2,82)	1:59:A:MET:HG3	1:136:A:LYS:HA	4	0.52
(2,28)	1:87:A:GLU:HG2	1:87:A:GLU:HB3	9	0.52
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD12	3	0.51
(2,1915)	1:79:A:SER:H	1:78:A:LYS:HG3	2	0.51
(2,1670)	1:77:A:ALA:HA	1:78:A:LYS:HA	2	0.51
(2,1662)	1:131:A:LEU:HA	1:61:A:ARG:HA	8	0.51
(2,1627)	1:95:A:PHE:HA	1:101:A:VAL:HB	3	0.51
(2,1572)	1:82:A:PHE:HE2	1:77:A:ALA:HA	2	0.51
(2,1471)	1:86:A:ILE:HD13	1:89:A:LEU:HB2	7	0.51
(2,1460)	1:104:A:ILE:HD12	1:102:A:THR:HB	3	0.51
(2,1456)	1:104:A:ILE:HD11	1:93:A:ILE:HA	7	0.51
(2,1418)	1:64:A:VAL:HG23	1:127:A:GLY:HA2	2	0.51
(2,1404)	1:102:A:THR:HG21	1:77:A:ALA:HA	9	0.51
(2,1401)	1:84:A:THR:HG22	1:89:A:LEU:HD22	6	0.51
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG21	1	0.51
(2,1393)	1:60:A:THR:HG23	1:62:A:LEU:HB3	9	0.51
(2,1367)	1:65:A:THR:HG21	1:100:A:GLY:HA2	1	0.51
(2,1324)	1:115:A:MET:HG3	1:108:A:LYS:HG3	10	0.51
(2,1190)	1:107:A:PRO:HB3	1:90:A:GLY:HA2	1	0.51
(2,1178)	1:85:A:ARG:H	1:86:A:ILE:HB	2	0.51
(2,1171)	1:58:A:GLU:HG2	1:58:A:GLU:HB3	9	0.51
(2,871)	1:87:A:GLU:H	1:92:A:SER:HB3	10	0.51
(2,772)	1:62:A:LEU:H	1:103:A:MET:HG3	5	0.51
(2,728)	1:124:A:ALA:HB1	1:120:A:HIS:HB2	5	0.51
(2,646)	1:106:A:LEU:HG	1:107:A:PRO:HD3	6	0.51
(2,333)	1:124:A:ALA:HB1	1:76:A:MET:HG3	2	0.51
(2,241)	1:106:A:LEU:HD22	1:110:A:VAL:HG12	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,241)	1:106:A:LEU:HD22	1:110:A:VAL:HG12	4	0.51
(2,1862)	1:121:A:ASP:H	1:116:A:ASP:HA	4	0.5
(2,1769)	1:121:A:ASP:HB2	1:82:A:PHE:HA	1	0.5
(2,1741)	1:136:A:LYS:HE2	1:136:A:LYS:HA	2	0.5
(2,1702)	1:106:A:LEU:HB2	1:86:A:ILE:HB	6	0.5
(2,1700)	1:107:A:PRO:HD2	1:106:A:LEU:HB2	6	0.5
(2,1675)	1:101:A:VAL:HG12	1:103:A:MET:HA	10	0.5
(2,1626)	1:118:A:LEU:HA	1:85:A:ARG:HG2	7	0.5
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG22	9	0.5
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB3	1	0.5
(2,1523)	1:110:A:VAL:HA	1:107:A:PRO:HG3	3	0.5
(2,1438)	1:104:A:ILE:HG23	1:62:A:LEU:HB2	4	0.5
(2,1433)	1:77:A:ALA:HB2	1:78:A:LYS:HB2	9	0.5
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG21	9	0.5
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG21	10	0.5
(2,1380)	1:64:A:VAL:HG11	1:128:A:VAL:HG23	3	0.5
(2,1357)	1:96:A:LEU:HD21	1:61:A:ARG:HD3	9	0.5
(2,1294)	1:106:A:LEU:HG	1:90:A:GLY:HA3	8	0.5
(2,1224)	1:115:A:MET:HB3	1:111:A:SER:HB2	1	0.5
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG21	3	0.5
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG23	7	0.5
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG21	10	0.5
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG21	5	0.5
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD22	5	0.5
(2,871)	1:87:A:GLU:H	1:92:A:SER:HB3	3	0.5
(2,871)	1:87:A:GLU:H	1:92:A:SER:HB3	5	0.5
(2,871)	1:87:A:GLU:H	1:92:A:SER:HB3	7	0.5
(2,759)	1:111:A:SER:H	1:114:A:ASP:HB3	5	0.5
(2,759)	1:111:A:SER:H	1:114:A:ASP:HB3	6	0.5
(2,759)	1:111:A:SER:H	1:114:A:ASP:HB3	9	0.5
(2,728)	1:124:A:ALA:HB3	1:120:A:HIS:HB2	1	0.5
(2,624)	1:101:A:VAL:HG12	1:63:A:MET:HA	6	0.5
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD11	5	0.5
(2,472)	1:82:A:PHE:HA	1:84:A:THR:HG21	8	0.5
(2,340)	1:124:A:ALA:HB3	1:121:A:ASP:HB2	5	0.5
(2,340)	1:124:A:ALA:HB1	1:121:A:ASP:HB2	8	0.5
(2,275)	1:64:A:VAL:HG12	1:102:A:THR:HB	2	0.5
(2,275)	1:64:A:VAL:HG13	1:102:A:THR:HB	8	0.5
(2,241)	1:106:A:LEU:HD23	1:110:A:VAL:HG12	6	0.5
(2,200)	1:118:A:LEU:HD11	1:86:A:ILE:HA	2	0.5
(2,121)	1:58:A:GLU:HB3	1:59:A:MET:HA	8	0.5
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG13	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1940)	1:127:A:GLY:H	1:123:A:LEU:HG	9	0.49
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG12	5	0.49
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG12	9	0.49
(2,1904)	1:66:A:GLU:H	1:71:A:LYS:HD3	9	0.49
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD13	3	0.49
(2,1810)	1:136:A:LYS:H	1:136:A:LYS:HD3	9	0.49
(2,1769)	1:121:A:ASP:HB2	1:82:A:PHE:HA	9	0.49
(2,1769)	1:121:A:ASP:HB2	1:82:A:PHE:HA	10	0.49
(2,1702)	1:106:A:LEU:HB2	1:86:A:ILE:HB	5	0.49
(2,1702)	1:106:A:LEU:HB2	1:86:A:ILE:HB	10	0.49
(2,1700)	1:107:A:PRO:HD2	1:106:A:LEU:HB2	2	0.49
(2,1675)	1:101:A:VAL:HG13	1:103:A:MET:HA	2	0.49
(2,1675)	1:101:A:VAL:HG13	1:103:A:MET:HA	5	0.49
(2,1670)	1:77:A:ALA:HA	1:78:A:LYS:HA	5	0.49
(2,1670)	1:77:A:ALA:HA	1:78:A:LYS:HA	7	0.49
(2,1627)	1:95:A:PHE:HA	1:101:A:VAL:HB	6	0.49
(2,1626)	1:118:A:LEU:HA	1:85:A:ARG:HG2	9	0.49
(2,1617)	1:79:A:SER:HA	1:78:A:LYS:HB3	9	0.49
(2,1607)	1:76:A:MET:HA	1:75:A:LYS:HG2	8	0.49
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG22	2	0.49
(2,1581)	1:104:A:ILE:HA	1:93:A:ILE:HG13	4	0.49
(2,1581)	1:104:A:ILE:HA	1:93:A:ILE:HG13	10	0.49
(2,1557)	1:95:A:PHE:HE2	1:102:A:THR:HB	10	0.49
(2,1460)	1:104:A:ILE:HD12	1:102:A:THR:HB	5	0.49
(2,1455)	1:93:A:ILE:HD11	1:78:A:LYS:HD3	10	0.49
(2,1429)	1:77:A:ALA:HB2	1:74:A:SER:HA	9	0.49
(2,1367)	1:65:A:THR:HG22	1:100:A:GLY:HA2	9	0.49
(2,1364)	1:119:A:LEU:HD21	1:104:A:ILE:HG12	5	0.49
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD21	10	0.49
(2,1274)	1:122:A:ILE:HG13	1:119:A:LEU:HB2	7	0.49
(2,1274)	1:122:A:ILE:HG13	1:119:A:LEU:HB2	9	0.49
(2,1178)	1:85:A:ARG:H	1:86:A:ILE:HB	1	0.49
(2,934)	1:60:A:THR:H	1:60:A:THR:HG23	8	0.49
(2,759)	1:111:A:SER:H	1:114:A:ASP:HB3	8	0.49
(2,664)	1:118:A:LEU:HD21	1:85:A:ARG:HD3	10	0.49
(2,646)	1:106:A:LEU:HG	1:107:A:PRO:HD3	5	0.49
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD13	10	0.49
(2,459)	1:77:A:ALA:HB1	1:74:A:SER:HB3	7	0.49
(2,459)	1:77:A:ALA:HB1	1:74:A:SER:HB3	10	0.49
(2,353)	1:86:A:ILE:HG23	1:104:A:ILE:HG21	5	0.49
(2,353)	1:86:A:ILE:HG21	1:104:A:ILE:HG22	7	0.49
(2,353)	1:86:A:ILE:HG23	1:104:A:ILE:HG21	10	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,340)	1:124:A:ALA:HB1	1:121:A:ASP:HB2	6	0.49
(2,288)	1:110:A:VAL:HG22	1:113:A:HIS:HB2	10	0.49
(2,275)	1:64:A:VAL:HG13	1:102:A:THR:HB	3	0.49
(2,246)	1:123:A:LEU:HD13	1:127:A:GLY:HA2	1	0.49
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG22	9	0.49
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG12	7	0.49
(2,1915)	1:79:A:SER:H	1:78:A:LYS:HG3	1	0.48
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD11	5	0.48
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD13	6	0.48
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD11	9	0.48
(2,1846)	1:106:A:LEU:H	1:105:A:GLU:HG3	3	0.48
(2,1769)	1:121:A:ASP:HB2	1:82:A:PHE:HA	2	0.48
(2,1759)	1:82:A:PHE:HB3	1:85:A:ARG:HG3	2	0.48
(2,1752)	1:78:A:LYS:HE2	1:75:A:LYS:HA	4	0.48
(2,1714)	1:106:A:LEU:HB2	1:91:A:GLY:HA2	2	0.48
(2,1702)	1:106:A:LEU:HB2	1:86:A:ILE:HB	8	0.48
(2,1700)	1:107:A:PRO:HD2	1:106:A:LEU:HB2	4	0.48
(2,1662)	1:131:A:LEU:HA	1:61:A:ARG:HA	5	0.48
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD1	2	0.48
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD2	6	0.48
(2,1617)	1:79:A:SER:HA	1:78:A:LYS:HB3	1	0.48
(2,1525)	1:86:A:ILE:HG22	1:110:A:VAL:HA	7	0.48
(2,1523)	1:135:A:VAL:HA	1:58:A:GLU:HG2	4	0.48
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD23	7	0.48
(2,1380)	1:64:A:VAL:HG12	1:128:A:VAL:HG22	7	0.48
(2,1325)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	7	0.48
(2,1311)	1:89:A:LEU:HD13	1:107:A:PRO:HG3	3	0.48
(2,1292)	1:118:A:LEU:HG	1:118:A:LEU:HB3	7	0.48
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD21	10	0.48
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG21	10	0.48
(2,934)	1:60:A:THR:H	1:60:A:THR:HG21	1	0.48
(2,759)	1:111:A:SER:H	1:114:A:ASP:HB3	7	0.48
(2,728)	1:124:A:ALA:HB2	1:120:A:HIS:HB2	7	0.48
(2,728)	1:124:A:ALA:HB3	1:120:A:HIS:HB2	9	0.48
(2,664)	1:118:A:LEU:HD23	1:85:A:ARG:HD3	1	0.48
(2,664)	1:118:A:LEU:HD22	1:85:A:ARG:HD3	4	0.48
(2,664)	1:118:A:LEU:HD23	1:85:A:ARG:HD3	5	0.48
(2,664)	1:118:A:LEU:HD22	1:85:A:ARG:HD3	9	0.48
(2,646)	1:106:A:LEU:HG	1:107:A:PRO:HD3	10	0.48
(2,333)	1:124:A:ALA:HB2	1:76:A:MET:HG3	1	0.48
(2,331)	1:125:A:ALA:HB3	1:121:A:ASP:HB3	9	0.48
(2,275)	1:64:A:VAL:HG11	1:102:A:THR:HB	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,264)	1:65:A:THR:HG23	1:64:A:VAL:HG12	1	0.48
(2,243)	1:123:A:LEU:HD11	1:128:A:VAL:HA	6	0.48
(2,241)	1:106:A:LEU:HD21	1:110:A:VAL:HG13	7	0.48
(2,241)	1:106:A:LEU:HD21	1:110:A:VAL:HG11	10	0.48
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG23	10	0.48
(2,34)	1:58:A:GLU:HG2	1:135:A:VAL:HG13	10	0.48
(2,1890)	1:76:A:MET:H	1:77:A:ALA:HA	9	0.47
(2,1878)	1:58:A:GLU:H	1:90:A:GLY:HA2	4	0.47
(2,1862)	1:121:A:ASP:H	1:116:A:ASP:HA	5	0.47
(2,1770)	1:116:A:ASP:HB2	1:112:A:GLU:HB3	7	0.47
(2,1769)	1:121:A:ASP:HB2	1:82:A:PHE:HA	8	0.47
(2,1759)	1:82:A:PHE:HB3	1:85:A:ARG:HG3	10	0.47
(2,1711)	1:104:A:ILE:HG22	1:91:A:GLY:HA2	9	0.47
(2,1702)	1:106:A:LEU:HB2	1:86:A:ILE:HB	7	0.47
(2,1700)	1:107:A:PRO:HD2	1:106:A:LEU:HB2	1	0.47
(2,1700)	1:107:A:PRO:HD2	1:106:A:LEU:HB2	10	0.47
(2,1651)	1:104:A:ILE:HG22	1:61:A:ARG:HA	3	0.47
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD1	3	0.47
(2,1626)	1:118:A:LEU:HA	1:85:A:ARG:HG2	2	0.47
(2,1626)	1:118:A:LEU:HA	1:85:A:ARG:HG2	5	0.47
(2,1582)	1:104:A:ILE:HD13	1:104:A:ILE:HA	1	0.47
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB3	7	0.47
(2,1525)	1:86:A:ILE:HG21	1:110:A:VAL:HA	5	0.47
(2,1502)	1:70:A:SER:HB2	1:71:A:LYS:HD3	9	0.47
(2,1471)	1:86:A:ILE:HD12	1:89:A:LEU:HB2	1	0.47
(2,1471)	1:86:A:ILE:HD13	1:89:A:LEU:HB2	8	0.47
(2,1460)	1:104:A:ILE:HD11	1:102:A:THR:HB	1	0.47
(2,1460)	1:104:A:ILE:HD11	1:102:A:THR:HB	2	0.47
(2,1456)	1:104:A:ILE:HD11	1:93:A:ILE:HA	10	0.47
(2,1438)	1:104:A:ILE:HG21	1:62:A:LEU:HB2	6	0.47
(2,1434)	1:86:A:ILE:HG22	1:106:A:LEU:HD13	1	0.47
(2,1429)	1:77:A:ALA:HB3	1:74:A:SER:HA	4	0.47
(2,1417)	1:64:A:VAL:HG21	1:62:A:LEU:HA	10	0.47
(2,1401)	1:84:A:THR:HG23	1:89:A:LEU:HD23	1	0.47
(2,1401)	1:84:A:THR:HG22	1:89:A:LEU:HD21	7	0.47
(2,1388)	1:109:A:THR:HG23	1:108:A:LYS:HE3	2	0.47
(2,1302)	1:62:A:LEU:HG	1:103:A:MET:HG2	5	0.47
(2,1285)	1:93:A:ILE:HG12	1:92:A:SER:HA	2	0.47
(2,1274)	1:122:A:ILE:HG13	1:119:A:LEU:HB2	6	0.47
(2,1265)	1:78:A:LYS:HD2	1:78:A:LYS:HA	5	0.47
(2,1256)	1:75:A:LYS:HD3	1:78:A:LYS:HE3	5	0.47
(2,1249)	1:117:A:GLN:HB2	1:114:A:ASP:HA	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD21	3	0.47
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD21	6	0.47
(2,1208)	1:66:A:GLU:HB3	1:74:A:SER:HA	1	0.47
(2,1178)	1:85:A:ARG:H	1:86:A:ILE:HB	9	0.47
(2,1171)	1:58:A:GLU:HG2	1:58:A:GLU:HB3	10	0.47
(2,1149)	1:58:A:GLU:H	1:58:A:GLU:HG2	8	0.47
(2,1148)	1:58:A:GLU:H	1:58:A:GLU:HB3	4	0.47
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG22	10	0.47
(2,1032)	1:84:A:THR:H	1:84:A:THR:HG22	6	0.47
(2,934)	1:60:A:THR:H	1:60:A:THR:HG23	2	0.47
(2,871)	1:87:A:GLU:H	1:92:A:SER:HB3	4	0.47
(2,728)	1:124:A:ALA:HB2	1:120:A:HIS:HB2	6	0.47
(2,724)	1:128:A:VAL:HG22	1:65:A:THR:HB	4	0.47
(2,664)	1:118:A:LEU:HD22	1:85:A:ARG:HD3	2	0.47
(2,664)	1:118:A:LEU:HD23	1:85:A:ARG:HD3	3	0.47
(2,664)	1:118:A:LEU:HD21	1:85:A:ARG:HD3	6	0.47
(2,353)	1:86:A:ILE:HG21	1:104:A:ILE:HG23	6	0.47
(2,340)	1:124:A:ALA:HB2	1:121:A:ASP:HB2	4	0.47
(2,318)	1:64:A:VAL:HG22	1:102:A:THR:HB	1	0.47
(2,241)	1:106:A:LEU:HD21	1:110:A:VAL:HG11	9	0.47
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG11	4	0.47
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG12	3	0.46
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG13	6	0.46
(2,1890)	1:76:A:MET:H	1:77:A:ALA:HA	3	0.46
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD12	2	0.46
(2,1711)	1:104:A:ILE:HG23	1:91:A:GLY:HA2	6	0.46
(2,1700)	1:107:A:PRO:HD2	1:106:A:LEU:HB2	3	0.46
(2,1700)	1:107:A:PRO:HD2	1:106:A:LEU:HB2	8	0.46
(2,1662)	1:131:A:LEU:HA	1:61:A:ARG:HA	9	0.46
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD1	9	0.46
(2,1627)	1:95:A:PHE:HA	1:101:A:VAL:HB	10	0.46
(2,1607)	1:76:A:MET:HA	1:78:A:LYS:HG3	3	0.46
(2,1545)	1:95:A:PHE:HE2	1:95:A:PHE:HA	1	0.46
(2,1544)	1:74:A:SER:HB3	1:75:A:LYS:HG2	6	0.46
(2,1540)	1:135:A:VAL:HA	1:109:A:THR:H	4	0.46
(2,1540)	1:135:A:VAL:HA	1:109:A:THR:H	5	0.46
(2,1525)	1:86:A:ILE:HG21	1:110:A:VAL:HA	9	0.46
(2,1488)	1:92:A:SER:HB2	1:93:A:ILE:HB	8	0.46
(2,1471)	1:86:A:ILE:HD13	1:89:A:LEU:HB2	5	0.46
(2,1460)	1:104:A:ILE:HD12	1:102:A:THR:HB	9	0.46
(2,1456)	1:104:A:ILE:HD11	1:93:A:ILE:HA	6	0.46
(2,1438)	1:104:A:ILE:HG21	1:62:A:LEU:HB2	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1438)	1:104:A:ILE:HG23	1:62:A:LEU:HB2	9	0.46
(2,1380)	1:64:A:VAL:HG13	1:128:A:VAL:HG21	9	0.46
(2,1372)	1:103:A:MET:HG2	1:101:A:VAL:HG13	5	0.46
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD22	4	0.46
(2,1324)	1:115:A:MET:HG3	1:108:A:LYS:HG3	7	0.46
(2,1324)	1:115:A:MET:HG3	1:108:A:LYS:HG3	9	0.46
(2,1274)	1:122:A:ILE:HG13	1:119:A:LEU:HB2	5	0.46
(2,1274)	1:122:A:ILE:HG13	1:119:A:LEU:HB2	8	0.46
(2,1269)	1:78:A:LYS:HD2	1:75:A:LYS:HE2	7	0.46
(2,1178)	1:85:A:ARG:H	1:86:A:ILE:HB	3	0.46
(2,1178)	1:85:A:ARG:H	1:86:A:ILE:HB	6	0.46
(2,1178)	1:85:A:ARG:H	1:86:A:ILE:HB	8	0.46
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG21	6	0.46
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG21	4	0.46
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG22	8	0.46
(2,934)	1:60:A:THR:H	1:60:A:THR:HG21	7	0.46
(2,812)	1:137:A:LEU:H	1:60:A:THR:HG23	10	0.46
(2,664)	1:118:A:LEU:HD22	1:85:A:ARG:HD3	7	0.46
(2,664)	1:118:A:LEU:HD21	1:85:A:ARG:HD3	8	0.46
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD12	3	0.46
(2,331)	1:125:A:ALA:HB3	1:121:A:ASP:HB3	8	0.46
(2,330)	1:64:A:VAL:HG12	1:125:A:ALA:HB3	2	0.46
(2,275)	1:64:A:VAL:HG12	1:102:A:THR:HB	5	0.46
(2,241)	1:106:A:LEU:HD22	1:110:A:VAL:HG13	1	0.46
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG23	6	0.46
(2,121)	1:58:A:GLU:HB3	1:59:A:MET:HA	2	0.46
(2,87)	1:59:A:MET:HG2	1:136:A:LYS:HG3	10	0.46
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG12	2	0.46
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD12	4	0.45
(2,1915)	1:79:A:SER:H	1:78:A:LYS:HG3	3	0.45
(2,1890)	1:76:A:MET:H	1:77:A:ALA:HA	4	0.45
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD13	8	0.45
(2,1711)	1:104:A:ILE:HG21	1:91:A:GLY:HA2	5	0.45
(2,1711)	1:104:A:ILE:HG22	1:91:A:GLY:HA2	7	0.45
(2,1702)	1:106:A:LEU:HB2	1:86:A:ILE:HB	2	0.45
(2,1700)	1:107:A:PRO:HD2	1:106:A:LEU:HB2	7	0.45
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB3	5	0.45
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB3	8	0.45
(2,1607)	1:76:A:MET:HA	1:75:A:LYS:HG2	2	0.45
(2,1545)	1:95:A:PHE:HE1	1:95:A:PHE:HA	3	0.45
(2,1545)	1:95:A:PHE:HE2	1:95:A:PHE:HA	5	0.45
(2,1443)	1:86:A:ILE:HG22	1:87:A:GLU:HA	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1439)	1:104:A:ILE:HG21	1:105:A:GLU:HG2	1	0.45
(2,1434)	1:86:A:ILE:HG23	1:106:A:LEU:HD13	8	0.45
(2,1433)	1:77:A:ALA:HB1	1:78:A:LYS:HB2	7	0.45
(2,1424)	1:125:A:ALA:HB1	1:72:A:ASN:HB3	1	0.45
(2,1424)	1:125:A:ALA:HB2	1:72:A:ASN:HB3	2	0.45
(2,1404)	1:102:A:THR:HG23	1:77:A:ALA:HA	6	0.45
(2,1396)	1:101:A:VAL:HG13	1:63:A:MET:HA	5	0.45
(2,1381)	1:64:A:VAL:HG12	1:125:A:ALA:HB1	5	0.45
(2,1381)	1:64:A:VAL:HG11	1:125:A:ALA:HB3	6	0.45
(2,1381)	1:64:A:VAL:HG13	1:125:A:ALA:HB2	8	0.45
(2,1380)	1:64:A:VAL:HG12	1:128:A:VAL:HG21	10	0.45
(2,1372)	1:89:A:LEU:HD23	1:88:A:GLU:HB3	2	0.45
(2,1372)	1:103:A:MET:HG2	1:101:A:VAL:HG12	6	0.45
(2,1372)	1:89:A:LEU:HD22	1:88:A:GLU:HB3	10	0.45
(2,1364)	1:119:A:LEU:HD23	1:104:A:ILE:HG12	6	0.45
(2,1344)	1:123:A:LEU:HD23	1:129:A:VAL:HG21	2	0.45
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD23	8	0.45
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD22	7	0.45
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD23	7	0.45
(2,1153)	1:72:A:ASN:HB3	1:76:A:MET:HG2	10	0.45
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG23	2	0.45
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG21	7	0.45
(2,934)	1:60:A:THR:H	1:60:A:THR:HG21	10	0.45
(2,871)	1:87:A:GLU:H	1:92:A:SER:HB3	1	0.45
(2,604)	1:131:A:LEU:HD21	1:131:A:LEU:HA	3	0.45
(2,589)	1:71:A:LYS:HG2	1:71:A:LYS:HA	8	0.45
(2,587)	1:71:A:LYS:HD3	1:71:A:LYS:HA	7	0.45
(2,568)	1:94:A:SER:HA	1:96:A:LEU:HD13	8	0.45
(2,494)	1:65:A:THR:HG21	1:99:A:THR:HA	10	0.45
(2,340)	1:124:A:ALA:HB1	1:121:A:ASP:HB2	7	0.45
(2,340)	1:124:A:ALA:HB2	1:121:A:ASP:HB2	9	0.45
(2,331)	1:125:A:ALA:HB1	1:121:A:ASP:HB3	3	0.45
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG12	8	0.45
(1,11)	1:66:A:GLU:HB3	1:101:A:VAL:HA	9	0.45
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD11	1	0.44
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD13	8	0.44
(2,1940)	1:127:A:GLY:H	1:123:A:LEU:HG	7	0.44
(2,1890)	1:76:A:MET:H	1:77:A:ALA:HA	2	0.44
(2,1890)	1:76:A:MET:H	1:77:A:ALA:HA	6	0.44
(2,1860)	1:77:A:ALA:H	1:76:A:MET:HG2	9	0.44
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD13	8	0.44
(2,1769)	1:121:A:ASP:HB2	1:82:A:PHE:HA	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1702)	1:106:A:LEU:HB2	1:86:A:ILE:HB	4	0.44
(2,1702)	1:106:A:LEU:HB2	1:86:A:ILE:HB	9	0.44
(2,1700)	1:107:A:PRO:HD2	1:106:A:LEU:HB2	9	0.44
(2,1675)	1:101:A:VAL:HG12	1:103:A:MET:HA	3	0.44
(2,1673)	1:93:A:ILE:HD13	1:77:A:ALA:HA	7	0.44
(2,1670)	1:77:A:ALA:HA	1:78:A:LYS:HA	6	0.44
(2,1661)	1:134:A:GLU:HB3	1:131:A:LEU:HA	9	0.44
(2,1651)	1:104:A:ILE:HG21	1:61:A:ARG:HA	2	0.44
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD1	1	0.44
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD2	10	0.44
(2,1627)	1:95:A:PHE:HA	1:101:A:VAL:HB	9	0.44
(2,1626)	1:118:A:LEU:HA	1:85:A:ARG:HG2	6	0.44
(2,1617)	1:79:A:SER:HA	1:78:A:LYS:HB3	8	0.44
(2,1601)	1:112:A:GLU:HA	1:111:A:SER:HA	3	0.44
(2,1582)	1:104:A:ILE:HD11	1:104:A:ILE:HA	9	0.44
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB3	8	0.44
(2,1545)	1:95:A:PHE:HE2	1:95:A:PHE:HA	10	0.44
(2,1540)	1:135:A:VAL:HA	1:109:A:THR:H	7	0.44
(2,1516)	1:107:A:PRO:HA	1:59:A:MET:HB3	8	0.44
(2,1471)	1:86:A:ILE:HD13	1:89:A:LEU:HB2	4	0.44
(2,1456)	1:104:A:ILE:HD12	1:93:A:ILE:HA	4	0.44
(2,1456)	1:104:A:ILE:HD12	1:93:A:ILE:HA	8	0.44
(2,1438)	1:104:A:ILE:HG22	1:62:A:LEU:HB2	3	0.44
(2,1396)	1:101:A:VAL:HG12	1:65:A:THR:HA	1	0.44
(2,1380)	1:64:A:VAL:HG13	1:128:A:VAL:HG22	5	0.44
(2,1345)	1:110:A:VAL:HG13	1:114:A:ASP:HB2	5	0.44
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD22	2	0.44
(2,1327)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	3	0.44
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD23	1	0.44
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD22	9	0.44
(2,1274)	1:122:A:ILE:HG13	1:119:A:LEU:HB2	4	0.44
(2,1238)	1:134:A:GLU:HB3	1:131:A:LEU:HA	9	0.44
(2,1171)	1:112:A:GLU:HG3	1:112:A:GLU:HB2	3	0.44
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG23	4	0.44
(2,1159)	1:72:A:ASN:HB3	1:76:A:MET:HB3	3	0.44
(2,1153)	1:72:A:ASN:HB3	1:76:A:MET:HG2	9	0.44
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG21	5	0.44
(2,871)	1:87:A:GLU:H	1:92:A:SER:HB3	2	0.44
(2,807)	1:67:A:LYS:H	1:71:A:LYS:HG3	8	0.44
(2,687)	1:108:A:LYS:HE3	1:60:A:THR:HA	10	0.44
(2,592)	1:61:A:ARG:HA	1:61:A:ARG:HD2	8	0.44
(2,494)	1:65:A:THR:HG21	1:99:A:THR:HA	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,333)	1:124:A:ALA:HB2	1:76:A:MET:HG3	4	0.44
(2,333)	1:124:A:ALA:HB1	1:76:A:MET:HG3	7	0.44
(2,333)	1:124:A:ALA:HB2	1:76:A:MET:HG3	9	0.44
(2,331)	1:125:A:ALA:HB2	1:121:A:ASP:HB3	4	0.44
(2,264)	1:65:A:THR:HG23	1:64:A:VAL:HG12	8	0.44
(2,240)	1:110:A:VAL:HG13	1:89:A:LEU:HB2	9	0.44
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG13	4	0.44
(2,182)	1:137:A:LEU:HG	1:61:A:ARG:HD3	1	0.44
(2,121)	1:58:A:GLU:HB3	1:59:A:MET:HA	5	0.44
(2,1940)	1:127:A:GLY:H	1:123:A:LEU:HG	3	0.43
(2,1890)	1:76:A:MET:H	1:77:A:ALA:HA	7	0.43
(2,1890)	1:76:A:MET:H	1:77:A:ALA:HA	10	0.43
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD11	2	0.43
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD13	7	0.43
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD11	10	0.43
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD21	10	0.43
(2,1769)	1:121:A:ASP:HB2	1:82:A:PHE:HA	6	0.43
(2,1721)	1:85:A:ARG:HA	1:85:A:ARG:HD2	10	0.43
(2,1702)	1:106:A:LEU:HB2	1:86:A:ILE:HB	3	0.43
(2,1635)	1:114:A:ASP:HA	1:118:A:LEU:HA	10	0.43
(2,1582)	1:104:A:ILE:HD13	1:104:A:ILE:HA	10	0.43
(2,1545)	1:95:A:PHE:HE2	1:95:A:PHE:HA	4	0.43
(2,1540)	1:135:A:VAL:HA	1:109:A:THR:H	3	0.43
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB1	1	0.43
(2,1429)	1:77:A:ALA:HB3	1:74:A:SER:HA	1	0.43
(2,1429)	1:77:A:ALA:HB1	1:74:A:SER:HA	2	0.43
(2,1367)	1:65:A:THR:HG21	1:100:A:GLY:HA2	4	0.43
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD22	1	0.43
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD22	5	0.43
(2,1294)	1:106:A:LEU:HG	1:90:A:GLY:HA3	9	0.43
(2,1288)	1:137:A:LEU:HG	1:132:A:ASP:HA	6	0.43
(2,1285)	1:93:A:ILE:HG12	1:92:A:SER:HA	1	0.43
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG23	2	0.43
(2,1043)	1:89:A:LEU:H	1:89:A:LEU:HB3	9	0.43
(2,934)	1:60:A:THR:H	1:60:A:THR:HG22	6	0.43
(2,870)	1:87:A:GLU:H	1:84:A:THR:HG22	5	0.43
(2,724)	1:128:A:VAL:HG22	1:65:A:THR:HB	2	0.43
(2,646)	1:106:A:LEU:HG	1:107:A:PRO:HD3	1	0.43
(2,646)	1:106:A:LEU:HG	1:107:A:PRO:HD3	4	0.43
(2,633)	1:120:A:HIS:HB2	1:120:A:HIS:HD2	4	0.43
(2,570)	1:121:A:ASP:HA	1:120:A:HIS:HB2	10	0.43
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG21	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG23	7	0.43
(2,433)	1:76:A:MET:HG3	1:82:A:PHE:HD1	6	0.43
(2,333)	1:124:A:ALA:HB3	1:76:A:MET:HG3	5	0.43
(2,333)	1:124:A:ALA:HB1	1:76:A:MET:HG3	8	0.43
(2,275)	1:64:A:VAL:HG12	1:102:A:THR:HB	4	0.43
(2,121)	1:58:A:GLU:HB3	1:59:A:MET:HA	3	0.43
(2,1925)	1:130:A:GLY:H	1:129:A:VAL:HG13	2	0.42
(2,1890)	1:76:A:MET:H	1:77:A:ALA:HA	8	0.42
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG22	7	0.42
(2,1774)	1:104:A:ILE:HB	1:103:A:MET:HG3	1	0.42
(2,1721)	1:85:A:ARG:HA	1:85:A:ARG:HD2	3	0.42
(2,1721)	1:85:A:ARG:HA	1:85:A:ARG:HD2	4	0.42
(2,1711)	1:104:A:ILE:HG22	1:91:A:GLY:HA2	4	0.42
(2,1694)	1:106:A:LEU:HD23	1:107:A:PRO:HD2	1	0.42
(2,1694)	1:106:A:LEU:HD22	1:107:A:PRO:HD2	7	0.42
(2,1694)	1:106:A:LEU:HD22	1:107:A:PRO:HD2	9	0.42
(2,1682)	1:62:A:LEU:HA	1:103:A:MET:HG3	1	0.42
(2,1651)	1:104:A:ILE:HG23	1:61:A:ARG:HA	4	0.42
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD2	4	0.42
(2,1634)	1:123:A:LEU:HA	1:73:A:PHE:HD2	7	0.42
(2,1626)	1:118:A:LEU:HA	1:85:A:ARG:HG2	10	0.42
(2,1601)	1:111:A:SER:HA	1:110:A:VAL:HA	5	0.42
(2,1582)	1:104:A:ILE:HD11	1:104:A:ILE:HA	3	0.42
(2,1581)	1:104:A:ILE:HA	1:93:A:ILE:HG13	5	0.42
(2,1572)	1:82:A:PHE:HE2	1:77:A:ALA:HA	1	0.42
(2,1557)	1:95:A:PHE:HE2	1:102:A:THR:HB	1	0.42
(2,1439)	1:104:A:ILE:HG21	1:105:A:GLU:HG2	8	0.42
(2,1429)	1:77:A:ALA:HB2	1:74:A:SER:HA	6	0.42
(2,1381)	1:64:A:VAL:HG13	1:125:A:ALA:HB2	1	0.42
(2,1364)	1:119:A:LEU:HD22	1:104:A:ILE:HG12	8	0.42
(2,1357)	1:96:A:LEU:HD23	1:61:A:ARG:HD3	4	0.42
(2,1351)	1:118:A:LEU:HD21	1:85:A:ARG:HD3	10	0.42
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD22	3	0.42
(2,1288)	1:137:A:LEU:HG	1:132:A:ASP:HA	8	0.42
(2,1274)	1:122:A:ILE:HG13	1:119:A:LEU:HB2	3	0.42
(2,1174)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	10	0.42
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG22	5	0.42
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG23	6	0.42
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD22	10	0.42
(2,1043)	1:89:A:LEU:H	1:89:A:LEU:HB3	3	0.42
(2,1042)	1:89:A:LEU:H	1:88:A:GLU:HB3	6	0.42
(2,1032)	1:84:A:THR:H	1:84:A:THR:HG23	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,943)	1:58:A:GLU:H	1:59:A:MET:H	8	0.42
(2,934)	1:60:A:THR:H	1:60:A:THR:HG23	5	0.42
(2,706)	1:122:A:ILE:HG21	1:123:A:LEU:HB2	5	0.42
(2,633)	1:120:A:HIS:HB2	1:120:A:HIS:HD2	1	0.42
(2,633)	1:120:A:HIS:HB2	1:120:A:HIS:HD2	6	0.42
(2,633)	1:120:A:HIS:HB2	1:120:A:HIS:HD2	9	0.42
(2,624)	1:101:A:VAL:HG13	1:63:A:MET:HA	8	0.42
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG22	6	0.42
(2,193)	1:106:A:LEU:HD13	1:106:A:LEU:HA	5	0.42
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG23	4	0.42
(2,121)	1:58:A:GLU:HB3	1:59:A:MET:HA	1	0.42
(2,64)	1:107:A:PRO:HB2	1:135:A:VAL:HG12	9	0.42
(1,26)	1:107:A:PRO:HA	1:59:A:MET:HG3	4	0.42
(1,11)	1:66:A:GLU:HB3	1:101:A:VAL:HA	1	0.42
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD12	7	0.41
(2,1932)	1:92:A:SER:H	1:93:A:ILE:HG13	8	0.41
(2,1890)	1:76:A:MET:H	1:77:A:ALA:HA	5	0.41
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD12	1	0.41
(2,1851)	1:122:A:ILE:H	1:122:A:ILE:HD12	4	0.41
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD21	3	0.41
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD21	6	0.41
(2,1770)	1:116:A:ASP:HB2	1:112:A:GLU:HB3	4	0.41
(2,1763)	1:82:A:PHE:HB2	1:85:A:ARG:HB3	10	0.41
(2,1752)	1:74:A:SER:HA	1:78:A:LYS:HE2	10	0.41
(2,1721)	1:85:A:ARG:HA	1:85:A:ARG:HD2	5	0.41
(2,1651)	1:104:A:ILE:HG23	1:61:A:ARG:HA	9	0.41
(2,1635)	1:114:A:ASP:HA	1:118:A:LEU:HA	2	0.41
(2,1572)	1:82:A:PHE:HE2	1:77:A:ALA:HA	5	0.41
(2,1471)	1:86:A:ILE:HD13	1:89:A:LEU:HB2	3	0.41
(2,1439)	1:104:A:ILE:HG21	1:105:A:GLU:HG2	6	0.41
(2,1429)	1:77:A:ALA:HB1	1:74:A:SER:HA	3	0.41
(2,1404)	1:102:A:THR:HG23	1:77:A:ALA:HA	7	0.41
(2,1380)	1:64:A:VAL:HG11	1:128:A:VAL:HG23	1	0.41
(2,1357)	1:96:A:LEU:HD23	1:61:A:ARG:HD2	1	0.41
(2,1351)	1:118:A:LEU:HD22	1:85:A:ARG:HD3	4	0.41
(2,1351)	1:118:A:LEU:HD23	1:85:A:ARG:HD3	5	0.41
(2,1351)	1:118:A:LEU:HD22	1:85:A:ARG:HD3	9	0.41
(2,1336)	1:115:A:MET:HB3	1:106:A:LEU:HD23	6	0.41
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD22	10	0.41
(2,1297)	1:86:A:ILE:HG13	1:82:A:PHE:HZ	8	0.41
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD23	5	0.41
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG22	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1159)	1:72:A:ASN:HB2	1:76:A:MET:HB3	10	0.41
(2,1043)	1:89:A:LEU:H	1:89:A:LEU:HB3	1	0.41
(2,934)	1:60:A:THR:H	1:60:A:THR:HG22	3	0.41
(2,728)	1:124:A:ALA:HB3	1:120:A:HIS:HB2	4	0.41
(2,646)	1:106:A:LEU:HG	1:107:A:PRO:HD3	7	0.41
(2,633)	1:120:A:HIS:HB2	1:120:A:HIS:HD2	3	0.41
(2,633)	1:120:A:HIS:HB2	1:120:A:HIS:HD2	8	0.41
(2,633)	1:120:A:HIS:HB2	1:120:A:HIS:HD2	10	0.41
(2,589)	1:71:A:LYS:HG2	1:71:A:LYS:HA	5	0.41
(2,570)	1:121:A:ASP:HA	1:120:A:HIS:HB2	8	0.41
(2,427)	1:111:A:SER:HB2	1:110:A:VAL:HG11	6	0.41
(2,331)	1:125:A:ALA:HB2	1:121:A:ASP:HB3	10	0.41
(2,193)	1:106:A:LEU:HD13	1:106:A:LEU:HA	2	0.41
(2,193)	1:106:A:LEU:HD11	1:106:A:LEU:HA	6	0.41
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG21	5	0.41
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG23	7	0.41
(2,121)	1:58:A:GLU:HB3	1:59:A:MET:HA	6	0.41
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG13	3	0.41
(2,1940)	1:127:A:GLY:H	1:123:A:LEU:HG	1	0.4
(2,1890)	1:76:A:MET:H	1:77:A:ALA:HA	1	0.4
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG23	9	0.4
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD23	7	0.4
(2,1770)	1:116:A:ASP:HB2	1:112:A:GLU:HB3	8	0.4
(2,1747)	1:78:A:LYS:HE3	1:75:A:LYS:HA	10	0.4
(2,1741)	1:136:A:LYS:HE2	1:136:A:LYS:HA	4	0.4
(2,1694)	1:106:A:LEU:HD23	1:107:A:PRO:HD2	4	0.4
(2,1694)	1:106:A:LEU:HD21	1:107:A:PRO:HD2	8	0.4
(2,1683)	1:131:A:LEU:HD11	1:62:A:LEU:HA	6	0.4
(2,1682)	1:62:A:LEU:HA	1:103:A:MET:HG3	9	0.4
(2,1651)	1:104:A:ILE:HG21	1:61:A:ARG:HA	6	0.4
(2,1582)	1:104:A:ILE:HD13	1:104:A:ILE:HA	2	0.4
(2,1582)	1:104:A:ILE:HD11	1:104:A:ILE:HA	5	0.4
(2,1581)	1:104:A:ILE:HA	1:93:A:ILE:HG13	7	0.4
(2,1540)	1:135:A:VAL:HA	1:109:A:THR:H	9	0.4
(2,1524)	1:136:A:LYS:HD2	1:135:A:VAL:HA	8	0.4
(2,1488)	1:92:A:SER:HB2	1:93:A:ILE:HB	6	0.4
(2,1439)	1:104:A:ILE:HG23	1:105:A:GLU:HG2	9	0.4
(2,1434)	1:86:A:ILE:HG21	1:106:A:LEU:HD12	9	0.4
(2,1429)	1:77:A:ALA:HB3	1:74:A:SER:HA	8	0.4
(2,1418)	1:64:A:VAL:HG21	1:127:A:GLY:HA2	3	0.4
(2,1400)	1:96:A:LEU:HB2	1:101:A:VAL:HG23	2	0.4
(2,1396)	1:101:A:VAL:HG13	1:65:A:THR:HA	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1351)	1:118:A:LEU:HD23	1:85:A:ARG:HD3	1	0.4
(2,1351)	1:118:A:LEU:HD21	1:85:A:ARG:HD3	6	0.4
(2,1297)	1:86:A:ILE:HG13	1:82:A:PHE:HZ	4	0.4
(2,1241)	1:120:A:HIS:HB3	1:123:A:LEU:HD23	9	0.4
(2,1224)	1:115:A:MET:HB3	1:111:A:SER:HB2	6	0.4
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG21	7	0.4
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD23	6	0.4
(2,1042)	1:89:A:LEU:H	1:88:A:GLU:HB3	4	0.4
(2,1042)	1:89:A:LEU:H	1:88:A:GLU:HB3	9	0.4
(2,934)	1:60:A:THR:H	1:60:A:THR:HG23	4	0.4
(2,813)	1:137:A:LEU:H	1:137:A:LEU:HD13	7	0.4
(2,724)	1:128:A:VAL:HG22	1:65:A:THR:HB	9	0.4
(2,706)	1:122:A:ILE:HG22	1:123:A:LEU:HB2	3	0.4
(2,654)	1:72:A:ASN:HB2	1:126:A:GLY:HA3	6	0.4
(2,633)	1:120:A:HIS:HB2	1:120:A:HIS:HD2	2	0.4
(2,633)	1:120:A:HIS:HB2	1:120:A:HIS:HD2	5	0.4
(2,633)	1:120:A:HIS:HB2	1:120:A:HIS:HD2	7	0.4
(2,570)	1:121:A:ASP:HA	1:120:A:HIS:HB2	1	0.4
(2,570)	1:121:A:ASP:HA	1:120:A:HIS:HB2	3	0.4
(2,570)	1:121:A:ASP:HA	1:120:A:HIS:HB2	5	0.4
(2,489)	1:95:A:PHE:HE2	1:78:A:LYS:HE3	9	0.4
(2,459)	1:77:A:ALA:HB2	1:74:A:SER:HB3	5	0.4
(2,343)	1:86:A:ILE:HG23	1:91:A:GLY:HA2	3	0.4
(2,333)	1:124:A:ALA:HB1	1:76:A:MET:HG3	3	0.4
(2,318)	1:64:A:VAL:HG21	1:102:A:THR:HB	2	0.4
(2,318)	1:64:A:VAL:HG21	1:102:A:THR:HB	9	0.4
(2,318)	1:64:A:VAL:HG23	1:102:A:THR:HB	10	0.4
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG23	8	0.4
(2,275)	1:64:A:VAL:HG11	1:102:A:THR:HB	6	0.4
(2,241)	1:106:A:LEU:HD22	1:110:A:VAL:HG11	2	0.4
(2,225)	1:115:A:MET:HG3	1:119:A:LEU:HD12	5	0.4
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG21	1	0.4
(2,132)	1:75:A:LYS:HD3	1:75:A:LYS:HA	7	0.4
(2,1940)	1:127:A:GLY:H	1:123:A:LEU:HG	2	0.39
(2,1940)	1:127:A:GLY:H	1:123:A:LEU:HG	8	0.39
(2,1932)	1:92:A:SER:H	1:93:A:ILE:HG13	2	0.39
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD21	2	0.39
(2,1796)	1:96:A:LEU:H	1:96:A:LEU:HB3	7	0.39
(2,1771)	1:111:A:SER:HB3	1:114:A:ASP:HB2	10	0.39
(2,1749)	1:95:A:PHE:HE2	1:78:A:LYS:HE3	9	0.39
(2,1745)	1:134:A:GLU:HB2	1:108:A:LYS:HE3	5	0.39
(2,1721)	1:85:A:ARG:HA	1:85:A:ARG:HD2	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1694)	1:106:A:LEU:HD23	1:107:A:PRO:HD2	2	0.39
(2,1694)	1:106:A:LEU:HD21	1:107:A:PRO:HD2	6	0.39
(2,1673)	1:93:A:ILE:HD13	1:77:A:ALA:HA	4	0.39
(2,1673)	1:93:A:ILE:HD11	1:77:A:ALA:HA	8	0.39
(2,1648)	1:136:A:LYS:HG2	1:136:A:LYS:HA	2	0.39
(2,1645)	1:71:A:LYS:HA	1:69:A:GLU:HB3	2	0.39
(2,1601)	1:112:A:GLU:HA	1:111:A:SER:HA	6	0.39
(2,1601)	1:112:A:GLU:HA	1:111:A:SER:HA	7	0.39
(2,1582)	1:104:A:ILE:HD13	1:104:A:ILE:HA	6	0.39
(2,1545)	1:95:A:PHE:HE1	1:95:A:PHE:HA	7	0.39
(2,1540)	1:135:A:VAL:HA	1:109:A:THR:H	1	0.39
(2,1488)	1:92:A:SER:HB2	1:93:A:ILE:HB	3	0.39
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB3	6	0.39
(2,1434)	1:86:A:ILE:HG22	1:106:A:LEU:HD12	7	0.39
(2,1433)	1:77:A:ALA:HB2	1:78:A:LYS:HB2	5	0.39
(2,1429)	1:77:A:ALA:HB1	1:74:A:SER:HA	7	0.39
(2,1364)	1:119:A:LEU:HD21	1:104:A:ILE:HG12	7	0.39
(2,1364)	1:119:A:LEU:HD22	1:104:A:ILE:HG12	9	0.39
(2,1351)	1:118:A:LEU:HD22	1:85:A:ARG:HD3	2	0.39
(2,1351)	1:118:A:LEU:HD23	1:85:A:ARG:HD3	3	0.39
(2,1351)	1:118:A:LEU:HD22	1:85:A:ARG:HD3	7	0.39
(2,1351)	1:118:A:LEU:HD21	1:85:A:ARG:HD3	8	0.39
(2,1345)	1:110:A:VAL:HG11	1:114:A:ASP:HB2	3	0.39
(2,1341)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	3	0.39
(2,1324)	1:115:A:MET:HG3	1:108:A:LYS:HG3	2	0.39
(2,1324)	1:115:A:MET:HG3	1:108:A:LYS:HG3	6	0.39
(2,1321)	1:62:A:LEU:HD11	1:82:A:PHE:HZ	4	0.39
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD23	2	0.39
(2,1297)	1:86:A:ILE:HG13	1:82:A:PHE:HZ	9	0.39
(2,1294)	1:106:A:LEU:HG	1:90:A:GLY:HA3	7	0.39
(2,1178)	1:85:A:ARG:H	1:86:A:ILE:HB	4	0.39
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD21	1	0.39
(2,1043)	1:89:A:LEU:H	1:89:A:LEU:HB3	8	0.39
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG21	7	0.39
(2,870)	1:87:A:GLU:H	1:84:A:THR:HG22	10	0.39
(2,744)	1:105:A:GLU:H	1:105:A:GLU:HG2	7	0.39
(2,706)	1:122:A:ILE:HG21	1:123:A:LEU:HB2	7	0.39
(2,706)	1:122:A:ILE:HG22	1:123:A:LEU:HB2	8	0.39
(2,706)	1:122:A:ILE:HG23	1:123:A:LEU:HB2	9	0.39
(2,706)	1:122:A:ILE:HG22	1:123:A:LEU:HB2	10	0.39
(2,649)	1:70:A:SER:HB2	1:126:A:GLY:HA3	1	0.39
(2,626)	1:64:A:VAL:HG11	1:63:A:MET:HA	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,626)	1:64:A:VAL:HG13	1:63:A:MET:HA	6	0.39
(2,626)	1:64:A:VAL:HG12	1:63:A:MET:HA	8	0.39
(2,626)	1:64:A:VAL:HG13	1:63:A:MET:HA	10	0.39
(2,583)	1:136:A:LYS:HA	1:133:A:SER:HB2	1	0.39
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG21	5	0.39
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG21	7	0.39
(2,246)	1:123:A:LEU:HD13	1:127:A:GLY:HA2	3	0.39
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG13	6	0.39
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG11	7	0.39
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG13	8	0.39
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG12	9	0.39
(2,225)	1:115:A:MET:HG3	1:119:A:LEU:HD13	7	0.39
(2,193)	1:106:A:LEU:HD11	1:106:A:LEU:HA	10	0.39
(2,131)	1:136:A:LYS:HD3	1:58:A:GLU:HG3	10	0.39
(1,13)	1:120:A:HIS:HB2	1:122:A:ILE:HG13	10	0.39
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD13	6	0.38
(2,1939)	1:127:A:GLY:H	1:122:A:ILE:HB	8	0.38
(2,1770)	1:116:A:ASP:HB2	1:112:A:GLU:HB3	1	0.38
(2,1739)	1:75:A:LYS:HG3	1:75:A:LYS:HE3	1	0.38
(2,1670)	1:77:A:ALA:HA	1:78:A:LYS:HA	3	0.38
(2,1661)	1:134:A:GLU:HB3	1:131:A:LEU:HA	2	0.38
(2,1582)	1:104:A:ILE:HD11	1:104:A:ILE:HA	7	0.38
(2,1582)	1:104:A:ILE:HD12	1:104:A:ILE:HA	8	0.38
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB3	3	0.38
(2,1572)	1:82:A:PHE:HE2	1:77:A:ALA:HA	4	0.38
(2,1572)	1:82:A:PHE:HE2	1:77:A:ALA:HA	7	0.38
(2,1545)	1:95:A:PHE:HE2	1:95:A:PHE:HA	2	0.38
(2,1545)	1:95:A:PHE:HE1	1:95:A:PHE:HA	6	0.38
(2,1524)	1:136:A:LYS:HD2	1:135:A:VAL:HA	1	0.38
(2,1488)	1:92:A:SER:HB2	1:93:A:ILE:HB	2	0.38
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB1	4	0.38
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB3	9	0.38
(2,1443)	1:86:A:ILE:HG22	1:87:A:GLU:HA	10	0.38
(2,1439)	1:104:A:ILE:HG23	1:105:A:GLU:HG2	4	0.38
(2,1417)	1:64:A:VAL:HG22	1:62:A:LEU:HA	2	0.38
(2,1412)	1:128:A:VAL:HG12	1:130:A:GLY:HA2	4	0.38
(2,1345)	1:110:A:VAL:HG12	1:114:A:ASP:HB2	7	0.38
(2,1317)	1:78:A:LYS:HG3	1:78:A:LYS:HA	2	0.38
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD21	6	0.38
(2,1238)	1:134:A:GLU:HB3	1:131:A:LEU:HA	2	0.38
(2,1225)	1:115:A:MET:HB2	1:107:A:PRO:HD2	3	0.38
(2,1225)	1:115:A:MET:HB2	1:107:A:PRO:HD2	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1159)	1:72:A:ASN:HB3	1:76:A:MET:HB3	6	0.38
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG22	3	0.38
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG23	9	0.38
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB3	8	0.38
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD23	4	0.38
(2,1043)	1:89:A:LEU:H	1:89:A:LEU:HB3	4	0.38
(2,1042)	1:89:A:LEU:H	1:88:A:GLU:HB3	8	0.38
(2,870)	1:87:A:GLU:H	1:84:A:THR:HG23	4	0.38
(2,570)	1:121:A:ASP:HA	1:120:A:HIS:HB2	2	0.38
(2,570)	1:121:A:ASP:HA	1:120:A:HIS:HB2	4	0.38
(2,343)	1:86:A:ILE:HG22	1:91:A:GLY:HA2	9	0.38
(2,333)	1:124:A:ALA:HB2	1:76:A:MET:HG3	10	0.38
(2,331)	1:125:A:ALA:HB2	1:121:A:ASP:HB3	7	0.38
(2,318)	1:64:A:VAL:HG22	1:102:A:THR:HB	3	0.38
(2,307)	1:102:A:THR:HG22	1:64:A:VAL:HB	6	0.38
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG13	1	0.38
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG11	9	0.38
(2,246)	1:123:A:LEU:HD12	1:127:A:GLY:HA2	9	0.38
(2,230)	1:62:A:LEU:HD11	1:122:A:ILE:HG12	9	0.38
(2,193)	1:106:A:LEU:HD11	1:106:A:LEU:HA	3	0.38
(2,193)	1:106:A:LEU:HD12	1:106:A:LEU:HA	4	0.38
(2,182)	1:137:A:LEU:HG	1:61:A:ARG:HD2	4	0.38
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG22	3	0.38
(1,60)	1:119:A:LEU:H	1:114:A:ASP:HB2	10	0.38
(2,1939)	1:127:A:GLY:H	1:122:A:ILE:HB	7	0.37
(2,1932)	1:92:A:SER:H	1:93:A:ILE:HG13	10	0.37
(2,1922)	1:86:A:ILE:H	1:87:A:GLU:HB2	9	0.37
(2,1915)	1:79:A:SER:H	1:78:A:LYS:HG3	10	0.37
(2,1891)	1:116:A:ASP:H	1:115:A:MET:HB2	9	0.37
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD21	1	0.37
(2,1860)	1:77:A:ALA:H	1:76:A:MET:HG2	5	0.37
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG22	3	0.37
(2,1721)	1:85:A:ARG:HA	1:85:A:ARG:HD2	6	0.37
(2,1721)	1:85:A:ARG:HA	1:85:A:ARG:HD2	9	0.37
(2,1694)	1:106:A:LEU:HD22	1:107:A:PRO:HD2	10	0.37
(2,1675)	1:101:A:VAL:HG12	1:103:A:MET:HA	7	0.37
(2,1607)	1:76:A:MET:HA	1:75:A:LYS:HG2	1	0.37
(2,1601)	1:112:A:GLU:HA	1:111:A:SER:HA	4	0.37
(2,1601)	1:112:A:GLU:HA	1:111:A:SER:HA	8	0.37
(2,1601)	1:112:A:GLU:HA	1:111:A:SER:HA	9	0.37
(2,1557)	1:95:A:PHE:HE2	1:102:A:THR:HB	4	0.37
(2,1545)	1:95:A:PHE:HE1	1:95:A:PHE:HA	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1540)	1:135:A:VAL:HA	1:109:A:THR:H	2	0.37
(2,1438)	1:104:A:ILE:HG22	1:62:A:LEU:HB2	10	0.37
(2,1434)	1:86:A:ILE:HG22	1:106:A:LEU:HD11	3	0.37
(2,1345)	1:110:A:VAL:HG12	1:114:A:ASP:HB2	1	0.37
(2,1294)	1:106:A:LEU:HG	1:90:A:GLY:HA3	5	0.37
(2,1288)	1:137:A:LEU:HG	1:132:A:ASP:HA	9	0.37
(2,1171)	1:88:A:GLU:HG2	1:88:A:GLU:HB2	7	0.37
(2,1159)	1:72:A:ASN:HB3	1:76:A:MET:HB3	9	0.37
(2,1154)	1:72:A:ASN:HB2	1:73:A:PHE:HD1	1	0.37
(2,1154)	1:72:A:ASN:HB2	1:73:A:PHE:HD2	7	0.37
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD23	2	0.37
(2,934)	1:60:A:THR:H	1:60:A:THR:HG23	9	0.37
(2,706)	1:122:A:ILE:HG22	1:123:A:LEU:HB2	1	0.37
(2,702)	1:123:A:LEU:HB2	1:129:A:VAL:HG21	3	0.37
(2,570)	1:121:A:ASP:HA	1:120:A:HIS:HB2	9	0.37
(2,340)	1:124:A:ALA:HB2	1:121:A:ASP:HB2	10	0.37
(2,318)	1:64:A:VAL:HG23	1:102:A:THR:HB	7	0.37
(2,318)	1:64:A:VAL:HG23	1:102:A:THR:HB	8	0.37
(2,307)	1:102:A:THR:HG23	1:64:A:VAL:HB	4	0.37
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG12	3	0.37
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG13	4	0.37
(2,246)	1:123:A:LEU:HD12	1:127:A:GLY:HA2	5	0.37
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG12	5	0.37
(2,193)	1:106:A:LEU:HD13	1:106:A:LEU:HA	1	0.37
(2,193)	1:106:A:LEU:HD12	1:106:A:LEU:HA	7	0.37
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG12	9	0.37
(2,36)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	4	0.37
(1,13)	1:120:A:HIS:HB2	1:122:A:ILE:HG13	2	0.37
(1,11)	1:66:A:GLU:HB3	1:101:A:VAL:HA	3	0.37
(2,1932)	1:92:A:SER:H	1:93:A:ILE:HG13	4	0.36
(2,1891)	1:116:A:ASP:H	1:115:A:MET:HB2	5	0.36
(2,1891)	1:116:A:ASP:H	1:115:A:MET:HB2	7	0.36
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD22	8	0.36
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD23	5	0.36
(2,1774)	1:104:A:ILE:HB	1:103:A:MET:HG3	9	0.36
(2,1651)	1:104:A:ILE:HG21	1:61:A:ARG:HA	8	0.36
(2,1643)	1:58:A:GLU:HA	1:58:A:GLU:HG3	3	0.36
(2,1582)	1:104:A:ILE:HD11	1:104:A:ILE:HA	4	0.36
(2,1581)	1:104:A:ILE:HA	1:93:A:ILE:HG13	6	0.36
(2,1557)	1:95:A:PHE:HE1	1:102:A:THR:HB	3	0.36
(2,1532)	1:87:A:GLU:HB3	1:83:A:SER:HA	10	0.36
(2,1439)	1:104:A:ILE:HG22	1:105:A:GLU:HG2	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1438)	1:104:A:ILE:HG23	1:62:A:LEU:HB2	7	0.36
(2,1344)	1:123:A:LEU:HD22	1:129:A:VAL:HG21	10	0.36
(2,1317)	1:78:A:LYS:HG3	1:78:A:LYS:HA	8	0.36
(2,1317)	1:78:A:LYS:HG3	1:78:A:LYS:HA	10	0.36
(2,1294)	1:106:A:LEU:HG	1:90:A:GLY:HA3	6	0.36
(2,1285)	1:93:A:ILE:HG12	1:92:A:SER:HA	3	0.36
(2,1285)	1:93:A:ILE:HG12	1:92:A:SER:HA	5	0.36
(2,1225)	1:115:A:MET:HB2	1:107:A:PRO:HD2	9	0.36
(2,1147)	1:126:A:GLY:H	1:122:A:ILE:HG22	1	0.36
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD22	7	0.36
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD23	8	0.36
(2,1043)	1:89:A:LEU:H	1:89:A:LEU:HB3	6	0.36
(2,1012)	1:119:A:LEU:H	1:119:A:LEU:HB3	2	0.36
(2,1012)	1:119:A:LEU:H	1:119:A:LEU:HB3	10	0.36
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG22	3	0.36
(2,728)	1:124:A:ALA:HB2	1:120:A:HIS:HB2	2	0.36
(2,626)	1:64:A:VAL:HG12	1:63:A:MET:HA	1	0.36
(2,626)	1:64:A:VAL:HG13	1:63:A:MET:HA	7	0.36
(2,624)	1:101:A:VAL:HG13	1:63:A:MET:HA	4	0.36
(2,604)	1:131:A:LEU:HD22	1:131:A:LEU:HA	6	0.36
(2,594)	1:61:A:ARG:HG2	1:61:A:ARG:HA	7	0.36
(2,570)	1:121:A:ASP:HA	1:120:A:HIS:HB2	7	0.36
(2,494)	1:65:A:THR:HG23	1:99:A:THR:HA	2	0.36
(2,374)	1:104:A:ILE:HD12	1:122:A:ILE:HG21	1	0.36
(2,374)	1:104:A:ILE:HD13	1:122:A:ILE:HG23	5	0.36
(2,374)	1:104:A:ILE:HD13	1:122:A:ILE:HG23	7	0.36
(2,369)	1:104:A:ILE:HD13	1:122:A:ILE:HG13	5	0.36
(2,369)	1:104:A:ILE:HD11	1:122:A:ILE:HG13	8	0.36
(2,307)	1:102:A:THR:HG22	1:64:A:VAL:HB	7	0.36
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG13	2	0.36
(2,297)	1:101:A:VAL:HB	1:101:A:VAL:HG12	10	0.36
(2,279)	1:64:A:VAL:HG12	1:122:A:ILE:HG23	5	0.36
(2,267)	1:110:A:VAL:HG21	1:114:A:ASP:HB3	6	0.36
(2,267)	1:110:A:VAL:HG23	1:114:A:ASP:HB3	8	0.36
(2,264)	1:65:A:THR:HG22	1:64:A:VAL:HG11	2	0.36
(2,230)	1:62:A:LEU:HD12	1:122:A:ILE:HG12	5	0.36
(2,230)	1:62:A:LEU:HD11	1:122:A:ILE:HG12	8	0.36
(2,225)	1:115:A:MET:HG3	1:119:A:LEU:HD11	6	0.36
(2,193)	1:106:A:LEU:HD13	1:106:A:LEU:HA	8	0.36
(2,182)	1:137:A:LEU:HG	1:61:A:ARG:HD2	3	0.36
(2,182)	1:137:A:LEU:HG	1:61:A:ARG:HD2	9	0.36
(2,133)	1:67:A:LYS:HD3	1:69:A:GLU:HB3	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,36)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	1	0.36
(2,36)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	5	0.36
(2,36)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	6	0.36
(2,36)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	8	0.36
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG23	8	0.35
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG22	9	0.35
(2,1932)	1:92:A:SER:H	1:93:A:ILE:HG13	1	0.35
(2,1891)	1:116:A:ASP:H	1:115:A:MET:HB2	2	0.35
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG21	2	0.35
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG22	6	0.35
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG23	8	0.35
(2,1721)	1:85:A:ARG:HA	1:85:A:ARG:HD2	7	0.35
(2,1711)	1:104:A:ILE:HG23	1:91:A:GLY:HA2	2	0.35
(2,1658)	1:60:A:THR:HG22	1:105:A:GLU:HA	3	0.35
(2,1601)	1:112:A:GLU:HA	1:111:A:SER:HA	1	0.35
(2,1572)	1:82:A:PHE:HE2	1:77:A:ALA:HA	9	0.35
(2,1572)	1:82:A:PHE:HE2	1:77:A:ALA:HA	10	0.35
(2,1546)	1:95:A:PHE:HE1	1:102:A:THR:HA	8	0.35
(2,1488)	1:92:A:SER:HB2	1:93:A:ILE:HB	1	0.35
(2,1488)	1:92:A:SER:HB2	1:93:A:ILE:HB	7	0.35
(2,1488)	1:92:A:SER:HB2	1:93:A:ILE:HB	10	0.35
(2,1443)	1:86:A:ILE:HG22	1:87:A:GLU:HA	2	0.35
(2,1429)	1:77:A:ALA:HB1	1:74:A:SER:HA	10	0.35
(2,1325)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	1	0.35
(2,1294)	1:106:A:LEU:HG	1:90:A:GLY:HA3	3	0.35
(2,1288)	1:137:A:LEU:HG	1:132:A:ASP:HA	10	0.35
(2,1222)	1:76:A:MET:HG3	1:77:A:ALA:HB1	1	0.35
(2,1159)	1:72:A:ASN:HB3	1:76:A:MET:HB3	2	0.35
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB3	8	0.35
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB1	2	0.35
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD23	3	0.35
(2,1043)	1:89:A:LEU:H	1:89:A:LEU:HB3	7	0.35
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG22	9	0.35
(2,813)	1:137:A:LEU:H	1:137:A:LEU:HD12	3	0.35
(2,744)	1:105:A:GLU:H	1:105:A:GLU:HG2	6	0.35
(2,744)	1:105:A:GLU:H	1:105:A:GLU:HG2	8	0.35
(2,706)	1:122:A:ILE:HG23	1:123:A:LEU:HB2	2	0.35
(2,706)	1:122:A:ILE:HG21	1:123:A:LEU:HB2	4	0.35
(2,706)	1:122:A:ILE:HG23	1:123:A:LEU:HB2	6	0.35
(2,654)	1:72:A:ASN:HB2	1:126:A:GLY:HA3	3	0.35
(2,626)	1:64:A:VAL:HG11	1:63:A:MET:HA	2	0.35
(2,530)	1:88:A:GLU:HA	1:88:A:GLU:HB2	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,530)	1:88:A:GLU:HA	1:88:A:GLU:HB2	3	0.35
(2,530)	1:88:A:GLU:HA	1:88:A:GLU:HB2	4	0.35
(2,530)	1:88:A:GLU:HA	1:88:A:GLU:HB2	5	0.35
(2,530)	1:88:A:GLU:HA	1:88:A:GLU:HB2	6	0.35
(2,530)	1:88:A:GLU:HA	1:88:A:GLU:HB2	9	0.35
(2,530)	1:88:A:GLU:HA	1:88:A:GLU:HB2	10	0.35
(2,472)	1:82:A:PHE:HA	1:84:A:THR:HG23	1	0.35
(2,436)	1:93:A:ILE:HG21	1:82:A:PHE:HD2	8	0.35
(2,423)	1:111:A:SER:HB2	1:114:A:ASP:HB3	2	0.35
(2,374)	1:104:A:ILE:HD13	1:122:A:ILE:HG22	9	0.35
(2,369)	1:104:A:ILE:HD13	1:122:A:ILE:HG13	3	0.35
(2,341)	1:77:A:ALA:HB1	1:78:A:LYS:HA	3	0.35
(2,267)	1:110:A:VAL:HG22	1:114:A:ASP:HB3	7	0.35
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG11	1	0.35
(2,230)	1:62:A:LEU:HD11	1:122:A:ILE:HG12	4	0.35
(2,230)	1:62:A:LEU:HD12	1:122:A:ILE:HG12	6	0.35
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG11	2	0.35
(2,36)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	2	0.35
(2,36)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	3	0.35
(2,36)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	9	0.35
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG11	10	0.35
(1,36)	1:85:A:ARG:HA	1:88:A:GLU:HB3	5	0.35
(1,13)	1:120:A:HIS:HB2	1:122:A:ILE:HG13	3	0.35
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD11	5	0.34
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD13	10	0.34
(2,1930)	1:92:A:SER:H	1:105:A:GLU:HG2	2	0.34
(2,1891)	1:116:A:ASP:H	1:115:A:MET:HB2	10	0.34
(2,1796)	1:96:A:LEU:H	1:101:A:VAL:HB	4	0.34
(2,1779)	1:120:A:HIS:HB3	1:123:A:LEU:HD23	9	0.34
(2,1774)	1:104:A:ILE:HB	1:103:A:MET:HG3	4	0.34
(2,1711)	1:104:A:ILE:HG21	1:91:A:GLY:HA2	3	0.34
(2,1694)	1:106:A:LEU:HD23	1:107:A:PRO:HD2	3	0.34
(2,1673)	1:93:A:ILE:HD11	1:77:A:ALA:HA	1	0.34
(2,1673)	1:93:A:ILE:HD13	1:77:A:ALA:HA	10	0.34
(2,1661)	1:134:A:GLU:HB3	1:131:A:LEU:HA	6	0.34
(2,1627)	1:95:A:PHE:HA	1:101:A:VAL:HB	1	0.34
(2,1601)	1:112:A:GLU:HA	1:111:A:SER:HA	2	0.34
(2,1601)	1:112:A:GLU:HA	1:111:A:SER:HA	10	0.34
(2,1581)	1:104:A:ILE:HA	1:93:A:ILE:HG13	3	0.34
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB2	2	0.34
(2,1557)	1:95:A:PHE:HE2	1:102:A:THR:HB	2	0.34
(2,1557)	1:95:A:PHE:HE1	1:102:A:THR:HB	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1553)	1:60:A:THR:HA	1:59:A:MET:HG2	6	0.34
(2,1540)	1:135:A:VAL:HA	1:109:A:THR:H	6	0.34
(2,1540)	1:135:A:VAL:HA	1:109:A:THR:H	10	0.34
(2,1524)	1:136:A:LYS:HD2	1:135:A:VAL:HA	3	0.34
(2,1488)	1:92:A:SER:HB2	1:93:A:ILE:HB	5	0.34
(2,1434)	1:86:A:ILE:HG22	1:106:A:LEU:HD12	4	0.34
(2,1403)	1:102:A:THR:HG21	1:74:A:SER:HA	10	0.34
(2,1396)	1:101:A:VAL:HG11	1:65:A:THR:HA	3	0.34
(2,1372)	1:89:A:LEU:HD21	1:88:A:GLU:HB3	1	0.34
(2,1324)	1:115:A:MET:HG3	1:108:A:LYS:HG3	4	0.34
(2,1317)	1:78:A:LYS:HG3	1:78:A:LYS:HA	1	0.34
(2,1297)	1:86:A:ILE:HG13	1:82:A:PHE:HZ	3	0.34
(2,1285)	1:93:A:ILE:HG12	1:92:A:SER:HA	7	0.34
(2,1238)	1:134:A:GLU:HB3	1:131:A:LEU:HA	6	0.34
(2,1224)	1:115:A:MET:HB3	1:111:A:SER:HB2	8	0.34
(2,1208)	1:66:A:GLU:HB3	1:74:A:SER:HA	4	0.34
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB3	1	0.34
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB2	6	0.34
(2,1012)	1:119:A:LEU:H	1:119:A:LEU:HB3	1	0.34
(2,990)	1:59:A:MET:H	1:59:A:MET:HB3	5	0.34
(2,813)	1:137:A:LEU:H	1:137:A:LEU:HD11	9	0.34
(2,744)	1:105:A:GLU:H	1:105:A:GLU:HG2	2	0.34
(2,744)	1:105:A:GLU:H	1:105:A:GLU:HG2	9	0.34
(2,646)	1:106:A:LEU:HG	1:107:A:PRO:HD3	9	0.34
(2,626)	1:64:A:VAL:HG12	1:63:A:MET:HA	3	0.34
(2,626)	1:64:A:VAL:HG11	1:63:A:MET:HA	5	0.34
(2,624)	1:101:A:VAL:HG11	1:63:A:MET:HA	9	0.34
(2,570)	1:121:A:ASP:HA	1:120:A:HIS:HB2	6	0.34
(2,530)	1:88:A:GLU:HA	1:88:A:GLU:HB2	2	0.34
(2,530)	1:88:A:GLU:HA	1:88:A:GLU:HB2	8	0.34
(2,369)	1:104:A:ILE:HD12	1:122:A:ILE:HG13	2	0.34
(2,369)	1:104:A:ILE:HD13	1:122:A:ILE:HG13	4	0.34
(2,369)	1:104:A:ILE:HD12	1:122:A:ILE:HG13	6	0.34
(2,369)	1:104:A:ILE:HD13	1:122:A:ILE:HG13	9	0.34
(2,359)	1:122:A:ILE:HG23	1:64:A:VAL:HA	8	0.34
(2,352)	1:104:A:ILE:HG21	1:73:A:PHE:HZ	7	0.34
(2,287)	1:84:A:THR:HG22	1:85:A:ARG:HD3	3	0.34
(2,264)	1:65:A:THR:HG21	1:64:A:VAL:HG13	6	0.34
(2,246)	1:123:A:LEU:HD11	1:127:A:GLY:HA2	8	0.34
(2,246)	1:123:A:LEU:HD12	1:127:A:GLY:HA2	10	0.34
(2,230)	1:62:A:LEU:HD11	1:122:A:ILE:HG12	2	0.34
(2,230)	1:62:A:LEU:HD13	1:122:A:ILE:HG12	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,230)	1:62:A:LEU:HD13	1:122:A:ILE:HG12	7	0.34
(2,230)	1:62:A:LEU:HD12	1:122:A:ILE:HG12	10	0.34
(2,193)	1:106:A:LEU:HD12	1:106:A:LEU:HA	9	0.34
(2,182)	1:137:A:LEU:HG	1:61:A:ARG:HD2	6	0.34
(1,60)	1:119:A:LEU:H	1:114:A:ASP:HB2	2	0.34
(1,13)	1:120:A:HIS:HB2	1:122:A:ILE:HG13	4	0.34
(2,1947)	1:90:A:GLY:H	1:89:A:LEU:HD11	2	0.33
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG23	1	0.33
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG22	7	0.33
(2,1930)	1:92:A:SER:H	1:105:A:GLU:HG2	4	0.33
(2,1930)	1:92:A:SER:H	1:105:A:GLU:HG2	10	0.33
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD21	8	0.33
(2,1796)	1:96:A:LEU:H	1:101:A:VAL:HB	5	0.33
(2,1721)	1:85:A:ARG:HA	1:85:A:ARG:HD2	1	0.33
(2,1721)	1:85:A:ARG:HA	1:85:A:ARG:HD2	8	0.33
(2,1683)	1:131:A:LEU:HD22	1:62:A:LEU:HA	2	0.33
(2,1662)	1:131:A:LEU:HA	1:61:A:ARG:HA	7	0.33
(2,1516)	1:107:A:PRO:HA	1:59:A:MET:HB3	5	0.33
(2,1488)	1:92:A:SER:HB2	1:93:A:ILE:HB	9	0.33
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB3	5	0.33
(2,1471)	1:86:A:ILE:HD13	1:89:A:LEU:HB2	6	0.33
(2,1367)	1:65:A:THR:HG21	1:100:A:GLY:HA2	8	0.33
(2,1344)	1:123:A:LEU:HD22	1:129:A:VAL:HG23	1	0.33
(2,1339)	1:106:A:LEU:HD23	1:135:A:VAL:HG12	3	0.33
(2,1288)	1:137:A:LEU:HG	1:132:A:ASP:HA	1	0.33
(2,1257)	1:75:A:LYS:HD3	1:78:A:LYS:HE2	6	0.33
(2,1249)	1:117:A:GLN:HB2	1:113:A:HIS:HA	8	0.33
(2,1225)	1:115:A:MET:HB2	1:107:A:PRO:HD2	4	0.33
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB3	5	0.33
(2,1012)	1:119:A:LEU:H	1:119:A:LEU:HB3	4	0.33
(2,1012)	1:119:A:LEU:H	1:119:A:LEU:HB3	5	0.33
(2,1012)	1:119:A:LEU:H	1:119:A:LEU:HB3	8	0.33
(2,1012)	1:119:A:LEU:H	1:119:A:LEU:HB3	9	0.33
(2,870)	1:87:A:GLU:H	1:84:A:THR:HG21	6	0.33
(2,845)	1:85:A:ARG:H	1:84:A:THR:HG22	3	0.33
(2,646)	1:106:A:LEU:HG	1:107:A:PRO:HD3	8	0.33
(2,604)	1:131:A:LEU:HD23	1:131:A:LEU:HA	8	0.33
(2,592)	1:61:A:ARG:HA	1:61:A:ARG:HD2	6	0.33
(2,463)	1:101:A:VAL:HA	1:65:A:THR:HG21	10	0.33
(2,436)	1:93:A:ILE:HG21	1:82:A:PHE:HD2	9	0.33
(2,369)	1:104:A:ILE:HD12	1:122:A:ILE:HG13	1	0.33
(2,369)	1:104:A:ILE:HD13	1:122:A:ILE:HG13	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,369)	1:104:A:ILE:HD12	1:122:A:ILE:HG13	10	0.33
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG21	2	0.33
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG22	4	0.33
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG21	6	0.33
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG22	7	0.33
(2,307)	1:102:A:THR:HG22	1:64:A:VAL:HB	1	0.33
(2,307)	1:102:A:THR:HG23	1:64:A:VAL:HB	10	0.33
(2,299)	1:101:A:VAL:HG12	1:102:A:THR:HA	7	0.33
(2,279)	1:64:A:VAL:HG13	1:122:A:ILE:HG21	3	0.33
(2,267)	1:110:A:VAL:HG22	1:114:A:ASP:HB3	4	0.33
(2,267)	1:110:A:VAL:HG21	1:114:A:ASP:HB3	5	0.33
(1,13)	1:120:A:HIS:HB2	1:122:A:ILE:HG13	1	0.33
(2,1932)	1:92:A:SER:H	1:93:A:ILE:HG13	5	0.32
(2,1932)	1:92:A:SER:H	1:93:A:ILE:HG13	7	0.32
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD22	1	0.32
(2,1915)	1:79:A:SER:H	1:78:A:LYS:HG3	5	0.32
(2,1770)	1:116:A:ASP:HB2	1:112:A:GLU:HB3	9	0.32
(2,1752)	1:78:A:LYS:HE2	1:75:A:LYS:HA	9	0.32
(2,1651)	1:104:A:ILE:HG22	1:61:A:ARG:HA	5	0.32
(2,1648)	1:136:A:LYS:HG3	1:136:A:LYS:HA	8	0.32
(2,1581)	1:104:A:ILE:HA	1:93:A:ILE:HG13	1	0.32
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB3	6	0.32
(2,1516)	1:107:A:PRO:HA	1:59:A:MET:HB3	6	0.32
(2,1443)	1:86:A:ILE:HG23	1:87:A:GLU:HA	7	0.32
(2,1397)	1:101:A:VAL:HG11	1:101:A:VAL:HA	6	0.32
(2,1383)	1:96:A:LEU:HB3	1:97:A:THR:HG22	8	0.32
(2,1363)	1:96:A:LEU:HB2	1:96:A:LEU:HD21	1	0.32
(2,1363)	1:131:A:LEU:HG	1:131:A:LEU:HD22	2	0.32
(2,1363)	1:96:A:LEU:HG	1:96:A:LEU:HD23	3	0.32
(2,1363)	1:96:A:LEU:HG	1:96:A:LEU:HD21	4	0.32
(2,1363)	1:137:A:LEU:HG	1:137:A:LEU:HD22	7	0.32
(2,1363)	1:131:A:LEU:HG	1:131:A:LEU:HD21	9	0.32
(2,1324)	1:115:A:MET:HG3	1:108:A:LYS:HG3	5	0.32
(2,1321)	1:62:A:LEU:HD12	1:82:A:PHE:HZ	10	0.32
(2,1317)	1:78:A:LYS:HG3	1:78:A:LYS:HA	6	0.32
(2,1285)	1:93:A:ILE:HG12	1:92:A:SER:HA	4	0.32
(2,1257)	1:136:A:LYS:HD3	1:58:A:GLU:HG3	4	0.32
(2,1253)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	10	0.32
(2,1252)	1:66:A:GLU:HG3	1:71:A:LYS:HD3	10	0.32
(2,1249)	1:117:A:GLN:HB2	1:113:A:HIS:HA	6	0.32
(2,1225)	1:115:A:MET:HB2	1:107:A:PRO:HD2	8	0.32
(2,1224)	1:115:A:MET:HB3	1:111:A:SER:HB2	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG21	9	0.32
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG22	8	0.32
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB3	1	0.32
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB3	4	0.32
(2,1043)	1:89:A:LEU:H	1:89:A:LEU:HB3	2	0.32
(2,1012)	1:119:A:LEU:H	1:119:A:LEU:HB3	3	0.32
(2,1012)	1:119:A:LEU:H	1:119:A:LEU:HB3	6	0.32
(2,1012)	1:119:A:LEU:H	1:119:A:LEU:HB3	7	0.32
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG21	1	0.32
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG23	2	0.32
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG21	4	0.32
(2,813)	1:137:A:LEU:H	1:137:A:LEU:HD13	6	0.32
(2,786)	1:102:A:THR:H	1:65:A:THR:HG21	7	0.32
(2,744)	1:105:A:GLU:H	1:105:A:GLU:HG2	3	0.32
(2,744)	1:105:A:GLU:H	1:105:A:GLU:HG2	4	0.32
(2,744)	1:105:A:GLU:H	1:105:A:GLU:HG2	10	0.32
(2,604)	1:131:A:LEU:HD21	1:131:A:LEU:HA	5	0.32
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG22	6	0.32
(2,385)	1:86:A:ILE:HD11	1:85:A:ARG:HA	2	0.32
(2,374)	1:104:A:ILE:HD13	1:122:A:ILE:HG23	4	0.32
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG23	1	0.32
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG22	5	0.32
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG23	8	0.32
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG23	10	0.32
(2,307)	1:102:A:THR:HG21	1:64:A:VAL:HB	2	0.32
(2,279)	1:64:A:VAL:HG12	1:122:A:ILE:HG23	4	0.32
(2,267)	1:110:A:VAL:HG23	1:114:A:ASP:HB3	9	0.32
(2,219)	1:75:A:LYS:HG3	1:75:A:LYS:HA	4	0.32
(1,13)	1:120:A:HIS:HB2	1:122:A:ILE:HG13	8	0.32
(2,1935)	1:78:A:LYS:H	1:78:A:LYS:HB3	3	0.31
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG23	6	0.31
(2,1932)	1:92:A:SER:H	1:93:A:ILE:HG13	9	0.31
(2,1874)	1:123:A:LEU:H	1:129:A:VAL:HG12	2	0.31
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD21	4	0.31
(2,1862)	1:121:A:ASP:H	1:116:A:ASP:HA	7	0.31
(2,1856)	1:94:A:SER:H	1:93:A:ILE:HB	3	0.31
(2,1796)	1:96:A:LEU:H	1:101:A:VAL:HB	3	0.31
(2,1796)	1:96:A:LEU:H	1:101:A:VAL:HB	6	0.31
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG23	5	0.31
(2,1774)	1:104:A:ILE:HB	1:103:A:MET:HG3	10	0.31
(2,1768)	1:89:A:LEU:HB2	1:114:A:ASP:HB3	10	0.31
(2,1649)	1:78:A:LYS:HD3	1:78:A:LYS:HA	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1648)	1:136:A:LYS:HG3	1:136:A:LYS:HA	4	0.31
(2,1540)	1:135:A:VAL:HA	1:109:A:THR:H	8	0.31
(2,1516)	1:107:A:PRO:HA	1:59:A:MET:HB3	2	0.31
(2,1488)	1:92:A:SER:HB2	1:93:A:ILE:HB	4	0.31
(2,1471)	1:86:A:ILE:HD12	1:89:A:LEU:HB2	9	0.31
(2,1443)	1:86:A:ILE:HG22	1:87:A:GLU:HA	5	0.31
(2,1404)	1:102:A:THR:HG21	1:77:A:ALA:HA	10	0.31
(2,1380)	1:64:A:VAL:HG11	1:128:A:VAL:HG21	8	0.31
(2,1363)	1:96:A:LEU:HG	1:96:A:LEU:HD23	5	0.31
(2,1317)	1:78:A:LYS:HG3	1:78:A:LYS:HA	3	0.31
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD23	5	0.31
(2,1297)	1:86:A:ILE:HG13	1:82:A:PHE:HZ	5	0.31
(2,1257)	1:136:A:LYS:HD2	1:59:A:MET:HG2	10	0.31
(2,1225)	1:115:A:MET:HB2	1:107:A:PRO:HD2	1	0.31
(2,1225)	1:115:A:MET:HB2	1:107:A:PRO:HD2	6	0.31
(2,1225)	1:115:A:MET:HB2	1:107:A:PRO:HD2	7	0.31
(2,1043)	1:89:A:LEU:H	1:89:A:LEU:HB3	10	0.31
(2,990)	1:59:A:MET:H	1:59:A:MET:HB3	6	0.31
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG21	5	0.31
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG22	6	0.31
(2,956)	1:101:A:VAL:H	1:65:A:THR:HG21	8	0.31
(2,931)	1:60:A:THR:H	1:59:A:MET:HG3	4	0.31
(2,813)	1:137:A:LEU:H	1:137:A:LEU:HD12	5	0.31
(2,788)	1:73:A:PHE:H	1:73:A:PHE:HD2	5	0.31
(2,744)	1:105:A:GLU:H	1:105:A:GLU:HG2	5	0.31
(2,687)	1:108:A:LYS:HE3	1:60:A:THR:HA	9	0.31
(2,592)	1:61:A:ARG:HA	1:61:A:ARG:HD2	4	0.31
(2,592)	1:61:A:ARG:HA	1:61:A:ARG:HD2	10	0.31
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG23	3	0.31
(2,361)	1:122:A:ILE:HG13	1:122:A:ILE:HG21	9	0.31
(2,359)	1:122:A:ILE:HG23	1:64:A:VAL:HA	1	0.31
(2,343)	1:86:A:ILE:HG23	1:91:A:GLY:HA2	4	0.31
(2,330)	1:64:A:VAL:HG12	1:125:A:ALA:HB1	5	0.31
(2,330)	1:64:A:VAL:HG11	1:125:A:ALA:HB3	6	0.31
(2,330)	1:64:A:VAL:HG13	1:125:A:ALA:HB2	8	0.31
(2,307)	1:102:A:THR:HG21	1:64:A:VAL:HB	5	0.31
(2,267)	1:110:A:VAL:HG23	1:114:A:ASP:HB3	1	0.31
(2,219)	1:75:A:LYS:HG3	1:75:A:LYS:HA	1	0.31
(2,182)	1:137:A:LEU:HG	1:61:A:ARG:HD2	8	0.31
(2,121)	1:58:A:GLU:HB3	1:59:A:MET:HA	10	0.31
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG13	10	0.31
(2,36)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:120:A:HIS:HB2	1:122:A:ILE:HG13	5	0.31
(1,13)	1:120:A:HIS:HB2	1:122:A:ILE:HG13	9	0.31
(1,3)	1:122:A:ILE:HB	1:62:A:LEU:HB2	7	0.31
(1,3)	1:122:A:ILE:HB	1:62:A:LEU:HB2	9	0.31
(2,1939)	1:127:A:GLY:H	1:122:A:ILE:HB	3	0.3
(2,1939)	1:127:A:GLY:H	1:122:A:ILE:HB	5	0.3
(2,1930)	1:92:A:SER:H	1:105:A:GLU:HG2	7	0.3
(2,1925)	1:130:A:GLY:H	1:128:A:VAL:HG12	4	0.3
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD23	4	0.3
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD21	3	0.3
(2,1864)	1:135:A:VAL:H	1:135:A:VAL:HB	3	0.3
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG23	4	0.3
(2,1676)	1:63:A:MET:HG3	1:63:A:MET:HA	2	0.3
(2,1649)	1:78:A:LYS:HD3	1:78:A:LYS:HA	3	0.3
(2,1627)	1:95:A:PHE:HA	1:101:A:VAL:HB	2	0.3
(2,1553)	1:60:A:THR:HA	1:59:A:MET:HG2	5	0.3
(2,1478)	1:97:A:THR:HB	1:78:A:LYS:HE2	4	0.3
(2,1443)	1:86:A:ILE:HG23	1:87:A:GLU:HA	3	0.3
(2,1443)	1:86:A:ILE:HG23	1:87:A:GLU:HA	4	0.3
(2,1439)	1:104:A:ILE:HG23	1:105:A:GLU:HG2	7	0.3
(2,1396)	1:101:A:VAL:HG13	1:63:A:MET:HA	2	0.3
(2,1363)	1:96:A:LEU:HG	1:96:A:LEU:HD23	6	0.3
(2,1363)	1:96:A:LEU:HG	1:96:A:LEU:HD21	10	0.3
(2,1321)	1:62:A:LEU:HD11	1:82:A:PHE:HZ	8	0.3
(2,1314)	1:108:A:LYS:HG3	1:106:A:LEU:HD23	4	0.3
(2,1294)	1:106:A:LEU:HG	1:90:A:GLY:HA3	4	0.3
(2,1285)	1:93:A:ILE:HG12	1:92:A:SER:HA	9	0.3
(2,1249)	1:117:A:GLN:HB2	1:113:A:HIS:HA	4	0.3
(2,1222)	1:76:A:MET:HG3	1:77:A:ALA:HB3	5	0.3
(2,1144)	1:126:A:GLY:H	1:127:A:GLY:HA2	5	0.3
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG21	8	0.3
(2,1043)	1:89:A:LEU:H	1:89:A:LEU:HB3	5	0.3
(2,1042)	1:89:A:LEU:H	1:88:A:GLU:HB3	2	0.3
(2,962)	1:114:A:ASP:H	1:114:A:ASP:HB3	3	0.3
(2,962)	1:114:A:ASP:H	1:114:A:ASP:HB3	8	0.3
(2,626)	1:64:A:VAL:HG11	1:63:A:MET:HA	9	0.3
(2,624)	1:101:A:VAL:HG13	1:63:A:MET:HA	1	0.3
(2,592)	1:61:A:ARG:HA	1:61:A:ARG:HD2	9	0.3
(2,464)	1:101:A:VAL:HG11	1:101:A:VAL:HA	6	0.3
(2,340)	1:124:A:ALA:HB1	1:121:A:ASP:HB2	2	0.3
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG13	3	0.3
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG12	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG21	7	0.3
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG22	10	0.3
(2,307)	1:102:A:THR:HG22	1:64:A:VAL:HB	3	0.3
(2,282)	1:97:A:THR:HG22	1:78:A:LYS:HE2	4	0.3
(2,279)	1:64:A:VAL:HG13	1:122:A:ILE:HG21	8	0.3
(2,279)	1:64:A:VAL:HG12	1:122:A:ILE:HG22	9	0.3
(2,246)	1:123:A:LEU:HD13	1:127:A:GLY:HA2	2	0.3
(2,1939)	1:127:A:GLY:H	1:122:A:ILE:HB	2	0.29
(2,1922)	1:86:A:ILE:H	1:87:A:GLU:HB2	4	0.29
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD23	5	0.29
(2,1796)	1:96:A:LEU:H	1:101:A:VAL:HB	10	0.29
(2,1747)	1:78:A:LYS:HE3	1:75:A:LYS:HA	2	0.29
(2,1741)	1:136:A:LYS:HE2	1:136:A:LYS:HA	1	0.29
(2,1711)	1:104:A:ILE:HG21	1:91:A:GLY:HA2	10	0.29
(2,1676)	1:63:A:MET:HG2	1:63:A:MET:HA	1	0.29
(2,1658)	1:60:A:THR:HG21	1:105:A:GLU:HA	1	0.29
(2,1658)	1:60:A:THR:HG23	1:105:A:GLU:HA	2	0.29
(2,1597)	1:75:A:LYS:HB3	1:75:A:LYS:HA	5	0.29
(2,1553)	1:60:A:THR:HA	1:59:A:MET:HG2	8	0.29
(2,1514)	1:86:A:ILE:HD13	1:82:A:PHE:HD1	9	0.29
(2,1481)	1:84:A:THR:HG23	1:84:A:THR:HB	5	0.29
(2,1443)	1:86:A:ILE:HG23	1:87:A:GLU:HA	1	0.29
(2,1438)	1:104:A:ILE:HG21	1:62:A:LEU:HB2	2	0.29
(2,1418)	1:64:A:VAL:HG23	1:127:A:GLY:HA2	5	0.29
(2,1372)	1:89:A:LEU:HD23	1:88:A:GLU:HB3	4	0.29
(2,1363)	1:96:A:LEU:HB2	1:96:A:LEU:HD22	8	0.29
(2,1345)	1:110:A:VAL:HG11	1:114:A:ASP:HB2	4	0.29
(2,1294)	1:106:A:LEU:HG	1:90:A:GLY:HA3	1	0.29
(2,1209)	1:110:A:VAL:HB	1:106:A:LEU:HG	2	0.29
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB3	4	0.29
(2,990)	1:59:A:MET:H	1:59:A:MET:HB3	7	0.29
(2,962)	1:114:A:ASP:H	1:114:A:ASP:HB3	1	0.29
(2,962)	1:114:A:ASP:H	1:114:A:ASP:HB3	4	0.29
(2,962)	1:114:A:ASP:H	1:114:A:ASP:HB3	7	0.29
(2,962)	1:114:A:ASP:H	1:114:A:ASP:HB3	9	0.29
(2,845)	1:85:A:ARG:H	1:84:A:THR:HG22	2	0.29
(2,813)	1:137:A:LEU:H	1:137:A:LEU:HD11	4	0.29
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG22	3	0.29
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG23	4	0.29
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG23	5	0.29
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG23	9	0.29
(2,744)	1:105:A:GLU:H	1:105:A:GLU:HG2	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,560)	1:70:A:SER:HB2	1:70:A:SER:HA	9	0.29
(2,521)	1:86:A:ILE:HG22	1:87:A:GLU:HA	9	0.29
(2,513)	1:113:A:HIS:HA	1:110:A:VAL:HG22	10	0.29
(2,464)	1:101:A:VAL:HG12	1:101:A:VAL:HA	5	0.29
(2,374)	1:104:A:ILE:HD12	1:122:A:ILE:HG21	10	0.29
(2,359)	1:122:A:ILE:HG21	1:64:A:VAL:HA	9	0.29
(2,343)	1:86:A:ILE:HG23	1:91:A:GLY:HA2	7	0.29
(2,343)	1:86:A:ILE:HG21	1:91:A:GLY:HA2	8	0.29
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG13	1	0.29
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG12	2	0.29
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG12	4	0.29
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG22	6	0.29
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG13	8	0.29
(2,314)	1:128:A:VAL:HB	1:128:A:VAL:HG13	9	0.29
(2,307)	1:102:A:THR:HG23	1:64:A:VAL:HB	9	0.29
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG12	10	0.29
(2,230)	1:62:A:LEU:HD11	1:122:A:ILE:HG12	1	0.29
(1,13)	1:120:A:HIS:HB2	1:122:A:ILE:HG13	6	0.29
(2,1949)	1:90:A:GLY:H	1:107:A:PRO:HG3	10	0.28
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG22	4	0.28
(2,1930)	1:92:A:SER:H	1:105:A:GLU:HG2	3	0.28
(2,1930)	1:92:A:SER:H	1:105:A:GLU:HG2	8	0.28
(2,1922)	1:86:A:ILE:H	1:87:A:GLU:HB2	2	0.28
(2,1922)	1:86:A:ILE:H	1:87:A:GLU:HB2	7	0.28
(2,1891)	1:116:A:ASP:H	1:115:A:MET:HB2	6	0.28
(2,1881)	1:114:A:ASP:H	1:115:A:MET:HB3	8	0.28
(2,1819)	1:136:A:LYS:H	1:58:A:GLU:HA	4	0.28
(2,1796)	1:96:A:LEU:H	1:101:A:VAL:HB	8	0.28
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG23	10	0.28
(2,1768)	1:89:A:LEU:HB2	1:114:A:ASP:HB3	2	0.28
(2,1676)	1:63:A:MET:HG3	1:63:A:MET:HA	7	0.28
(2,1676)	1:63:A:MET:HG3	1:63:A:MET:HA	10	0.28
(2,1662)	1:131:A:LEU:HA	1:61:A:ARG:HA	6	0.28
(2,1629)	1:95:A:PHE:HA	1:96:A:LEU:HD21	7	0.28
(2,1514)	1:86:A:ILE:HD11	1:82:A:PHE:HD1	8	0.28
(2,1481)	1:84:A:THR:HG23	1:84:A:THR:HB	2	0.28
(2,1481)	1:84:A:THR:HG22	1:84:A:THR:HB	4	0.28
(2,1481)	1:84:A:THR:HG23	1:84:A:THR:HB	6	0.28
(2,1481)	1:97:A:THR:HG22	1:97:A:THR:HB	10	0.28
(2,1383)	1:96:A:LEU:HB3	1:97:A:THR:HG23	1	0.28
(2,1380)	1:64:A:VAL:HG13	1:128:A:VAL:HG21	2	0.28
(2,1334)	1:131:A:LEU:HG	1:131:A:LEU:HD11	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1334)	1:131:A:LEU:HG	1:131:A:LEU:HD11	3	0.28
(2,1334)	1:131:A:LEU:HG	1:131:A:LEU:HD13	9	0.28
(2,1305)	1:118:A:LEU:HD13	1:85:A:ARG:HA	1	0.28
(2,1295)	1:106:A:LEU:HG	1:89:A:LEU:HB3	5	0.28
(2,1285)	1:93:A:ILE:HG12	1:92:A:SER:HA	6	0.28
(2,1285)	1:93:A:ILE:HG12	1:92:A:SER:HA	10	0.28
(2,1261)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	2	0.28
(2,1225)	1:115:A:MET:HB2	1:107:A:PRO:HD2	2	0.28
(2,1225)	1:115:A:MET:HB2	1:107:A:PRO:HD2	10	0.28
(2,1224)	1:115:A:MET:HB3	1:111:A:SER:HB2	4	0.28
(2,1222)	1:76:A:MET:HG3	1:77:A:ALA:HB2	10	0.28
(2,1200)	1:136:A:LYS:HB3	1:59:A:MET:HA	3	0.28
(2,1181)	1:101:A:VAL:HB	1:103:A:MET:HA	6	0.28
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG22	7	0.28
(2,1152)	1:96:A:LEU:HB3	1:97:A:THR:HG23	1	0.28
(2,1062)	1:120:A:HIS:H	1:119:A:LEU:HB3	9	0.28
(2,1045)	1:89:A:LEU:H	1:89:A:LEU:HD21	9	0.28
(2,990)	1:59:A:MET:H	1:59:A:MET:HB3	8	0.28
(2,962)	1:114:A:ASP:H	1:114:A:ASP:HB3	6	0.28
(2,788)	1:73:A:PHE:H	1:73:A:PHE:HD2	3	0.28
(2,530)	1:88:A:GLU:HA	1:88:A:GLU:HB2	7	0.28
(2,488)	1:74:A:SER:HB3	1:95:A:PHE:HE2	2	0.28
(2,359)	1:122:A:ILE:HG21	1:64:A:VAL:HA	2	0.28
(2,343)	1:86:A:ILE:HG22	1:91:A:GLY:HA2	2	0.28
(2,343)	1:86:A:ILE:HG23	1:91:A:GLY:HA2	6	0.28
(2,330)	1:64:A:VAL:HG13	1:125:A:ALA:HB2	1	0.28
(2,267)	1:110:A:VAL:HG23	1:114:A:ASP:HB3	3	0.28
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG22	2	0.28
(1,46)	1:108:A:LYS:HE3	1:59:A:MET:HA	1	0.28
(1,3)	1:122:A:ILE:HB	1:62:A:LEU:HB2	5	0.28
(2,1935)	1:78:A:LYS:H	1:78:A:LYS:HB3	6	0.27
(2,1929)	1:92:A:SER:H	1:107:A:PRO:HD3	3	0.27
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD22	10	0.27
(2,1881)	1:114:A:ASP:H	1:115:A:MET:HB3	1	0.27
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB2	6	0.27
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB2	8	0.27
(2,1856)	1:94:A:SER:H	1:93:A:ILE:HB	6	0.27
(2,1805)	1:61:A:ARG:H	1:137:A:LEU:HD23	4	0.27
(2,1796)	1:96:A:LEU:H	1:101:A:VAL:HB	9	0.27
(2,1793)	1:103:A:MET:H	1:102:A:THR:HG22	1	0.27
(2,1774)	1:104:A:ILE:HB	1:103:A:MET:HG3	3	0.27
(2,1741)	1:136:A:LYS:HE2	1:136:A:LYS:HA	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1686)	1:120:A:HIS:HD2	1:123:A:LEU:HA	5	0.27
(2,1676)	1:63:A:MET:HG3	1:63:A:MET:HA	5	0.27
(2,1676)	1:63:A:MET:HG3	1:63:A:MET:HA	8	0.27
(2,1658)	1:60:A:THR:HG23	1:105:A:GLU:HA	9	0.27
(2,1628)	1:95:A:PHE:HA	1:96:A:LEU:HB2	2	0.27
(2,1628)	1:95:A:PHE:HA	1:96:A:LEU:HB2	6	0.27
(2,1628)	1:95:A:PHE:HA	1:96:A:LEU:HB2	8	0.27
(2,1618)	1:79:A:SER:HA	1:78:A:LYS:HB2	7	0.27
(2,1581)	1:104:A:ILE:HA	1:93:A:ILE:HG13	9	0.27
(2,1544)	1:74:A:SER:HB3	1:75:A:LYS:HG2	2	0.27
(2,1481)	1:84:A:THR:HG22	1:84:A:THR:HB	7	0.27
(2,1481)	1:84:A:THR:HG23	1:84:A:THR:HB	9	0.27
(2,1434)	1:86:A:ILE:HG21	1:106:A:LEU:HD11	10	0.27
(2,1345)	1:110:A:VAL:HG11	1:114:A:ASP:HB2	8	0.27
(2,1334)	1:137:A:LEU:HG	1:137:A:LEU:HD13	1	0.27
(2,1334)	1:131:A:LEU:HG	1:131:A:LEU:HD11	5	0.27
(2,1334)	1:131:A:LEU:HG	1:131:A:LEU:HD13	6	0.27
(2,1334)	1:131:A:LEU:HG	1:131:A:LEU:HD11	7	0.27
(2,1334)	1:137:A:LEU:HG	1:137:A:LEU:HD12	8	0.27
(2,1321)	1:62:A:LEU:HD12	1:82:A:PHE:HZ	6	0.27
(2,1297)	1:86:A:ILE:HG13	1:82:A:PHE:HZ	6	0.27
(2,1297)	1:86:A:ILE:HG13	1:82:A:PHE:HZ	7	0.27
(2,1261)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	7	0.27
(2,1261)	1:71:A:LYS:HD2	1:71:A:LYS:HG3	10	0.27
(2,1254)	1:136:A:LYS:HD2	1:135:A:VAL:HA	2	0.27
(2,1158)	1:72:A:ASN:HB2	1:70:A:SER:HB3	10	0.27
(2,990)	1:59:A:MET:H	1:59:A:MET:HB3	1	0.27
(2,990)	1:59:A:MET:H	1:59:A:MET:HB3	9	0.27
(2,962)	1:114:A:ASP:H	1:114:A:ASP:HB3	5	0.27
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG22	6	0.27
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD12	1	0.27
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD11	2	0.27
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD13	7	0.27
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG21	1	0.27
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG23	2	0.27
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG22	6	0.27
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG21	7	0.27
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG23	8	0.27
(2,728)	1:124:A:ALA:HB3	1:120:A:HIS:HB2	10	0.27
(2,630)	1:77:A:ALA:HA	1:93:A:ILE:HG23	5	0.27
(2,624)	1:101:A:VAL:HG13	1:63:A:MET:HA	5	0.27
(2,538)	1:120:A:HIS:HB2	1:117:A:GLN:HA	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,463)	1:101:A:VAL:HA	1:65:A:THR:HG21	7	0.27
(2,426)	1:111:A:SER:HB2	1:110:A:VAL:HG21	2	0.27
(2,374)	1:104:A:ILE:HD12	1:122:A:ILE:HG22	2	0.27
(2,364)	1:104:A:ILE:HD11	1:82:A:PHE:HE2	2	0.27
(2,359)	1:122:A:ILE:HG21	1:64:A:VAL:HA	6	0.27
(2,343)	1:86:A:ILE:HG23	1:91:A:GLY:HA2	1	0.27
(2,299)	1:101:A:VAL:HG12	1:102:A:THR:HA	3	0.27
(2,295)	1:101:A:VAL:HG13	1:103:A:MET:HA	1	0.27
(2,246)	1:123:A:LEU:HD13	1:127:A:GLY:HA2	7	0.27
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG12	2	0.27
(2,225)	1:115:A:MET:HG3	1:119:A:LEU:HD11	9	0.27
(2,219)	1:75:A:LYS:HG3	1:75:A:LYS:HA	2	0.27
(2,219)	1:75:A:LYS:HG3	1:75:A:LYS:HA	8	0.27
(2,106)	1:103:A:MET:HG2	1:94:A:SER:HB2	6	0.27
(1,41)	1:105:A:GLU:HA	1:132:A:ASP:HB2	1	0.27
(1,13)	1:120:A:HIS:HB2	1:122:A:ILE:HG13	7	0.27
(2,1939)	1:127:A:GLY:H	1:122:A:ILE:HB	9	0.26
(2,1932)	1:92:A:SER:H	1:93:A:ILE:HG13	3	0.26
(2,1932)	1:92:A:SER:H	1:93:A:ILE:HG13	6	0.26
(2,1930)	1:92:A:SER:H	1:105:A:GLU:HG2	1	0.26
(2,1922)	1:86:A:ILE:H	1:87:A:GLU:HB2	3	0.26
(2,1922)	1:86:A:ILE:H	1:87:A:GLU:HB2	10	0.26
(2,1904)	1:66:A:GLU:H	1:71:A:LYS:HD3	8	0.26
(2,1881)	1:114:A:ASP:H	1:115:A:MET:HB3	4	0.26
(2,1878)	1:58:A:GLU:H	1:90:A:GLY:HA2	6	0.26
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD21	10	0.26
(2,1861)	1:77:A:ALA:H	1:78:A:LYS:HE3	7	0.26
(2,1819)	1:136:A:LYS:H	1:58:A:GLU:HA	7	0.26
(2,1819)	1:136:A:LYS:H	1:58:A:GLU:HA	10	0.26
(2,1814)	1:62:A:LEU:H	1:62:A:LEU:HB3	7	0.26
(2,1785)	1:103:A:MET:H	1:103:A:MET:HG2	2	0.26
(2,1686)	1:120:A:HIS:HD2	1:123:A:LEU:HA	7	0.26
(2,1683)	1:131:A:LEU:HD12	1:62:A:LEU:HA	8	0.26
(2,1662)	1:131:A:LEU:HA	1:61:A:ARG:HA	3	0.26
(2,1658)	1:60:A:THR:HG23	1:105:A:GLU:HA	8	0.26
(2,1628)	1:95:A:PHE:HA	1:96:A:LEU:HB2	5	0.26
(2,1567)	1:99:A:THR:HA	1:100:A:GLY:HA2	3	0.26
(2,1541)	1:81:A:SER:HB2	1:81:A:SER:HA	9	0.26
(2,1523)	1:135:A:VAL:HA	1:58:A:GLU:HG2	1	0.26
(2,1481)	1:84:A:THR:HG22	1:84:A:THR:HB	3	0.26
(2,1481)	1:84:A:THR:HG22	1:84:A:THR:HB	8	0.26
(2,1429)	1:77:A:ALA:HB2	1:74:A:SER:HA	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1406)	1:135:A:VAL:HG12	1:107:A:PRO:HD3	2	0.26
(2,1344)	1:123:A:LEU:HD22	1:129:A:VAL:HG22	4	0.26
(2,1325)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	6	0.26
(2,1321)	1:62:A:LEU:HD12	1:82:A:PHE:HZ	5	0.26
(2,1269)	1:78:A:LYS:HD2	1:75:A:LYS:HE3	10	0.26
(2,1261)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	1	0.26
(2,1261)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	3	0.26
(2,1261)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	4	0.26
(2,1261)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	6	0.26
(2,1184)	1:59:A:MET:HB3	1:90:A:GLY:HA2	5	0.26
(2,1149)	1:58:A:GLU:H	1:58:A:GLU:HG2	5	0.26
(2,1144)	1:126:A:GLY:H	1:127:A:GLY:HA2	3	0.26
(2,1062)	1:120:A:HIS:H	1:119:A:LEU:HB3	1	0.26
(2,1062)	1:120:A:HIS:H	1:119:A:LEU:HB3	4	0.26
(2,1062)	1:120:A:HIS:H	1:119:A:LEU:HB3	6	0.26
(2,1062)	1:120:A:HIS:H	1:119:A:LEU:HB3	8	0.26
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG22	3	0.26
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG23	7	0.26
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG22	9	0.26
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD12	3	0.26
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD13	5	0.26
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD13	6	0.26
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD12	8	0.26
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD11	9	0.26
(2,770)	1:62:A:LEU:H	1:60:A:THR:HG21	10	0.26
(2,724)	1:128:A:VAL:HG21	1:65:A:THR:HB	1	0.26
(2,649)	1:70:A:SER:HB2	1:126:A:GLY:HA3	2	0.26
(2,604)	1:131:A:LEU:HD22	1:131:A:LEU:HA	1	0.26
(2,506)	1:118:A:LEU:HD22	1:82:A:PHE:HE1	9	0.26
(2,385)	1:86:A:ILE:HD12	1:85:A:ARG:HA	1	0.26
(2,385)	1:86:A:ILE:HD11	1:85:A:ARG:HA	10	0.26
(2,374)	1:104:A:ILE:HD13	1:122:A:ILE:HG21	3	0.26
(2,374)	1:104:A:ILE:HD11	1:122:A:ILE:HG21	8	0.26
(2,299)	1:101:A:VAL:HG12	1:102:A:THR:HA	10	0.26
(2,287)	1:84:A:THR:HG22	1:85:A:ARG:HD3	2	0.26
(2,279)	1:64:A:VAL:HG12	1:122:A:ILE:HG22	2	0.26
(2,264)	1:65:A:THR:HG23	1:64:A:VAL:HG11	4	0.26
(2,264)	1:65:A:THR:HG23	1:64:A:VAL:HG11	5	0.26
(1,41)	1:105:A:GLU:HA	1:132:A:ASP:HB2	6	0.26
(2,1949)	1:90:A:GLY:H	1:107:A:PRO:HG3	5	0.25
(2,1915)	1:79:A:SER:H	1:78:A:LYS:HG3	7	0.25
(2,1912)	1:89:A:LEU:H	1:88:A:GLU:HG3	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB3	1	0.25
(2,1861)	1:77:A:ALA:H	1:78:A:LYS:HE3	5	0.25
(2,1814)	1:62:A:LEU:H	1:62:A:LEU:HB3	3	0.25
(2,1814)	1:62:A:LEU:H	1:62:A:LEU:HB3	10	0.25
(2,1785)	1:103:A:MET:H	1:103:A:MET:HG2	3	0.25
(2,1784)	1:104:A:ILE:H	1:103:A:MET:HG3	1	0.25
(2,1774)	1:104:A:ILE:HB	1:103:A:MET:HG3	2	0.25
(2,1760)	1:95:A:PHE:HE2	1:82:A:PHE:HB3	8	0.25
(2,1686)	1:120:A:HIS:HD2	1:123:A:LEU:HA	9	0.25
(2,1682)	1:62:A:LEU:HA	1:103:A:MET:HG3	3	0.25
(2,1682)	1:62:A:LEU:HA	1:103:A:MET:HG3	4	0.25
(2,1661)	1:134:A:GLU:HB3	1:131:A:LEU:HA	10	0.25
(2,1628)	1:95:A:PHE:HA	1:96:A:LEU:HB2	1	0.25
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB3	9	0.25
(2,1553)	1:60:A:THR:HA	1:59:A:MET:HG2	7	0.25
(2,1544)	1:74:A:SER:HB3	1:71:A:LYS:HG2	9	0.25
(2,1532)	1:87:A:GLU:HB3	1:83:A:SER:HA	9	0.25
(2,1531)	1:87:A:GLU:HG3	1:83:A:SER:HA	4	0.25
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB2	7	0.25
(2,1423)	1:125:A:ALA:HB1	1:126:A:GLY:HA2	5	0.25
(2,1344)	1:123:A:LEU:HD23	1:129:A:VAL:HG23	8	0.25
(2,1325)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	9	0.25
(2,1321)	1:62:A:LEU:HD11	1:82:A:PHE:HZ	1	0.25
(2,1291)	1:131:A:LEU:HG	1:131:A:LEU:HD22	2	0.25
(2,1291)	1:131:A:LEU:HG	1:131:A:LEU:HD21	9	0.25
(2,1288)	1:137:A:LEU:HG	1:132:A:ASP:HA	7	0.25
(2,1261)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	8	0.25
(2,1256)	1:75:A:LYS:HD3	1:78:A:LYS:HE3	4	0.25
(2,1238)	1:134:A:GLU:HB3	1:131:A:LEU:HA	10	0.25
(2,990)	1:59:A:MET:H	1:59:A:MET:HB3	2	0.25
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG22	2	0.25
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG23	4	0.25
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG21	8	0.25
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG21	10	0.25
(2,630)	1:77:A:ALA:HA	1:93:A:ILE:HG23	1	0.25
(2,630)	1:77:A:ALA:HA	1:93:A:ILE:HG22	7	0.25
(2,592)	1:61:A:ARG:HA	1:61:A:ARG:HD2	3	0.25
(2,560)	1:70:A:SER:HB2	1:70:A:SER:HA	7	0.25
(2,506)	1:118:A:LEU:HD21	1:82:A:PHE:HE1	8	0.25
(2,374)	1:104:A:ILE:HD12	1:122:A:ILE:HG22	6	0.25
(2,364)	1:104:A:ILE:HD11	1:82:A:PHE:HE2	1	0.25
(2,364)	1:104:A:ILE:HD12	1:82:A:PHE:HE2	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,363)	1:93:A:ILE:HD13	1:77:A:ALA:HA	7	0.25
(2,343)	1:86:A:ILE:HG22	1:91:A:GLY:HA2	10	0.25
(2,307)	1:102:A:THR:HG23	1:64:A:VAL:HB	8	0.25
(2,246)	1:123:A:LEU:HD13	1:127:A:GLY:HA2	4	0.25
(2,239)	1:107:A:PRO:HG3	1:110:A:VAL:HG13	3	0.25
(2,106)	1:103:A:MET:HG2	1:94:A:SER:HB2	8	0.25
(1,3)	1:122:A:ILE:HB	1:62:A:LEU:HB2	10	0.25
(2,1949)	1:90:A:GLY:H	1:107:A:PRO:HG3	3	0.24
(2,1935)	1:78:A:LYS:H	1:78:A:LYS:HB3	4	0.24
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD23	3	0.24
(2,1904)	1:66:A:GLU:H	1:71:A:LYS:HD3	7	0.24
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD23	7	0.24
(2,1863)	1:121:A:ASP:H	1:122:A:ILE:HB	8	0.24
(2,1849)	1:106:A:LEU:H	1:104:A:ILE:HG22	10	0.24
(2,1814)	1:62:A:LEU:H	1:104:A:ILE:HB	4	0.24
(2,1800)	1:105:A:GLU:H	1:86:A:ILE:HG23	2	0.24
(2,1739)	1:71:A:LYS:HE2	1:71:A:LYS:HG3	2	0.24
(2,1676)	1:63:A:MET:HG3	1:63:A:MET:HA	6	0.24
(2,1669)	1:73:A:PHE:HE2	1:77:A:ALA:HA	6	0.24
(2,1661)	1:134:A:GLU:HB3	1:131:A:LEU:HA	8	0.24
(2,1658)	1:60:A:THR:HG23	1:105:A:GLU:HA	5	0.24
(2,1648)	1:136:A:LYS:HG3	1:136:A:LYS:HA	1	0.24
(2,1628)	1:95:A:PHE:HA	1:96:A:LEU:HB2	4	0.24
(2,1628)	1:95:A:PHE:HA	1:96:A:LEU:HB2	9	0.24
(2,1628)	1:95:A:PHE:HA	1:96:A:LEU:HB2	10	0.24
(2,1557)	1:95:A:PHE:HE1	1:102:A:THR:HB	7	0.24
(2,1481)	1:84:A:THR:HG21	1:84:A:THR:HB	1	0.24
(2,1416)	1:64:A:VAL:HG22	1:73:A:PHE:HE1	1	0.24
(2,1403)	1:102:A:THR:HG21	1:74:A:SER:HA	4	0.24
(2,1334)	1:137:A:LEU:HD12	1:137:A:LEU:HB3	4	0.24
(2,1323)	1:75:A:LYS:HG3	1:75:A:LYS:HE3	5	0.24
(2,1306)	1:106:A:LEU:HD11	1:106:A:LEU:HG	2	0.24
(2,1291)	1:118:A:LEU:HG	1:118:A:LEU:HD21	3	0.24
(2,1291)	1:118:A:LEU:HG	1:118:A:LEU:HD23	4	0.24
(2,1291)	1:96:A:LEU:HG	1:96:A:LEU:HD23	5	0.24
(2,1291)	1:96:A:LEU:HG	1:96:A:LEU:HD11	8	0.24
(2,1288)	1:137:A:LEU:HG	1:132:A:ASP:HA	3	0.24
(2,1288)	1:137:A:LEU:HG	1:132:A:ASP:HA	5	0.24
(2,1261)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	9	0.24
(2,1249)	1:117:A:GLN:HB2	1:113:A:HIS:HA	1	0.24
(2,1240)	1:120:A:HIS:HB3	1:122:A:ILE:HG13	2	0.24
(2,1238)	1:134:A:GLU:HB3	1:131:A:LEU:HA	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1184)	1:59:A:MET:HB3	1:90:A:GLY:HA2	6	0.24
(2,1144)	1:126:A:GLY:H	1:127:A:GLY:HA2	2	0.24
(2,1062)	1:120:A:HIS:H	1:119:A:LEU:HB3	3	0.24
(2,1047)	1:79:A:SER:H	1:82:A:PHE:HD2	8	0.24
(2,933)	1:60:A:THR:H	1:106:A:LEU:HB3	3	0.24
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG23	5	0.24
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD12	4	0.24
(2,840)	1:85:A:ARG:H	1:86:A:ILE:HD11	10	0.24
(2,688)	1:108:A:LYS:HD3	1:108:A:LYS:HE3	1	0.24
(2,688)	1:108:A:LYS:HD3	1:108:A:LYS:HE3	5	0.24
(2,688)	1:108:A:LYS:HD3	1:108:A:LYS:HE3	6	0.24
(2,649)	1:70:A:SER:HB2	1:126:A:GLY:HA3	8	0.24
(2,624)	1:101:A:VAL:HG12	1:63:A:MET:HA	3	0.24
(2,592)	1:61:A:ARG:HA	1:61:A:ARG:HD2	2	0.24
(2,472)	1:82:A:PHE:HA	1:84:A:THR:HG22	7	0.24
(2,385)	1:86:A:ILE:HD12	1:85:A:ARG:HA	4	0.24
(2,385)	1:86:A:ILE:HD13	1:85:A:ARG:HA	6	0.24
(2,385)	1:86:A:ILE:HD13	1:85:A:ARG:HA	7	0.24
(2,385)	1:86:A:ILE:HD12	1:85:A:ARG:HA	8	0.24
(2,364)	1:104:A:ILE:HD13	1:82:A:PHE:HE2	8	0.24
(2,299)	1:101:A:VAL:HG13	1:102:A:THR:HA	2	0.24
(2,295)	1:101:A:VAL:HG13	1:103:A:MET:HA	4	0.24
(2,292)	1:60:A:THR:HG21	1:108:A:LYS:HE3	8	0.24
(2,225)	1:115:A:MET:HG3	1:119:A:LEU:HD11	10	0.24
(2,1939)	1:127:A:GLY:H	1:122:A:ILE:HB	10	0.23
(2,1935)	1:78:A:LYS:H	1:78:A:LYS:HB3	2	0.23
(2,1935)	1:78:A:LYS:H	1:78:A:LYS:HB3	10	0.23
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG21	5	0.23
(2,1930)	1:92:A:SER:H	1:105:A:GLU:HG2	9	0.23
(2,1922)	1:86:A:ILE:H	1:87:A:GLU:HB2	8	0.23
(2,1881)	1:114:A:ASP:H	1:115:A:MET:HB3	6	0.23
(2,1881)	1:114:A:ASP:H	1:115:A:MET:HB3	7	0.23
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB2	3	0.23
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB2	7	0.23
(2,1849)	1:106:A:LEU:H	1:104:A:ILE:HG21	2	0.23
(2,1774)	1:104:A:ILE:HB	1:103:A:MET:HG3	7	0.23
(2,1770)	1:116:A:ASP:HB2	1:112:A:GLU:HB2	3	0.23
(2,1765)	1:116:A:ASP:HA	1:116:A:ASP:HB3	5	0.23
(2,1765)	1:116:A:ASP:HA	1:116:A:ASP:HB3	7	0.23
(2,1765)	1:116:A:ASP:HA	1:116:A:ASP:HB3	9	0.23
(2,1752)	1:78:A:LYS:HE2	1:75:A:LYS:HA	6	0.23
(2,1752)	1:78:A:LYS:HE2	1:75:A:LYS:HA	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1715)	1:85:A:ARG:HD3	1:82:A:PHE:HE1	7	0.23
(2,1686)	1:120:A:HIS:HD2	1:123:A:LEU:HA	1	0.23
(2,1676)	1:63:A:MET:HG3	1:63:A:MET:HA	3	0.23
(2,1676)	1:63:A:MET:HG3	1:63:A:MET:HA	9	0.23
(2,1662)	1:131:A:LEU:HA	1:61:A:ARG:HA	1	0.23
(2,1662)	1:131:A:LEU:HA	1:61:A:ARG:HA	4	0.23
(2,1658)	1:60:A:THR:HG21	1:105:A:GLU:HA	10	0.23
(2,1648)	1:136:A:LYS:HG3	1:136:A:LYS:HA	6	0.23
(2,1557)	1:95:A:PHE:HE1	1:102:A:THR:HB	6	0.23
(2,1545)	1:95:A:PHE:HE1	1:95:A:PHE:HA	8	0.23
(2,1541)	1:81:A:SER:HB3	1:81:A:SER:HA	6	0.23
(2,1531)	1:87:A:GLU:HG3	1:83:A:SER:HA	3	0.23
(2,1514)	1:86:A:ILE:HD12	1:82:A:PHE:HD1	5	0.23
(2,1443)	1:86:A:ILE:HG23	1:87:A:GLU:HA	6	0.23
(2,1443)	1:86:A:ILE:HG21	1:87:A:GLU:HA	8	0.23
(2,1383)	1:66:A:GLU:HB2	1:97:A:THR:HG22	6	0.23
(2,1381)	1:64:A:VAL:HG13	1:125:A:ALA:HB3	3	0.23
(2,1325)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	5	0.23
(2,1317)	1:78:A:LYS:HG3	1:78:A:LYS:HA	4	0.23
(2,1305)	1:118:A:LEU:HD13	1:85:A:ARG:HA	4	0.23
(2,1291)	1:118:A:LEU:HG	1:118:A:LEU:HD21	1	0.23
(2,1291)	1:96:A:LEU:HG	1:96:A:LEU:HD23	6	0.23
(2,1291)	1:96:A:LEU:HG	1:96:A:LEU:HD21	10	0.23
(2,1249)	1:117:A:GLN:HB2	1:113:A:HIS:HA	3	0.23
(2,1209)	1:110:A:VAL:HB	1:106:A:LEU:HG	1	0.23
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB1	10	0.23
(2,940)	1:108:A:LYS:H	1:108:A:LYS:HD3	1	0.23
(2,860)	1:122:A:ILE:H	1:122:A:ILE:HG21	1	0.23
(2,813)	1:137:A:LEU:H	1:137:A:LEU:HD12	10	0.23
(2,724)	1:128:A:VAL:HG23	1:65:A:THR:HB	3	0.23
(2,688)	1:108:A:LYS:HD3	1:108:A:LYS:HE3	4	0.23
(2,672)	1:61:A:ARG:HB2	1:61:A:ARG:HD2	8	0.23
(2,624)	1:101:A:VAL:HG12	1:63:A:MET:HA	10	0.23
(2,564)	1:95:A:PHE:HD2	1:95:A:PHE:HA	1	0.23
(2,506)	1:118:A:LEU:HD22	1:82:A:PHE:HE1	4	0.23
(2,464)	1:101:A:VAL:HG12	1:101:A:VAL:HA	8	0.23
(2,364)	1:104:A:ILE:HD11	1:82:A:PHE:HE2	6	0.23
(2,352)	1:104:A:ILE:HG21	1:73:A:PHE:HZ	4	0.23
(2,342)	1:77:A:ALA:HB1	1:64:A:VAL:HG13	8	0.23
(2,322)	1:64:A:VAL:HG13	1:64:A:VAL:HG22	4	0.23
(2,219)	1:75:A:LYS:HG3	1:75:A:LYS:HA	10	0.23
(2,211)	1:78:A:LYS:HG3	1:78:A:LYS:HE2	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,72)	1:59:A:MET:HG3	1:136:A:LYS:HB3	7	0.23
(1,46)	1:108:A:LYS:HE3	1:59:A:MET:HA	4	0.23
(1,46)	1:108:A:LYS:HE3	1:59:A:MET:HA	5	0.23
(1,41)	1:105:A:GLU:HA	1:132:A:ASP:HB2	4	0.23
(2,1940)	1:127:A:GLY:H	1:123:A:LEU:HG	6	0.22
(2,1935)	1:78:A:LYS:H	1:78:A:LYS:HB3	8	0.22
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG23	2	0.22
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG21	3	0.22
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD23	5	0.22
(2,1891)	1:116:A:ASP:H	1:115:A:MET:HB2	4	0.22
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD23	9	0.22
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB1	5	0.22
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB3	9	0.22
(2,1863)	1:121:A:ASP:H	1:122:A:ILE:HB	3	0.22
(2,1856)	1:94:A:SER:H	1:93:A:ILE:HB	9	0.22
(2,1819)	1:136:A:LYS:H	1:58:A:GLU:HA	8	0.22
(2,1798)	1:105:A:GLU:H	1:62:A:LEU:HG	7	0.22
(2,1765)	1:116:A:ASP:HA	1:116:A:ASP:HB3	1	0.22
(2,1765)	1:116:A:ASP:HA	1:116:A:ASP:HB3	2	0.22
(2,1765)	1:116:A:ASP:HA	1:116:A:ASP:HB3	4	0.22
(2,1765)	1:116:A:ASP:HA	1:116:A:ASP:HB3	6	0.22
(2,1765)	1:116:A:ASP:HA	1:116:A:ASP:HB3	8	0.22
(2,1765)	1:116:A:ASP:HA	1:116:A:ASP:HB3	10	0.22
(2,1747)	1:78:A:LYS:HE3	1:75:A:LYS:HA	1	0.22
(2,1715)	1:85:A:ARG:HD3	1:82:A:PHE:HE1	4	0.22
(2,1694)	1:106:A:LEU:HD23	1:107:A:PRO:HD2	5	0.22
(2,1676)	1:63:A:MET:HG3	1:63:A:MET:HA	4	0.22
(2,1661)	1:134:A:GLU:HB3	1:131:A:LEU:HA	1	0.22
(2,1661)	1:134:A:GLU:HB3	1:131:A:LEU:HA	4	0.22
(2,1651)	1:104:A:ILE:HG21	1:61:A:ARG:HA	1	0.22
(2,1642)	1:72:A:ASN:HA	1:72:A:ASN:HB3	5	0.22
(2,1637)	1:116:A:ASP:HA	1:116:A:ASP:HB3	10	0.22
(2,1628)	1:95:A:PHE:HA	1:96:A:LEU:HB2	3	0.22
(2,1602)	1:118:A:LEU:HG	1:118:A:LEU:HA	6	0.22
(2,1600)	1:79:A:SER:HB2	1:79:A:SER:HA	4	0.22
(2,1597)	1:75:A:LYS:HB3	1:75:A:LYS:HA	7	0.22
(2,1567)	1:99:A:THR:HA	1:100:A:GLY:HA2	5	0.22
(2,1566)	1:99:A:THR:HA	1:98:A:GLU:HA	3	0.22
(2,1555)	1:86:A:ILE:HB	1:86:A:ILE:HA	1	0.22
(2,1555)	1:86:A:ILE:HB	1:86:A:ILE:HA	2	0.22
(2,1555)	1:86:A:ILE:HB	1:86:A:ILE:HA	3	0.22
(2,1555)	1:86:A:ILE:HB	1:86:A:ILE:HA	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1555)	1:86:A:ILE:HB	1:86:A:ILE:HA	6	0.22
(2,1555)	1:86:A:ILE:HB	1:86:A:ILE:HA	7	0.22
(2,1555)	1:86:A:ILE:HB	1:86:A:ILE:HA	8	0.22
(2,1555)	1:86:A:ILE:HB	1:86:A:ILE:HA	9	0.22
(2,1541)	1:81:A:SER:HB3	1:81:A:SER:HA	8	0.22
(2,1416)	1:64:A:VAL:HG23	1:73:A:PHE:HE2	10	0.22
(2,1381)	1:64:A:VAL:HG11	1:125:A:ALA:HB1	7	0.22
(2,1321)	1:62:A:LEU:HD11	1:82:A:PHE:HZ	2	0.22
(2,1305)	1:118:A:LEU:HD13	1:85:A:ARG:HA	8	0.22
(2,1291)	1:96:A:LEU:HG	1:96:A:LEU:HD13	7	0.22
(2,1265)	1:78:A:LYS:HD3	1:78:A:LYS:HA	4	0.22
(2,1238)	1:134:A:GLU:HB3	1:131:A:LEU:HA	1	0.22
(2,1238)	1:134:A:GLU:HB3	1:131:A:LEU:HA	4	0.22
(2,1144)	1:126:A:GLY:H	1:127:A:GLY:HA2	1	0.22
(2,1144)	1:126:A:GLY:H	1:127:A:GLY:HA2	9	0.22
(2,1047)	1:79:A:SER:H	1:82:A:PHE:HD2	1	0.22
(2,1047)	1:79:A:SER:H	1:82:A:PHE:HD2	6	0.22
(2,1042)	1:89:A:LEU:H	1:88:A:GLU:HB3	10	0.22
(2,649)	1:70:A:SER:HB2	1:126:A:GLY:HA3	6	0.22
(2,564)	1:95:A:PHE:HD1	1:95:A:PHE:HA	3	0.22
(2,564)	1:95:A:PHE:HD2	1:95:A:PHE:HA	5	0.22
(2,538)	1:120:A:HIS:HB2	1:117:A:GLN:HA	7	0.22
(2,521)	1:86:A:ILE:HG22	1:87:A:GLU:HA	10	0.22
(2,400)	1:109:A:THR:HG23	1:109:A:THR:HB	6	0.22
(2,385)	1:86:A:ILE:HD11	1:85:A:ARG:HA	9	0.22
(2,343)	1:86:A:ILE:HG22	1:91:A:GLY:HA2	5	0.22
(2,219)	1:75:A:LYS:HG3	1:75:A:LYS:HA	6	0.22
(2,186)	1:96:A:LEU:HG	1:103:A:MET:HG2	9	0.22
(2,72)	1:59:A:MET:HG3	1:136:A:LYS:HB3	5	0.22
(1,3)	1:122:A:ILE:HB	1:62:A:LEU:HB2	8	0.22
(2,1939)	1:127:A:GLY:H	1:122:A:ILE:HB	1	0.21
(2,1930)	1:92:A:SER:H	1:105:A:GLU:HG2	5	0.21
(2,1922)	1:86:A:ILE:H	1:87:A:GLU:HB2	1	0.21
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD21	9	0.21
(2,1863)	1:121:A:ASP:H	1:122:A:ILE:HB	1	0.21
(2,1863)	1:121:A:ASP:H	1:122:A:ILE:HB	4	0.21
(2,1863)	1:121:A:ASP:H	1:122:A:ILE:HB	6	0.21
(2,1863)	1:121:A:ASP:H	1:122:A:ILE:HB	10	0.21
(2,1856)	1:94:A:SER:H	1:93:A:ILE:HB	7	0.21
(2,1856)	1:94:A:SER:H	1:93:A:ILE:HB	10	0.21
(2,1819)	1:136:A:LYS:H	1:58:A:GLU:HA	2	0.21
(2,1791)	1:103:A:MET:H	1:103:A:MET:HB3	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1785)	1:103:A:MET:H	1:103:A:MET:HG2	7	0.21
(2,1764)	1:116:A:ASP:HB3	1:117:A:GLN:HB2	5	0.21
(2,1747)	1:78:A:LYS:HE3	1:75:A:LYS:HA	3	0.21
(2,1743)	1:136:A:LYS:HG2	1:136:A:LYS:HE2	3	0.21
(2,1686)	1:120:A:HIS:HD2	1:123:A:LEU:HA	2	0.21
(2,1686)	1:120:A:HIS:HD2	1:123:A:LEU:HA	3	0.21
(2,1686)	1:120:A:HIS:HD2	1:123:A:LEU:HA	10	0.21
(2,1683)	1:131:A:LEU:HD12	1:62:A:LEU:HA	7	0.21
(2,1680)	1:104:A:ILE:HD11	1:63:A:MET:HA	7	0.21
(2,1658)	1:60:A:THR:HG22	1:105:A:GLU:HA	6	0.21
(2,1648)	1:136:A:LYS:HG3	1:136:A:LYS:HA	5	0.21
(2,1637)	1:116:A:ASP:HA	1:116:A:ASP:HB3	2	0.21
(2,1602)	1:118:A:LEU:HG	1:118:A:LEU:HA	5	0.21
(2,1567)	1:99:A:THR:HA	1:100:A:GLY:HA2	1	0.21
(2,1567)	1:99:A:THR:HA	1:100:A:GLY:HA2	2	0.21
(2,1567)	1:99:A:THR:HA	1:100:A:GLY:HA2	4	0.21
(2,1567)	1:99:A:THR:HA	1:100:A:GLY:HA2	8	0.21
(2,1567)	1:99:A:THR:HA	1:100:A:GLY:HA2	9	0.21
(2,1566)	1:99:A:THR:HA	1:98:A:GLU:HA	8	0.21
(2,1560)	1:95:A:PHE:HE2	1:97:A:THR:HG21	4	0.21
(2,1555)	1:86:A:ILE:HB	1:86:A:ILE:HA	10	0.21
(2,1541)	1:81:A:SER:HB3	1:81:A:SER:HA	1	0.21
(2,1541)	1:81:A:SER:HB3	1:81:A:SER:HA	2	0.21
(2,1541)	1:81:A:SER:HB3	1:81:A:SER:HA	10	0.21
(2,1531)	1:87:A:GLU:HG3	1:83:A:SER:HA	1	0.21
(2,1531)	1:87:A:GLU:HG3	1:83:A:SER:HA	2	0.21
(2,1531)	1:87:A:GLU:HG3	1:83:A:SER:HA	7	0.21
(2,1510)	1:110:A:VAL:HA	1:89:A:LEU:HD21	8	0.21
(2,1502)	1:133:A:SER:HB3	1:136:A:LYS:HB2	6	0.21
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB2	2	0.21
(2,1423)	1:125:A:ALA:HB3	1:126:A:GLY:HA2	2	0.21
(2,1418)	1:64:A:VAL:HG23	1:127:A:GLY:HA2	9	0.21
(2,1408)	1:135:A:VAL:HG22	1:134:A:GLU:HA	5	0.21
(2,1344)	1:123:A:LEU:HD21	1:129:A:VAL:HG21	7	0.21
(2,1337)	1:96:A:LEU:HG	1:96:A:LEU:HD13	2	0.21
(2,1337)	1:96:A:LEU:HG	1:96:A:LEU:HD11	9	0.21
(2,1334)	1:137:A:LEU:HD11	1:137:A:LEU:HB3	10	0.21
(2,1321)	1:62:A:LEU:HD13	1:82:A:PHE:HZ	3	0.21
(2,1306)	1:106:A:LEU:HD11	1:106:A:LEU:HG	1	0.21
(2,1306)	1:106:A:LEU:HD12	1:106:A:LEU:HG	3	0.21
(2,1306)	1:106:A:LEU:HD13	1:106:A:LEU:HG	4	0.21
(2,1306)	1:106:A:LEU:HD12	1:106:A:LEU:HG	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1297)	1:86:A:ILE:HG13	1:82:A:PHE:HZ	1	0.21
(2,1297)	1:86:A:ILE:HG13	1:82:A:PHE:HZ	10	0.21
(2,1272)	1:78:A:LYS:HB2	1:78:A:LYS:HD2	6	0.21
(2,1217)	1:66:A:GLU:HB3	1:73:A:PHE:HD1	6	0.21
(2,1209)	1:110:A:VAL:HB	1:106:A:LEU:HG	10	0.21
(2,1181)	1:101:A:VAL:HB	1:103:A:MET:HA	5	0.21
(2,1144)	1:126:A:GLY:H	1:127:A:GLY:HA2	8	0.21
(2,1062)	1:120:A:HIS:H	1:119:A:LEU:HB3	5	0.21
(2,1047)	1:79:A:SER:H	1:82:A:PHE:HD2	2	0.21
(2,807)	1:67:A:LYS:H	1:71:A:LYS:HG3	5	0.21
(2,749)	1:61:A:ARG:H	1:61:A:ARG:HD2	8	0.21
(2,724)	1:128:A:VAL:HG22	1:65:A:THR:HB	7	0.21
(2,630)	1:77:A:ALA:HA	1:93:A:ILE:HG22	4	0.21
(2,604)	1:131:A:LEU:HD23	1:131:A:LEU:HA	10	0.21
(2,564)	1:95:A:PHE:HD2	1:95:A:PHE:HA	4	0.21
(2,564)	1:95:A:PHE:HD2	1:95:A:PHE:HA	10	0.21
(2,520)	1:87:A:GLU:HA	1:93:A:ILE:HD13	8	0.21
(2,506)	1:118:A:LEU:HD22	1:82:A:PHE:HE1	7	0.21
(2,433)	1:76:A:MET:HG3	1:82:A:PHE:HD1	8	0.21
(2,414)	1:92:A:SER:HB3	1:92:A:SER:HA	8	0.21
(2,400)	1:109:A:THR:HG23	1:109:A:THR:HB	1	0.21
(2,400)	1:109:A:THR:HG21	1:109:A:THR:HB	2	0.21
(2,400)	1:109:A:THR:HG22	1:109:A:THR:HB	3	0.21
(2,400)	1:109:A:THR:HG23	1:109:A:THR:HB	5	0.21
(2,400)	1:109:A:THR:HG22	1:109:A:THR:HB	7	0.21
(2,385)	1:86:A:ILE:HD12	1:85:A:ARG:HA	3	0.21
(2,365)	1:93:A:ILE:HD11	1:82:A:PHE:HD2	8	0.21
(2,359)	1:122:A:ILE:HG23	1:64:A:VAL:HA	3	0.21
(2,318)	1:64:A:VAL:HG23	1:102:A:THR:HB	4	0.21
(2,299)	1:101:A:VAL:HG13	1:102:A:THR:HA	4	0.21
(2,299)	1:101:A:VAL:HG13	1:102:A:THR:HA	8	0.21
(2,243)	1:123:A:LEU:HD11	1:128:A:VAL:HA	1	0.21
(2,28)	1:87:A:GLU:HG2	1:87:A:GLU:HB3	1	0.21
(1,47)	1:103:A:MET:H	1:95:A:PHE:HB3	3	0.21
(1,43)	1:132:A:ASP:HA	1:103:A:MET:HG2	9	0.21
(1,3)	1:122:A:ILE:HB	1:62:A:LEU:HB2	3	0.21
(1,3)	1:122:A:ILE:HB	1:62:A:LEU:HB2	4	0.21
(2,1935)	1:78:A:LYS:H	1:78:A:LYS:HB3	1	0.2
(2,1935)	1:78:A:LYS:H	1:78:A:LYS:HB3	7	0.2
(2,1930)	1:92:A:SER:H	1:105:A:GLU:HG2	6	0.2
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD22	6	0.2
(2,1819)	1:136:A:LYS:H	1:58:A:GLU:HA	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1796)	1:96:A:LEU:H	1:101:A:VAL:HB	1	0.2
(2,1791)	1:103:A:MET:H	1:103:A:MET:HB3	4	0.2
(2,1765)	1:116:A:ASP:HA	1:116:A:ASP:HB3	3	0.2
(2,1764)	1:116:A:ASP:HB3	1:117:A:GLN:HB2	3	0.2
(2,1755)	1:104:A:ILE:HB	1:102:A:THR:HB	8	0.2
(2,1686)	1:120:A:HIS:HD2	1:123:A:LEU:HA	6	0.2
(2,1686)	1:120:A:HIS:HD2	1:123:A:LEU:HA	8	0.2
(2,1682)	1:62:A:LEU:HA	1:103:A:MET:HG3	10	0.2
(2,1642)	1:72:A:ASN:HA	1:72:A:ASN:HB3	1	0.2
(2,1584)	1:104:A:ILE:HA	1:93:A:ILE:HG22	8	0.2
(2,1544)	1:74:A:SER:HB3	1:71:A:LYS:HG2	4	0.2
(2,1541)	1:81:A:SER:HB3	1:81:A:SER:HA	4	0.2
(2,1541)	1:81:A:SER:HB3	1:81:A:SER:HA	5	0.2
(2,1532)	1:87:A:GLU:HB3	1:83:A:SER:HA	5	0.2
(2,1531)	1:87:A:GLU:HG3	1:83:A:SER:HA	10	0.2
(2,1474)	1:99:A:THR:HB	1:101:A:VAL:HB	10	0.2
(2,1436)	1:104:A:ILE:HG21	1:62:A:LEU:HG	1	0.2
(2,1408)	1:135:A:VAL:HG12	1:58:A:GLU:HA	9	0.2
(2,1404)	1:102:A:THR:HG22	1:77:A:ALA:HA	2	0.2
(2,1401)	1:84:A:THR:HG23	1:118:A:LEU:HD21	5	0.2
(2,1396)	1:101:A:VAL:HG12	1:63:A:MET:HA	7	0.2
(2,1361)	1:122:A:ILE:HG13	1:119:A:LEU:HD22	8	0.2
(2,1341)	1:136:A:LYS:HG2	1:58:A:GLU:HG2	10	0.2
(2,1337)	1:137:A:LEU:HG	1:137:A:LEU:HD13	1	0.2
(2,1337)	1:96:A:LEU:HG	1:96:A:LEU:HD11	3	0.2
(2,1337)	1:96:A:LEU:HG	1:96:A:LEU:HD13	5	0.2
(2,1337)	1:131:A:LEU:HG	1:131:A:LEU:HD13	6	0.2
(2,1306)	1:106:A:LEU:HD11	1:106:A:LEU:HG	8	0.2
(2,1306)	1:106:A:LEU:HD12	1:106:A:LEU:HG	10	0.2
(2,1294)	1:106:A:LEU:HG	1:90:A:GLY:HA3	2	0.2
(2,1269)	1:78:A:LYS:HD2	1:75:A:LYS:HE2	2	0.2
(2,1256)	1:75:A:LYS:HD3	1:78:A:LYS:HE3	9	0.2
(2,1247)	1:68:A:GLN:HB3	1:67:A:LYS:HA	7	0.2
(2,1204)	1:59:A:MET:HG3	1:58:A:GLU:HA	3	0.2
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB2	5	0.2
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB1	7	0.2
(2,1047)	1:79:A:SER:H	1:82:A:PHE:HD2	4	0.2
(2,990)	1:59:A:MET:H	1:59:A:MET:HB3	10	0.2
(2,788)	1:73:A:PHE:H	1:73:A:PHE:HD2	2	0.2
(2,688)	1:108:A:LYS:HD3	1:108:A:LYS:HE3	7	0.2
(2,659)	1:90:A:GLY:HA2	1:89:A:LEU:HA	5	0.2
(2,649)	1:70:A:SER:HB2	1:126:A:GLY:HA3	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,506)	1:118:A:LEU:HD21	1:82:A:PHE:HE1	6	0.2
(2,479)	1:128:A:VAL:HG13	1:128:A:VAL:HA	10	0.2
(2,400)	1:109:A:THR:HG23	1:109:A:THR:HB	4	0.2
(2,400)	1:109:A:THR:HG21	1:109:A:THR:HB	9	0.2
(2,400)	1:109:A:THR:HG22	1:109:A:THR:HB	10	0.2
(2,363)	1:93:A:ILE:HD11	1:77:A:ALA:HA	8	0.2
(2,352)	1:104:A:ILE:HG23	1:73:A:PHE:HZ	10	0.2
(2,299)	1:101:A:VAL:HG11	1:102:A:THR:HA	9	0.2
(2,295)	1:101:A:VAL:HG12	1:103:A:MET:HA	6	0.2
(2,262)	1:65:A:THR:HG21	1:65:A:THR:HB	4	0.2
(2,262)	1:65:A:THR:HG22	1:65:A:THR:HB	5	0.2
(2,262)	1:65:A:THR:HG21	1:65:A:THR:HB	7	0.2
(2,262)	1:65:A:THR:HG21	1:65:A:THR:HB	8	0.2
(2,225)	1:115:A:MET:HG3	1:119:A:LEU:HD13	1	0.2
(2,219)	1:75:A:LYS:HG3	1:75:A:LYS:HA	3	0.2
(2,54)	1:129:A:VAL:HB	1:122:A:ILE:HG21	6	0.2
(1,3)	1:122:A:ILE:HB	1:62:A:LEU:HB2	6	0.2
(2,1949)	1:90:A:GLY:H	1:107:A:PRO:HG3	9	0.19
(2,1935)	1:78:A:LYS:H	1:78:A:LYS:HB3	5	0.19
(2,1904)	1:66:A:GLU:H	1:71:A:LYS:HD3	4	0.19
(2,1892)	1:65:A:THR:H	1:128:A:VAL:HB	5	0.19
(2,1881)	1:114:A:ASP:H	1:115:A:MET:HB3	5	0.19
(2,1863)	1:121:A:ASP:H	1:122:A:ILE:HB	5	0.19
(2,1863)	1:121:A:ASP:H	1:122:A:ILE:HB	7	0.19
(2,1863)	1:121:A:ASP:H	1:122:A:ILE:HB	9	0.19
(2,1739)	1:71:A:LYS:HE2	1:71:A:LYS:HG3	6	0.19
(2,1683)	1:131:A:LEU:HD11	1:62:A:LEU:HA	10	0.19
(2,1615)	1:64:A:VAL:HB	1:73:A:PHE:HZ	8	0.19
(2,1602)	1:118:A:LEU:HG	1:118:A:LEU:HA	7	0.19
(2,1567)	1:99:A:THR:HA	1:100:A:GLY:HA2	6	0.19
(2,1567)	1:99:A:THR:HA	1:100:A:GLY:HA2	7	0.19
(2,1566)	1:99:A:THR:HA	1:100:A:GLY:HA3	2	0.19
(2,1566)	1:99:A:THR:HA	1:100:A:GLY:HA3	5	0.19
(2,1566)	1:99:A:THR:HA	1:100:A:GLY:HA3	7	0.19
(2,1541)	1:81:A:SER:HB3	1:81:A:SER:HA	3	0.19
(2,1476)	1:102:A:THR:HB	1:77:A:ALA:HB2	10	0.19
(2,1474)	1:99:A:THR:HB	1:101:A:VAL:HB	6	0.19
(2,1384)	1:84:A:THR:HG23	1:84:A:THR:HB	5	0.19
(2,1367)	1:65:A:THR:HG22	1:100:A:GLY:HA2	6	0.19
(2,1337)	1:96:A:LEU:HG	1:96:A:LEU:HD11	8	0.19
(2,1306)	1:106:A:LEU:HD11	1:106:A:LEU:HG	5	0.19
(2,1306)	1:106:A:LEU:HD13	1:106:A:LEU:HG	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1306)	1:106:A:LEU:HD13	1:106:A:LEU:HG	9	0.19
(2,1305)	1:118:A:LEU:HD11	1:85:A:ARG:HA	6	0.19
(2,1295)	1:106:A:LEU:HG	1:89:A:LEU:HB3	7	0.19
(2,1252)	1:136:A:LYS:HD3	1:59:A:MET:HG2	3	0.19
(2,1186)	1:105:A:GLU:HB3	1:59:A:MET:HG3	4	0.19
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG21	3	0.19
(2,1062)	1:120:A:HIS:H	1:119:A:LEU:HB3	7	0.19
(2,990)	1:59:A:MET:H	1:59:A:MET:HB3	3	0.19
(2,918)	1:71:A:LYS:H	1:67:A:LYS:HA	3	0.19
(2,724)	1:128:A:VAL:HG22	1:65:A:THR:HB	5	0.19
(2,642)	1:113:A:HIS:HB2	1:113:A:HIS:HD2	3	0.19
(2,506)	1:118:A:LEU:HD23	1:82:A:PHE:HE1	5	0.19
(2,414)	1:92:A:SER:HB3	1:92:A:SER:HA	4	0.19
(2,414)	1:92:A:SER:HB3	1:92:A:SER:HA	9	0.19
(2,400)	1:109:A:THR:HG22	1:109:A:THR:HB	8	0.19
(2,385)	1:86:A:ILE:HD13	1:85:A:ARG:HA	5	0.19
(2,364)	1:104:A:ILE:HD12	1:82:A:PHE:HE2	3	0.19
(2,364)	1:104:A:ILE:HD12	1:82:A:PHE:HE2	9	0.19
(2,363)	1:93:A:ILE:HD13	1:77:A:ALA:HA	4	0.19
(2,322)	1:64:A:VAL:HG11	1:64:A:VAL:HG23	7	0.19
(2,308)	1:102:A:THR:HG23	1:104:A:ILE:HG13	4	0.19
(2,262)	1:65:A:THR:HG23	1:65:A:THR:HB	2	0.19
(2,262)	1:65:A:THR:HG22	1:65:A:THR:HB	6	0.19
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG21	7	0.19
(2,177)	1:123:A:LEU:HG	1:122:A:ILE:HG21	5	0.19
(2,177)	1:123:A:LEU:HG	1:122:A:ILE:HG23	6	0.19
(2,106)	1:103:A:MET:HG2	1:94:A:SER:HB2	5	0.19
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG11	5	0.19
(2,72)	1:59:A:MET:HG3	1:136:A:LYS:HB3	9	0.19
(2,28)	1:87:A:GLU:HG2	1:87:A:GLU:HB3	2	0.19
(2,8)	1:122:A:ILE:HB	1:64:A:VAL:HG13	4	0.19
(1,47)	1:103:A:MET:H	1:95:A:PHE:HB3	9	0.19
(2,1934)	1:92:A:SER:H	1:104:A:ILE:HG21	10	0.18
(2,1922)	1:86:A:ILE:H	1:87:A:GLU:HB2	6	0.18
(2,1901)	1:119:A:LEU:H	1:120:A:HIS:HB2	10	0.18
(2,1863)	1:121:A:ASP:H	1:122:A:ILE:HB	2	0.18
(2,1814)	1:62:A:LEU:H	1:104:A:ILE:HB	6	0.18
(2,1791)	1:103:A:MET:H	1:103:A:MET:HB3	1	0.18
(2,1791)	1:103:A:MET:H	1:103:A:MET:HB3	3	0.18
(2,1791)	1:103:A:MET:H	1:103:A:MET:HB3	8	0.18
(2,1785)	1:103:A:MET:H	1:103:A:MET:HG2	9	0.18
(2,1785)	1:103:A:MET:H	1:103:A:MET:HG2	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1764)	1:116:A:ASP:HB3	1:117:A:GLN:HB2	4	0.18
(2,1685)	1:62:A:LEU:HA	1:103:A:MET:HB3	1	0.18
(2,1649)	1:78:A:LYS:HG3	1:78:A:LYS:HA	5	0.18
(2,1649)	1:78:A:LYS:HG3	1:78:A:LYS:HA	7	0.18
(2,1623)	1:115:A:MET:HA	1:119:A:LEU:HG	6	0.18
(2,1602)	1:118:A:LEU:HG	1:118:A:LEU:HA	9	0.18
(2,1594)	1:89:A:LEU:HG	1:111:A:SER:HA	4	0.18
(2,1581)	1:104:A:ILE:HA	1:93:A:ILE:HG13	2	0.18
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB3	5	0.18
(2,1567)	1:99:A:THR:HA	1:100:A:GLY:HA2	10	0.18
(2,1566)	1:99:A:THR:HA	1:100:A:GLY:HA3	1	0.18
(2,1544)	1:74:A:SER:HB3	1:75:A:LYS:HG2	1	0.18
(2,1541)	1:81:A:SER:HB3	1:81:A:SER:HA	7	0.18
(2,1516)	1:107:A:PRO:HA	1:59:A:MET:HB3	1	0.18
(2,1514)	1:86:A:ILE:HD12	1:82:A:PHE:HD1	7	0.18
(2,1422)	1:125:A:ALA:HB1	1:76:A:MET:HA	6	0.18
(2,1384)	1:84:A:THR:HG23	1:84:A:THR:HB	6	0.18
(2,1384)	1:109:A:THR:HG22	1:109:A:THR:HA	10	0.18
(2,1383)	1:66:A:GLU:HB2	1:97:A:THR:HG21	2	0.18
(2,1382)	1:64:A:VAL:HG12	1:62:A:LEU:HB2	10	0.18
(2,1344)	1:123:A:LEU:HD22	1:129:A:VAL:HG21	6	0.18
(2,1305)	1:118:A:LEU:HD11	1:85:A:ARG:HA	3	0.18
(2,1305)	1:118:A:LEU:HD11	1:85:A:ARG:HA	7	0.18
(2,1269)	1:78:A:LYS:HD3	1:75:A:LYS:HE3	9	0.18
(2,1261)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	5	0.18
(2,1253)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	2	0.18
(2,1253)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	7	0.18
(2,1235)	1:76:A:MET:HG2	1:122:A:ILE:HA	4	0.18
(2,1149)	1:58:A:GLU:H	1:58:A:GLU:HG2	6	0.18
(2,1131)	1:99:A:THR:H	1:65:A:THR:HG23	2	0.18
(2,1047)	1:79:A:SER:H	1:82:A:PHE:HD2	7	0.18
(2,932)	1:60:A:THR:H	1:59:A:MET:HB2	2	0.18
(2,918)	1:71:A:LYS:H	1:67:A:LYS:HA	5	0.18
(2,918)	1:71:A:LYS:H	1:67:A:LYS:HA	6	0.18
(2,893)	1:115:A:MET:H	1:114:A:ASP:HB3	9	0.18
(2,794)	1:82:A:PHE:H	1:82:A:PHE:HD1	2	0.18
(2,794)	1:82:A:PHE:H	1:82:A:PHE:HD1	8	0.18
(2,788)	1:73:A:PHE:H	1:73:A:PHE:HD2	8	0.18
(2,659)	1:90:A:GLY:HA2	1:89:A:LEU:HA	1	0.18
(2,659)	1:90:A:GLY:HA2	1:89:A:LEU:HA	7	0.18
(2,659)	1:90:A:GLY:HA2	1:89:A:LEU:HA	8	0.18
(2,654)	1:72:A:ASN:HB2	1:126:A:GLY:HA3	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,521)	1:86:A:ILE:HG22	1:87:A:GLU:HA	2	0.18
(2,414)	1:92:A:SER:HB3	1:92:A:SER:HA	6	0.18
(2,414)	1:92:A:SER:HB3	1:92:A:SER:HA	7	0.18
(2,414)	1:92:A:SER:HB3	1:92:A:SER:HA	10	0.18
(2,405)	1:64:A:VAL:HG11	1:122:A:ILE:HA	6	0.18
(2,359)	1:122:A:ILE:HG23	1:64:A:VAL:HA	10	0.18
(2,322)	1:64:A:VAL:HG12	1:64:A:VAL:HG21	5	0.18
(2,322)	1:64:A:VAL:HG12	1:64:A:VAL:HG23	6	0.18
(2,322)	1:64:A:VAL:HG11	1:64:A:VAL:HG23	10	0.18
(2,318)	1:64:A:VAL:HG21	1:102:A:THR:HB	5	0.18
(2,308)	1:102:A:THR:HG22	1:104:A:ILE:HG13	6	0.18
(2,279)	1:64:A:VAL:HG13	1:122:A:ILE:HG21	1	0.18
(2,262)	1:65:A:THR:HG22	1:65:A:THR:HB	9	0.18
(2,195)	1:89:A:LEU:HG	1:89:A:LEU:HA	5	0.18
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG23	5	0.18
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG23	10	0.18
(2,103)	1:103:A:MET:HG3	1:61:A:ARG:HD3	5	0.18
(2,72)	1:59:A:MET:HG3	1:136:A:LYS:HB3	8	0.18
(2,28)	1:87:A:GLU:HG2	1:87:A:GLU:HB3	3	0.18
(2,28)	1:87:A:GLU:HG2	1:87:A:GLU:HB3	7	0.18
(1,46)	1:108:A:LYS:HE3	1:59:A:MET:HA	6	0.18
(1,6)	1:101:A:VAL:HB	1:103:A:MET:HG2	8	0.18
(2,1928)	1:83:A:SER:H	1:85:A:ARG:HB3	8	0.17
(2,1914)	1:79:A:SER:H	1:78:A:LYS:HB3	6	0.17
(2,1881)	1:114:A:ASP:H	1:115:A:MET:HB3	9	0.17
(2,1827)	1:95:A:PHE:H	1:93:A:ILE:HB	3	0.17
(2,1784)	1:104:A:ILE:H	1:103:A:MET:HG3	9	0.17
(2,1740)	1:128:A:VAL:HG22	1:67:A:LYS:HE2	10	0.17
(2,1739)	1:71:A:LYS:HE2	1:71:A:LYS:HG3	3	0.17
(2,1688)	1:125:A:ALA:HA	1:72:A:ASN:HB3	10	0.17
(2,1686)	1:120:A:HIS:HD2	1:123:A:LEU:HA	4	0.17
(2,1680)	1:104:A:ILE:HD13	1:63:A:MET:HA	1	0.17
(2,1680)	1:104:A:ILE:HD13	1:63:A:MET:HA	2	0.17
(2,1680)	1:104:A:ILE:HD11	1:63:A:MET:HA	3	0.17
(2,1680)	1:104:A:ILE:HD12	1:63:A:MET:HA	8	0.17
(2,1656)	1:105:A:GLU:HA	1:62:A:LEU:HG	7	0.17
(2,1648)	1:136:A:LYS:HG3	1:136:A:LYS:HA	7	0.17
(2,1642)	1:72:A:ASN:HA	1:72:A:ASN:HB3	7	0.17
(2,1611)	1:104:A:ILE:HG12	1:82:A:PHE:HZ	6	0.17
(2,1600)	1:79:A:SER:HB2	1:79:A:SER:HA	8	0.17
(2,1600)	1:79:A:SER:HB2	1:79:A:SER:HA	10	0.17
(2,1597)	1:75:A:LYS:HB2	1:75:A:LYS:HA	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1594)	1:89:A:LEU:HG	1:111:A:SER:HA	1	0.17
(2,1566)	1:99:A:THR:HA	1:100:A:GLY:HA3	4	0.17
(2,1566)	1:99:A:THR:HA	1:100:A:GLY:HA3	6	0.17
(2,1555)	1:86:A:ILE:HA	1:89:A:LEU:HB3	5	0.17
(2,1544)	1:74:A:SER:HB3	1:71:A:LYS:HG2	10	0.17
(2,1436)	1:104:A:ILE:HG21	1:62:A:LEU:HG	2	0.17
(2,1434)	1:86:A:ILE:HG21	1:106:A:LEU:HD13	2	0.17
(2,1384)	1:109:A:THR:HG22	1:109:A:THR:HA	4	0.17
(2,1384)	1:84:A:THR:HG22	1:84:A:THR:HB	7	0.17
(2,1384)	1:84:A:THR:HG23	1:84:A:THR:HB	9	0.17
(2,1381)	1:64:A:VAL:HG12	1:125:A:ALA:HB2	9	0.17
(2,1337)	1:137:A:LEU:HD12	1:137:A:LEU:HB3	4	0.17
(2,1337)	1:96:A:LEU:HG	1:96:A:LEU:HD13	7	0.17
(2,1295)	1:106:A:LEU:HG	1:89:A:LEU:HB3	8	0.17
(2,1272)	1:78:A:LYS:HB2	1:78:A:LYS:HD2	8	0.17
(2,1253)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	3	0.17
(2,1253)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	4	0.17
(2,1253)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	6	0.17
(2,1240)	1:120:A:HIS:HB3	1:122:A:ILE:HG13	3	0.17
(2,1159)	1:72:A:ASN:HB3	1:76:A:MET:HB3	1	0.17
(2,1154)	1:72:A:ASN:HB2	1:73:A:PHE:HD1	8	0.17
(2,1153)	1:72:A:ASN:HB3	1:76:A:MET:HG2	7	0.17
(2,1062)	1:120:A:HIS:H	1:119:A:LEU:HB3	10	0.17
(2,1047)	1:79:A:SER:H	1:82:A:PHE:HD2	9	0.17
(2,933)	1:60:A:THR:H	1:106:A:LEU:HB3	2	0.17
(2,918)	1:71:A:LYS:H	1:67:A:LYS:HA	1	0.17
(2,918)	1:71:A:LYS:H	1:67:A:LYS:HA	4	0.17
(2,749)	1:61:A:ARG:H	1:61:A:ARG:HD3	1	0.17
(2,724)	1:128:A:VAL:HG22	1:65:A:THR:HB	8	0.17
(2,659)	1:90:A:GLY:HA2	1:89:A:LEU:HA	4	0.17
(2,659)	1:90:A:GLY:HA2	1:89:A:LEU:HA	6	0.17
(2,659)	1:90:A:GLY:HA2	1:89:A:LEU:HA	9	0.17
(2,489)	1:95:A:PHE:HE2	1:78:A:LYS:HE3	6	0.17
(2,479)	1:128:A:VAL:HG12	1:128:A:VAL:HA	5	0.17
(2,464)	1:101:A:VAL:HG12	1:101:A:VAL:HA	1	0.17
(2,414)	1:92:A:SER:HB3	1:92:A:SER:HA	2	0.17
(2,365)	1:93:A:ILE:HD13	1:82:A:PHE:HD2	6	0.17
(2,364)	1:104:A:ILE:HD12	1:82:A:PHE:HE2	4	0.17
(2,352)	1:104:A:ILE:HG21	1:73:A:PHE:HZ	9	0.17
(2,341)	1:77:A:ALA:HB2	1:78:A:LYS:HA	6	0.17
(2,322)	1:64:A:VAL:HG12	1:64:A:VAL:HG21	2	0.17
(2,322)	1:64:A:VAL:HG13	1:64:A:VAL:HG22	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,295)	1:101:A:VAL:HG11	1:103:A:MET:HA	9	0.17
(2,291)	1:60:A:THR:HG21	1:60:A:THR:HA	3	0.17
(2,291)	1:60:A:THR:HG22	1:60:A:THR:HA	9	0.17
(2,262)	1:65:A:THR:HG21	1:65:A:THR:HB	10	0.17
(2,195)	1:89:A:LEU:HG	1:89:A:LEU:HA	10	0.17
(2,186)	1:96:A:LEU:HG	1:103:A:MET:HG2	7	0.17
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG23	2	0.17
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG21	4	0.17
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG21	6	0.17
(2,177)	1:123:A:LEU:HG	1:122:A:ILE:HG23	9	0.17
(2,140)	1:66:A:GLU:HB2	1:71:A:LYS:HD3	2	0.17
(1,41)	1:105:A:GLU:HA	1:132:A:ASP:HB2	10	0.17
(1,8)	1:107:A:PRO:HB2	1:90:A:GLY:HA2	1	0.17
(2,1949)	1:90:A:GLY:H	1:107:A:PRO:HG3	7	0.16
(2,1928)	1:83:A:SER:H	1:85:A:ARG:HB3	6	0.16
(2,1892)	1:65:A:THR:H	1:128:A:VAL:HB	3	0.16
(2,1874)	1:123:A:LEU:H	1:123:A:LEU:HD21	6	0.16
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB3	4	0.16
(2,1856)	1:94:A:SER:H	1:93:A:ILE:HB	5	0.16
(2,1814)	1:62:A:LEU:H	1:104:A:ILE:HB	8	0.16
(2,1814)	1:62:A:LEU:H	1:62:A:LEU:HB3	9	0.16
(2,1810)	1:136:A:LYS:H	1:136:A:LYS:HD2	2	0.16
(2,1791)	1:103:A:MET:H	1:103:A:MET:HB3	7	0.16
(2,1791)	1:103:A:MET:H	1:103:A:MET:HB3	10	0.16
(2,1767)	1:89:A:LEU:HD21	1:114:A:ASP:HB3	10	0.16
(2,1764)	1:116:A:ASP:HB3	1:117:A:GLN:HB2	8	0.16
(2,1743)	1:75:A:LYS:HG2	1:75:A:LYS:HE2	7	0.16
(2,1740)	1:128:A:VAL:HG22	1:67:A:LYS:HE2	5	0.16
(2,1740)	1:128:A:VAL:HG23	1:67:A:LYS:HE2	7	0.16
(2,1710)	1:90:A:GLY:HA3	1:107:A:PRO:HG2	3	0.16
(2,1680)	1:104:A:ILE:HD13	1:63:A:MET:HA	10	0.16
(2,1611)	1:104:A:ILE:HG12	1:82:A:PHE:HZ	5	0.16
(2,1602)	1:118:A:LEU:HG	1:118:A:LEU:HA	8	0.16
(2,1600)	1:79:A:SER:HB2	1:79:A:SER:HA	5	0.16
(2,1600)	1:79:A:SER:HB2	1:79:A:SER:HA	7	0.16
(2,1600)	1:79:A:SER:HB2	1:79:A:SER:HA	9	0.16
(2,1597)	1:75:A:LYS:HB3	1:75:A:LYS:HA	3	0.16
(2,1566)	1:99:A:THR:HA	1:100:A:GLY:HA3	9	0.16
(2,1566)	1:99:A:THR:HA	1:100:A:GLY:HA3	10	0.16
(2,1560)	1:78:A:LYS:HG3	1:95:A:PHE:HE2	3	0.16
(2,1523)	1:135:A:VAL:HA	1:58:A:GLU:HG2	9	0.16
(2,1493)	1:111:A:SER:HB3	1:112:A:GLU:HB3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1416)	1:64:A:VAL:HG21	1:73:A:PHE:HE2	2	0.16
(2,1409)	1:135:A:VAL:HG11	1:108:A:LYS:HA	3	0.16
(2,1404)	1:102:A:THR:HG23	1:77:A:ALA:HA	3	0.16
(2,1384)	1:109:A:THR:HG21	1:109:A:THR:HA	2	0.16
(2,1384)	1:84:A:THR:HG22	1:84:A:THR:HB	3	0.16
(2,1384)	1:84:A:THR:HG22	1:84:A:THR:HB	8	0.16
(2,1383)	1:66:A:GLU:HB2	1:97:A:THR:HG22	3	0.16
(2,1381)	1:64:A:VAL:HG12	1:125:A:ALA:HB1	4	0.16
(2,1362)	1:101:A:VAL:HB	1:96:A:LEU:HD23	3	0.16
(2,1362)	1:96:A:LEU:HB3	1:96:A:LEU:HD22	7	0.16
(2,1345)	1:110:A:VAL:HG13	1:114:A:ASP:HB2	9	0.16
(2,1339)	1:106:A:LEU:HD22	1:135:A:VAL:HG12	9	0.16
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD12	7	0.16
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD13	9	0.16
(2,1295)	1:106:A:LEU:HG	1:89:A:LEU:HB3	6	0.16
(2,1253)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	1	0.16
(2,1253)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	8	0.16
(2,1240)	1:120:A:HIS:HB3	1:122:A:ILE:HG13	7	0.16
(2,1233)	1:76:A:MET:HG2	1:82:A:PHE:HD2	6	0.16
(2,1230)	1:71:A:LYS:HB2	1:71:A:LYS:HE3	1	0.16
(2,1230)	1:71:A:LYS:HB2	1:71:A:LYS:HE2	4	0.16
(2,1181)	1:101:A:VAL:HB	1:103:A:MET:HA	8	0.16
(2,1153)	1:72:A:ASN:HB3	1:76:A:MET:HG2	8	0.16
(2,989)	1:59:A:MET:H	1:58:A:GLU:HG2	3	0.16
(2,918)	1:71:A:LYS:H	1:67:A:LYS:HA	2	0.16
(2,918)	1:71:A:LYS:H	1:67:A:LYS:HA	9	0.16
(2,918)	1:71:A:LYS:H	1:67:A:LYS:HA	10	0.16
(2,794)	1:82:A:PHE:H	1:82:A:PHE:HD1	4	0.16
(2,659)	1:90:A:GLY:HA2	1:89:A:LEU:HA	2	0.16
(2,659)	1:90:A:GLY:HA2	1:89:A:LEU:HA	10	0.16
(2,649)	1:70:A:SER:HB2	1:126:A:GLY:HA3	3	0.16
(2,617)	1:103:A:MET:HG2	1:103:A:MET:HA	1	0.16
(2,583)	1:136:A:LYS:HA	1:133:A:SER:HB2	10	0.16
(2,488)	1:74:A:SER:HB3	1:95:A:PHE:HE2	4	0.16
(2,479)	1:128:A:VAL:HG11	1:128:A:VAL:HA	6	0.16
(2,464)	1:101:A:VAL:HG12	1:101:A:VAL:HA	4	0.16
(2,433)	1:76:A:MET:HG3	1:82:A:PHE:HD1	9	0.16
(2,420)	1:79:A:SER:HB2	1:82:A:PHE:HB3	9	0.16
(2,414)	1:92:A:SER:HB3	1:92:A:SER:HA	3	0.16
(2,365)	1:93:A:ILE:HD11	1:82:A:PHE:HD2	3	0.16
(2,365)	1:93:A:ILE:HD13	1:82:A:PHE:HD2	4	0.16
(2,326)	1:125:A:ALA:HB2	1:125:A:ALA:HA	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,308)	1:102:A:THR:HG22	1:104:A:ILE:HG13	7	0.16
(2,295)	1:101:A:VAL:HG13	1:103:A:MET:HA	8	0.16
(2,290)	1:60:A:THR:HG23	1:62:A:LEU:HA	4	0.16
(2,262)	1:65:A:THR:HG21	1:65:A:THR:HB	1	0.16
(2,262)	1:65:A:THR:HG22	1:65:A:THR:HB	3	0.16
(2,256)	1:89:A:LEU:HD21	1:89:A:LEU:HA	9	0.16
(2,246)	1:123:A:LEU:HD13	1:127:A:GLY:HA2	6	0.16
(2,202)	1:118:A:LEU:HD11	1:114:A:ASP:HB2	4	0.16
(2,195)	1:89:A:LEU:HG	1:89:A:LEU:HA	6	0.16
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG21	1	0.16
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG21	3	0.16
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG23	9	0.16
(2,177)	1:123:A:LEU:HG	1:122:A:ILE:HG22	3	0.16
(2,163)	1:93:A:ILE:HG13	1:93:A:ILE:HG22	8	0.16
(2,132)	1:75:A:LYS:HD3	1:75:A:LYS:HA	10	0.16
(1,47)	1:103:A:MET:H	1:95:A:PHE:HB3	4	0.16
(1,43)	1:132:A:ASP:HA	1:103:A:MET:HG2	2	0.16
(1,36)	1:85:A:ARG:HA	1:88:A:GLU:HB3	3	0.16
(1,3)	1:122:A:ILE:HB	1:62:A:LEU:HB2	2	0.16
(2,1904)	1:66:A:GLU:H	1:71:A:LYS:HD3	5	0.15
(2,1856)	1:94:A:SER:H	1:93:A:ILE:HB	1	0.15
(2,1856)	1:94:A:SER:H	1:93:A:ILE:HB	4	0.15
(2,1827)	1:95:A:PHE:H	1:93:A:ILE:HB	9	0.15
(2,1791)	1:103:A:MET:H	1:103:A:MET:HB3	2	0.15
(2,1749)	1:95:A:PHE:HE2	1:78:A:LYS:HE3	6	0.15
(2,1682)	1:62:A:LEU:HA	1:103:A:MET:HG3	7	0.15
(2,1673)	1:93:A:ILE:HD13	1:77:A:ALA:HA	5	0.15
(2,1648)	1:136:A:LYS:HG3	1:136:A:LYS:HA	9	0.15
(2,1643)	1:58:A:GLU:HA	1:59:A:MET:HG2	2	0.15
(2,1642)	1:72:A:ASN:HA	1:72:A:ASN:HB3	8	0.15
(2,1602)	1:118:A:LEU:HG	1:118:A:LEU:HA	1	0.15
(2,1600)	1:79:A:SER:HB2	1:79:A:SER:HA	1	0.15
(2,1600)	1:79:A:SER:HB2	1:79:A:SER:HA	2	0.15
(2,1600)	1:79:A:SER:HB2	1:79:A:SER:HA	3	0.15
(2,1600)	1:79:A:SER:HB2	1:79:A:SER:HA	6	0.15
(2,1597)	1:75:A:LYS:HB3	1:75:A:LYS:HA	10	0.15
(2,1594)	1:89:A:LEU:HG	1:111:A:SER:HA	8	0.15
(2,1531)	1:87:A:GLU:HG3	1:83:A:SER:HA	5	0.15
(2,1526)	1:95:A:PHE:HD1	1:102:A:THR:HA	8	0.15
(2,1484)	1:122:A:ILE:HA	1:123:A:LEU:HA	6	0.15
(2,1474)	1:99:A:THR:HB	1:101:A:VAL:HB	8	0.15
(2,1384)	1:84:A:THR:HG21	1:84:A:THR:HB	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD12	5	0.15
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD11	6	0.15
(2,1325)	1:136:A:LYS:HG3	1:58:A:GLU:HG2	8	0.15
(2,1253)	1:136:A:LYS:HD3	1:136:A:LYS:HG3	9	0.15
(2,1240)	1:120:A:HIS:HB3	1:122:A:ILE:HG13	5	0.15
(2,1240)	1:120:A:HIS:HB3	1:122:A:ILE:HG13	10	0.15
(2,1230)	1:71:A:LYS:HB2	1:71:A:LYS:HE3	9	0.15
(2,1223)	1:103:A:MET:HG2	1:96:A:LEU:HD21	9	0.15
(2,1181)	1:101:A:VAL:HB	1:103:A:MET:HA	1	0.15
(2,1159)	1:72:A:ASN:HB3	1:76:A:MET:HB3	4	0.15
(2,1144)	1:126:A:GLY:H	1:127:A:GLY:HA2	6	0.15
(2,1144)	1:126:A:GLY:H	1:127:A:GLY:HA2	7	0.15
(2,1097)	1:92:A:SER:H	1:92:A:SER:HB3	1	0.15
(2,1053)	1:79:A:SER:H	1:77:A:ALA:HB2	9	0.15
(2,1047)	1:79:A:SER:H	1:82:A:PHE:HD2	3	0.15
(2,1042)	1:89:A:LEU:H	1:88:A:GLU:HB3	7	0.15
(2,794)	1:82:A:PHE:H	1:82:A:PHE:HD1	1	0.15
(2,788)	1:73:A:PHE:H	1:73:A:PHE:HD1	4	0.15
(2,788)	1:73:A:PHE:H	1:73:A:PHE:HD1	6	0.15
(2,745)	1:105:A:GLU:H	1:105:A:GLU:HB3	3	0.15
(2,659)	1:90:A:GLY:HA2	1:89:A:LEU:HA	3	0.15
(2,617)	1:103:A:MET:HG2	1:103:A:MET:HA	4	0.15
(2,608)	1:124:A:ALA:HB3	1:124:A:ALA:HA	1	0.15
(2,595)	1:60:A:THR:HG22	1:61:A:ARG:HA	6	0.15
(2,521)	1:86:A:ILE:HG23	1:87:A:GLU:HA	7	0.15
(2,514)	1:115:A:MET:HG3	1:112:A:GLU:HA	10	0.15
(2,506)	1:118:A:LEU:HD23	1:82:A:PHE:HE1	3	0.15
(2,479)	1:128:A:VAL:HG13	1:128:A:VAL:HA	3	0.15
(2,472)	1:82:A:PHE:HA	1:84:A:THR:HG22	9	0.15
(2,464)	1:101:A:VAL:HG11	1:101:A:VAL:HA	3	0.15
(2,464)	1:101:A:VAL:HG11	1:101:A:VAL:HA	7	0.15
(2,433)	1:76:A:MET:HG3	1:82:A:PHE:HD1	1	0.15
(2,414)	1:92:A:SER:HB3	1:92:A:SER:HA	5	0.15
(2,365)	1:93:A:ILE:HD11	1:82:A:PHE:HD2	1	0.15
(2,365)	1:93:A:ILE:HD12	1:82:A:PHE:HD2	2	0.15
(2,363)	1:93:A:ILE:HD11	1:77:A:ALA:HA	1	0.15
(2,363)	1:93:A:ILE:HD13	1:77:A:ALA:HA	10	0.15
(2,326)	1:125:A:ALA:HB1	1:125:A:ALA:HA	2	0.15
(2,322)	1:64:A:VAL:HG13	1:64:A:VAL:HG23	8	0.15
(2,322)	1:64:A:VAL:HG12	1:64:A:VAL:HG21	9	0.15
(2,309)	1:102:A:THR:HG21	1:77:A:ALA:HB2	8	0.15
(2,308)	1:102:A:THR:HG23	1:104:A:ILE:HG13	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,293)	1:110:A:VAL:HG23	1:106:A:LEU:HG	2	0.15
(2,291)	1:60:A:THR:HG22	1:60:A:THR:HA	4	0.15
(2,291)	1:60:A:THR:HG22	1:60:A:THR:HA	5	0.15
(2,286)	1:88:A:GLU:HG3	1:84:A:THR:HG23	4	0.15
(2,243)	1:123:A:LEU:HD11	1:128:A:VAL:HA	4	0.15
(2,231)	1:123:A:LEU:HD21	1:120:A:HIS:HA	1	0.15
(2,195)	1:89:A:LEU:HG	1:89:A:LEU:HA	1	0.15
(2,195)	1:89:A:LEU:HG	1:89:A:LEU:HA	2	0.15
(2,195)	1:89:A:LEU:HG	1:89:A:LEU:HA	3	0.15
(2,195)	1:89:A:LEU:HG	1:89:A:LEU:HA	4	0.15
(2,195)	1:89:A:LEU:HG	1:89:A:LEU:HA	7	0.15
(2,195)	1:89:A:LEU:HG	1:89:A:LEU:HA	8	0.15
(2,195)	1:89:A:LEU:HG	1:89:A:LEU:HA	9	0.15
(2,178)	1:86:A:ILE:HG12	1:86:A:ILE:HG22	8	0.15
(2,177)	1:123:A:LEU:HG	1:122:A:ILE:HG21	7	0.15
(2,72)	1:59:A:MET:HG3	1:136:A:LYS:HB3	6	0.15
(1,47)	1:103:A:MET:H	1:95:A:PHE:HB3	2	0.15
(1,43)	1:132:A:ASP:HA	1:103:A:MET:HG2	3	0.15
(1,43)	1:132:A:ASP:HA	1:103:A:MET:HG2	4	0.15
(1,36)	1:85:A:ARG:HA	1:88:A:GLU:HB3	1	0.15
(2,1940)	1:127:A:GLY:H	1:123:A:LEU:HG	10	0.14
(2,1892)	1:65:A:THR:H	1:128:A:VAL:HB	9	0.14
(2,1891)	1:116:A:ASP:H	1:115:A:MET:HB2	1	0.14
(2,1891)	1:116:A:ASP:H	1:115:A:MET:HB2	3	0.14
(2,1891)	1:116:A:ASP:H	1:115:A:MET:HB2	8	0.14
(2,1785)	1:103:A:MET:H	1:103:A:MET:HG2	4	0.14
(2,1740)	1:128:A:VAL:HG22	1:67:A:LYS:HE2	8	0.14
(2,1685)	1:62:A:LEU:HA	1:103:A:MET:HB3	6	0.14
(2,1669)	1:73:A:PHE:HE2	1:77:A:ALA:HA	3	0.14
(2,1648)	1:136:A:LYS:HG3	1:136:A:LYS:HA	3	0.14
(2,1623)	1:115:A:MET:HA	1:119:A:LEU:HG	1	0.14
(2,1611)	1:104:A:ILE:HG12	1:82:A:PHE:HZ	7	0.14
(2,1611)	1:104:A:ILE:HG12	1:82:A:PHE:HZ	9	0.14
(2,1611)	1:104:A:ILE:HG12	1:82:A:PHE:HZ	10	0.14
(2,1602)	1:118:A:LEU:HG	1:118:A:LEU:HA	4	0.14
(2,1531)	1:87:A:GLU:HG3	1:83:A:SER:HA	6	0.14
(2,1531)	1:87:A:GLU:HG3	1:83:A:SER:HA	8	0.14
(2,1515)	1:93:A:ILE:HD11	1:82:A:PHE:HD2	8	0.14
(2,1490)	1:96:A:LEU:HD23	1:94:A:SER:HB2	7	0.14
(2,1484)	1:122:A:ILE:HA	1:123:A:LEU:HA	3	0.14
(2,1484)	1:122:A:ILE:HA	1:123:A:LEU:HA	9	0.14
(2,1474)	1:99:A:THR:HB	1:101:A:VAL:HB	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1417)	1:64:A:VAL:HG23	1:62:A:LEU:HA	1	0.14
(2,1403)	1:102:A:THR:HG23	1:74:A:SER:HA	1	0.14
(2,1391)	1:60:A:THR:HG22	1:61:A:ARG:HA	6	0.14
(2,1383)	1:66:A:GLU:HB2	1:97:A:THR:HG21	4	0.14
(2,1337)	1:137:A:LEU:HD11	1:137:A:LEU:HB3	10	0.14
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD11	10	0.14
(2,1324)	1:115:A:MET:HG3	1:108:A:LYS:HG3	3	0.14
(2,1323)	1:75:A:LYS:HG3	1:75:A:LYS:HE3	1	0.14
(2,1297)	1:86:A:ILE:HG13	1:82:A:PHE:HZ	2	0.14
(2,1295)	1:106:A:LEU:HG	1:89:A:LEU:HB3	10	0.14
(2,1290)	1:118:A:LEU:HG	1:114:A:ASP:HB2	3	0.14
(2,1288)	1:137:A:LEU:HG	1:132:A:ASP:HA	2	0.14
(2,1272)	1:78:A:LYS:HB2	1:78:A:LYS:HD2	2	0.14
(2,1259)	1:136:A:LYS:HD2	1:58:A:GLU:HA	8	0.14
(2,1240)	1:120:A:HIS:HB3	1:122:A:ILE:HG13	9	0.14
(2,1230)	1:71:A:LYS:HB2	1:71:A:LYS:HE2	10	0.14
(2,1224)	1:115:A:MET:HB3	1:111:A:SER:HB2	7	0.14
(2,1213)	1:76:A:MET:HB2	1:73:A:PHE:HD2	4	0.14
(2,1193)	1:128:A:VAL:HB	1:128:A:VAL:HG13	3	0.14
(2,1184)	1:59:A:MET:HB3	1:90:A:GLY:HA2	8	0.14
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG21	10	0.14
(2,1144)	1:126:A:GLY:H	1:127:A:GLY:HA2	4	0.14
(2,1088)	1:83:A:SER:H	1:82:A:PHE:HB2	6	0.14
(2,868)	1:87:A:GLU:H	1:86:A:ILE:HG22	2	0.14
(2,868)	1:87:A:GLU:H	1:86:A:ILE:HG23	4	0.14
(2,868)	1:87:A:GLU:H	1:86:A:ILE:HG22	10	0.14
(2,788)	1:73:A:PHE:H	1:73:A:PHE:HD2	1	0.14
(2,617)	1:103:A:MET:HG2	1:103:A:MET:HA	10	0.14
(2,608)	1:124:A:ALA:HB3	1:124:A:ALA:HA	3	0.14
(2,598)	1:66:A:GLU:HA	1:73:A:PHE:HD1	7	0.14
(2,595)	1:60:A:THR:HG21	1:61:A:ARG:HA	1	0.14
(2,595)	1:60:A:THR:HG21	1:61:A:ARG:HA	7	0.14
(2,580)	1:134:A:GLU:HA	1:62:A:LEU:HD22	10	0.14
(2,569)	1:95:A:PHE:HD1	1:94:A:SER:HA	4	0.14
(2,564)	1:95:A:PHE:HD1	1:95:A:PHE:HA	7	0.14
(2,523)	1:87:A:GLU:HG3	1:87:A:GLU:HA	1	0.14
(2,523)	1:87:A:GLU:HG3	1:87:A:GLU:HA	7	0.14
(2,521)	1:86:A:ILE:HG23	1:87:A:GLU:HA	3	0.14
(2,521)	1:86:A:ILE:HG23	1:87:A:GLU:HA	4	0.14
(2,521)	1:86:A:ILE:HG22	1:87:A:GLU:HA	5	0.14
(2,514)	1:115:A:MET:HG3	1:112:A:GLU:HA	2	0.14
(2,506)	1:118:A:LEU:HD23	1:82:A:PHE:HE1	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,500)	1:82:A:PHE:HE1	1:119:A:LEU:HA	1	0.14
(2,500)	1:82:A:PHE:HE1	1:119:A:LEU:HA	10	0.14
(2,479)	1:128:A:VAL:HG11	1:128:A:VAL:HA	7	0.14
(2,464)	1:101:A:VAL:HG13	1:101:A:VAL:HA	9	0.14
(2,451)	1:76:A:MET:HG3	1:73:A:PHE:HA	6	0.14
(2,433)	1:76:A:MET:HG3	1:82:A:PHE:HD1	4	0.14
(2,414)	1:92:A:SER:HB3	1:92:A:SER:HA	1	0.14
(2,365)	1:93:A:ILE:HD13	1:82:A:PHE:HD2	7	0.14
(2,341)	1:77:A:ALA:HB1	1:78:A:LYS:HA	2	0.14
(2,322)	1:64:A:VAL:HG13	1:64:A:VAL:HG22	1	0.14
(2,295)	1:101:A:VAL:HG12	1:103:A:MET:HA	10	0.14
(2,291)	1:60:A:THR:HG23	1:60:A:THR:HA	10	0.14
(2,290)	1:60:A:THR:HG22	1:62:A:LEU:HA	6	0.14
(2,259)	1:97:A:THR:HG23	1:96:A:LEU:HA	9	0.14
(2,256)	1:89:A:LEU:HD23	1:89:A:LEU:HA	4	0.14
(2,256)	1:89:A:LEU:HD23	1:89:A:LEU:HA	8	0.14
(2,231)	1:123:A:LEU:HD22	1:120:A:HIS:HA	2	0.14
(2,225)	1:115:A:MET:HG3	1:119:A:LEU:HD11	8	0.14
(2,202)	1:118:A:LEU:HD12	1:114:A:ASP:HB2	3	0.14
(2,177)	1:123:A:LEU:HG	1:122:A:ILE:HG22	10	0.14
(2,84)	1:63:A:MET:HB3	1:101:A:VAL:HG13	7	0.14
(2,48)	1:86:A:ILE:HB	1:86:A:ILE:HD11	10	0.14
(2,28)	1:87:A:GLU:HG2	1:87:A:GLU:HB3	6	0.14
(1,47)	1:103:A:MET:H	1:95:A:PHE:HB3	6	0.14
(1,47)	1:103:A:MET:H	1:95:A:PHE:HB3	7	0.14
(2,1939)	1:127:A:GLY:H	1:122:A:ILE:HB	4	0.13
(2,1935)	1:78:A:LYS:H	1:78:A:LYS:HB3	9	0.13
(2,1892)	1:65:A:THR:H	1:128:A:VAL:HB	2	0.13
(2,1869)	1:121:A:ASP:H	1:124:A:ALA:HB3	10	0.13
(2,1791)	1:103:A:MET:H	1:103:A:MET:HB3	6	0.13
(2,1784)	1:104:A:ILE:H	1:103:A:MET:HG3	10	0.13
(2,1748)	1:78:A:LYS:HD2	1:78:A:LYS:HE3	9	0.13
(2,1685)	1:62:A:LEU:HA	1:103:A:MET:HB3	3	0.13
(2,1685)	1:62:A:LEU:HA	1:103:A:MET:HB3	5	0.13
(2,1685)	1:62:A:LEU:HA	1:103:A:MET:HB3	8	0.13
(2,1685)	1:62:A:LEU:HA	1:103:A:MET:HB3	9	0.13
(2,1658)	1:60:A:THR:HG21	1:105:A:GLU:HA	7	0.13
(2,1642)	1:72:A:ASN:HB2	1:72:A:ASN:HA	2	0.13
(2,1611)	1:104:A:ILE:HG12	1:82:A:PHE:HZ	3	0.13
(2,1611)	1:104:A:ILE:HG12	1:82:A:PHE:HZ	4	0.13
(2,1602)	1:118:A:LEU:HG	1:118:A:LEU:HA	3	0.13
(2,1602)	1:118:A:LEU:HG	1:118:A:LEU:HA	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1596)	1:84:A:THR:HG22	1:85:A:ARG:HA	3	0.13
(2,1573)	1:82:A:PHE:HE1	1:85:A:ARG:HB2	10	0.13
(2,1553)	1:60:A:THR:HA	1:59:A:MET:HG2	1	0.13
(2,1514)	1:86:A:ILE:HD11	1:82:A:PHE:HD1	4	0.13
(2,1507)	1:133:A:SER:HB3	1:138:A:ALA:HB1	2	0.13
(2,1484)	1:122:A:ILE:HA	1:123:A:LEU:HA	1	0.13
(2,1484)	1:122:A:ILE:HA	1:123:A:LEU:HA	2	0.13
(2,1484)	1:122:A:ILE:HA	1:123:A:LEU:HA	4	0.13
(2,1484)	1:122:A:ILE:HA	1:123:A:LEU:HA	7	0.13
(2,1423)	1:125:A:ALA:HB3	1:126:A:GLY:HA2	6	0.13
(2,1391)	1:60:A:THR:HG21	1:61:A:ARG:HA	1	0.13
(2,1391)	1:60:A:THR:HG21	1:61:A:ARG:HA	7	0.13
(2,1383)	1:66:A:GLU:HB2	1:97:A:THR:HG22	10	0.13
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD13	1	0.13
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD13	2	0.13
(2,1329)	1:136:A:LYS:HG2	1:136:A:LYS:HD2	2	0.13
(2,1329)	1:136:A:LYS:HG2	1:136:A:LYS:HD2	6	0.13
(2,1247)	1:68:A:GLN:HB3	1:67:A:LYS:HA	4	0.13
(2,1240)	1:120:A:HIS:HB3	1:122:A:ILE:HG13	8	0.13
(2,1209)	1:110:A:VAL:HB	1:106:A:LEU:HG	4	0.13
(2,1193)	1:129:A:VAL:HB	1:129:A:VAL:HG11	1	0.13
(2,1193)	1:129:A:VAL:HB	1:129:A:VAL:HG13	2	0.13
(2,1193)	1:129:A:VAL:HB	1:129:A:VAL:HG13	4	0.13
(2,1193)	1:129:A:VAL:HB	1:129:A:VAL:HG12	5	0.13
(2,1193)	1:129:A:VAL:HB	1:129:A:VAL:HG13	6	0.13
(2,1193)	1:129:A:VAL:HB	1:129:A:VAL:HG11	8	0.13
(2,1193)	1:128:A:VAL:HB	1:128:A:VAL:HG13	9	0.13
(2,1181)	1:101:A:VAL:HB	1:103:A:MET:HA	4	0.13
(2,1170)	1:98:A:GLU:HG3	1:101:A:VAL:HG22	5	0.13
(2,1159)	1:72:A:ASN:HB3	1:76:A:MET:HB3	8	0.13
(2,1097)	1:92:A:SER:H	1:92:A:SER:HB3	5	0.13
(2,1088)	1:83:A:SER:H	1:82:A:PHE:HB2	2	0.13
(2,1062)	1:120:A:HIS:H	1:119:A:LEU:HB3	2	0.13
(2,995)	1:125:A:ALA:H	1:126:A:GLY:HA2	7	0.13
(2,937)	1:108:A:LYS:H	1:107:A:PRO:HB3	3	0.13
(2,932)	1:60:A:THR:H	1:59:A:MET:HB2	3	0.13
(2,918)	1:71:A:LYS:H	1:67:A:LYS:HA	7	0.13
(2,893)	1:115:A:MET:H	1:114:A:ASP:HB3	5	0.13
(2,868)	1:87:A:GLU:H	1:86:A:ILE:HG22	9	0.13
(2,812)	1:137:A:LEU:H	1:60:A:THR:HG23	7	0.13
(2,794)	1:82:A:PHE:H	1:82:A:PHE:HD1	7	0.13
(2,788)	1:73:A:PHE:H	1:73:A:PHE:HD2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,788)	1:73:A:PHE:H	1:73:A:PHE:HD1	10	0.13
(2,625)	1:64:A:VAL:HG22	1:63:A:MET:HA	9	0.13
(2,617)	1:103:A:MET:HG2	1:103:A:MET:HA	3	0.13
(2,617)	1:103:A:MET:HG2	1:103:A:MET:HA	9	0.13
(2,608)	1:124:A:ALA:HB3	1:124:A:ALA:HA	6	0.13
(2,608)	1:124:A:ALA:HB3	1:124:A:ALA:HA	7	0.13
(2,608)	1:124:A:ALA:HB3	1:124:A:ALA:HA	8	0.13
(2,580)	1:134:A:GLU:HA	1:62:A:LEU:HD23	5	0.13
(2,569)	1:95:A:PHE:HD2	1:94:A:SER:HA	8	0.13
(2,569)	1:95:A:PHE:HD1	1:94:A:SER:HA	10	0.13
(2,523)	1:87:A:GLU:HG3	1:87:A:GLU:HA	2	0.13
(2,500)	1:82:A:PHE:HE1	1:119:A:LEU:HA	5	0.13
(2,484)	1:86:A:ILE:HG13	1:86:A:ILE:HA	10	0.13
(2,479)	1:128:A:VAL:HG12	1:128:A:VAL:HA	2	0.13
(2,464)	1:101:A:VAL:HG12	1:101:A:VAL:HA	2	0.13
(2,405)	1:64:A:VAL:HG13	1:122:A:ILE:HA	8	0.13
(2,373)	1:104:A:ILE:HD12	1:122:A:ILE:HD13	10	0.13
(2,366)	1:93:A:ILE:HD13	1:82:A:PHE:HB2	7	0.13
(2,341)	1:77:A:ALA:HB3	1:78:A:LYS:HA	8	0.13
(2,308)	1:102:A:THR:HG23	1:104:A:ILE:HG13	10	0.13
(2,295)	1:101:A:VAL:HG13	1:103:A:MET:HA	2	0.13
(2,295)	1:101:A:VAL:HG13	1:103:A:MET:HA	5	0.13
(2,291)	1:60:A:THR:HG22	1:60:A:THR:HA	2	0.13
(2,279)	1:64:A:VAL:HG11	1:122:A:ILE:HG23	7	0.13
(2,256)	1:89:A:LEU:HD21	1:89:A:LEU:HA	1	0.13
(2,256)	1:89:A:LEU:HD22	1:89:A:LEU:HA	7	0.13
(2,231)	1:123:A:LEU:HD21	1:120:A:HIS:HA	4	0.13
(2,186)	1:96:A:LEU:HG	1:103:A:MET:HG2	1	0.13
(2,186)	1:96:A:LEU:HG	1:103:A:MET:HG2	2	0.13
(2,186)	1:96:A:LEU:HG	1:103:A:MET:HG2	3	0.13
(2,167)	1:61:A:ARG:HG2	1:105:A:GLU:HA	4	0.13
(2,167)	1:61:A:ARG:HG2	1:105:A:GLU:HA	9	0.13
(1,47)	1:103:A:MET:H	1:95:A:PHE:HB3	5	0.13
(1,46)	1:108:A:LYS:HE3	1:59:A:MET:HA	3	0.13
(1,24)	1:75:A:LYS:HG3	1:78:A:LYS:HE3	6	0.13
(2,1949)	1:90:A:GLY:H	1:107:A:PRO:HG3	2	0.12
(2,1928)	1:83:A:SER:H	1:85:A:ARG:HB3	1	0.12
(2,1928)	1:83:A:SER:H	1:85:A:ARG:HB3	9	0.12
(2,1921)	1:86:A:ILE:H	1:85:A:ARG:HA	2	0.12
(2,1921)	1:86:A:ILE:H	1:85:A:ARG:HA	3	0.12
(2,1921)	1:86:A:ILE:H	1:85:A:ARG:HA	4	0.12
(2,1921)	1:86:A:ILE:H	1:85:A:ARG:HA	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1921)	1:86:A:ILE:H	1:85:A:ARG:HA	7	0.12
(2,1921)	1:86:A:ILE:H	1:85:A:ARG:HA	9	0.12
(2,1921)	1:86:A:ILE:H	1:85:A:ARG:HA	10	0.12
(2,1914)	1:79:A:SER:H	1:78:A:LYS:HB3	5	0.12
(2,1800)	1:105:A:GLU:H	1:86:A:ILE:HG23	10	0.12
(2,1755)	1:104:A:ILE:HB	1:102:A:THR:HB	5	0.12
(2,1742)	1:75:A:LYS:HE2	1:75:A:LYS:HA	5	0.12
(2,1715)	1:85:A:ARG:HD3	1:82:A:PHE:HE1	1	0.12
(2,1715)	1:85:A:ARG:HD3	1:82:A:PHE:HE1	9	0.12
(2,1658)	1:60:A:THR:HG23	1:105:A:GLU:HA	4	0.12
(2,1618)	1:79:A:SER:HA	1:78:A:LYS:HB2	6	0.12
(2,1615)	1:64:A:VAL:HB	1:73:A:PHE:HZ	5	0.12
(2,1611)	1:104:A:ILE:HG12	1:82:A:PHE:HZ	2	0.12
(2,1597)	1:75:A:LYS:HB3	1:75:A:LYS:HA	6	0.12
(2,1594)	1:89:A:LEU:HG	1:111:A:SER:HA	5	0.12
(2,1553)	1:60:A:THR:HA	1:107:A:PRO:HB3	9	0.12
(2,1534)	1:135:A:VAL:HA	1:107:A:PRO:HB3	5	0.12
(2,1514)	1:86:A:ILE:HD11	1:82:A:PHE:HD1	3	0.12
(2,1484)	1:122:A:ILE:HA	1:123:A:LEU:HA	10	0.12
(2,1403)	1:102:A:THR:HG22	1:74:A:SER:HA	2	0.12
(2,1377)	1:64:A:VAL:HG11	1:73:A:PHE:HE1	10	0.12
(2,1365)	1:89:A:LEU:HG	1:89:A:LEU:HD23	1	0.12
(2,1365)	1:89:A:LEU:HG	1:89:A:LEU:HD22	4	0.12
(2,1365)	1:89:A:LEU:HG	1:89:A:LEU:HD22	6	0.12
(2,1365)	1:89:A:LEU:HG	1:89:A:LEU:HD23	9	0.12
(2,1353)	1:118:A:LEU:HD22	1:118:A:LEU:HD11	7	0.12
(2,1353)	1:118:A:LEU:HD23	1:118:A:LEU:HD13	9	0.12
(2,1349)	1:118:A:LEU:HG	1:118:A:LEU:HD22	5	0.12
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD13	3	0.12
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD12	4	0.12
(2,1335)	1:119:A:LEU:HG	1:119:A:LEU:HD11	8	0.12
(2,1329)	1:136:A:LYS:HG2	1:136:A:LYS:HD2	1	0.12
(2,1323)	1:75:A:LYS:HG3	1:75:A:LYS:HE3	8	0.12
(2,1321)	1:62:A:LEU:HD11	1:82:A:PHE:HZ	9	0.12
(2,1240)	1:120:A:HIS:HB3	1:122:A:ILE:HG13	4	0.12
(2,1222)	1:76:A:MET:HG3	1:77:A:ALA:HB2	7	0.12
(2,1209)	1:110:A:VAL:HB	1:106:A:LEU:HG	6	0.12
(2,1200)	1:136:A:LYS:HB3	1:59:A:MET:HA	9	0.12
(2,1193)	1:129:A:VAL:HB	1:129:A:VAL:HG13	7	0.12
(2,1193)	1:129:A:VAL:HB	1:129:A:VAL:HG12	10	0.12
(2,1184)	1:59:A:MET:HB3	1:90:A:GLY:HA2	2	0.12
(2,1184)	1:59:A:MET:HB3	1:90:A:GLY:HA2	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1144)	1:126:A:GLY:H	1:127:A:GLY:HA2	10	0.12
(2,1097)	1:92:A:SER:H	1:92:A:SER:HB3	2	0.12
(2,1097)	1:92:A:SER:H	1:92:A:SER:HB3	3	0.12
(2,1088)	1:83:A:SER:H	1:82:A:PHE:HB2	1	0.12
(2,1047)	1:79:A:SER:H	1:82:A:PHE:HD2	10	0.12
(2,995)	1:125:A:ALA:H	1:126:A:GLY:HA2	1	0.12
(2,933)	1:60:A:THR:H	1:106:A:LEU:HB3	4	0.12
(2,933)	1:60:A:THR:H	1:106:A:LEU:HB3	7	0.12
(2,817)	1:110:A:VAL:H	1:107:A:PRO:HG2	2	0.12
(2,794)	1:82:A:PHE:H	1:82:A:PHE:HD1	3	0.12
(2,794)	1:82:A:PHE:H	1:82:A:PHE:HD1	6	0.12
(2,724)	1:128:A:VAL:HG21	1:65:A:THR:HB	10	0.12
(2,702)	1:123:A:LEU:HB2	1:129:A:VAL:HG21	9	0.12
(2,642)	1:113:A:HIS:HB2	1:113:A:HIS:HD2	10	0.12
(2,624)	1:101:A:VAL:HG13	1:63:A:MET:HA	2	0.12
(2,617)	1:103:A:MET:HG2	1:103:A:MET:HA	2	0.12
(2,608)	1:124:A:ALA:HB3	1:124:A:ALA:HA	2	0.12
(2,608)	1:124:A:ALA:HB2	1:124:A:ALA:HA	5	0.12
(2,608)	1:124:A:ALA:HB1	1:124:A:ALA:HA	9	0.12
(2,608)	1:124:A:ALA:HB1	1:124:A:ALA:HA	10	0.12
(2,598)	1:66:A:GLU:HA	1:73:A:PHE:HD2	3	0.12
(2,598)	1:66:A:GLU:HA	1:73:A:PHE:HD2	5	0.12
(2,598)	1:66:A:GLU:HA	1:73:A:PHE:HD1	10	0.12
(2,595)	1:60:A:THR:HG23	1:61:A:ARG:HA	8	0.12
(2,583)	1:136:A:LYS:HA	1:133:A:SER:HB2	2	0.12
(2,569)	1:95:A:PHE:HD1	1:94:A:SER:HA	9	0.12
(2,564)	1:95:A:PHE:HD2	1:95:A:PHE:HA	2	0.12
(2,564)	1:95:A:PHE:HD1	1:95:A:PHE:HA	6	0.12
(2,564)	1:95:A:PHE:HD1	1:95:A:PHE:HA	9	0.12
(2,521)	1:86:A:ILE:HG23	1:87:A:GLU:HA	1	0.12
(2,514)	1:115:A:MET:HG3	1:112:A:GLU:HA	1	0.12
(2,514)	1:115:A:MET:HG3	1:112:A:GLU:HA	3	0.12
(2,464)	1:101:A:VAL:HG11	1:101:A:VAL:HA	10	0.12
(2,458)	1:74:A:SER:HA	1:74:A:SER:HB3	4	0.12
(2,384)	1:86:A:ILE:HD12	1:106:A:LEU:HA	2	0.12
(2,366)	1:93:A:ILE:HD11	1:82:A:PHE:HB2	8	0.12
(2,359)	1:122:A:ILE:HG22	1:64:A:VAL:HA	4	0.12
(2,359)	1:122:A:ILE:HG22	1:64:A:VAL:HA	7	0.12
(2,339)	1:124:A:ALA:HB2	1:121:A:ASP:HB3	1	0.12
(2,291)	1:60:A:THR:HG21	1:60:A:THR:HA	6	0.12
(2,256)	1:89:A:LEU:HD23	1:89:A:LEU:HA	2	0.12
(2,231)	1:123:A:LEU:HD22	1:120:A:HIS:HA	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,225)	1:115:A:MET:HG3	1:119:A:LEU:HD12	4	0.12
(2,186)	1:96:A:LEU:HG	1:103:A:MET:HG2	4	0.12
(2,167)	1:61:A:ARG:HG2	1:105:A:GLU:HA	6	0.12
(2,156)	1:107:A:PRO:HG2	1:107:A:PRO:HD3	2	0.12
(2,156)	1:107:A:PRO:HG2	1:107:A:PRO:HD3	3	0.12
(2,132)	1:75:A:LYS:HD3	1:75:A:LYS:HA	3	0.12
(2,54)	1:129:A:VAL:HB	1:122:A:ILE:HG22	4	0.12
(2,48)	1:86:A:ILE:HB	1:86:A:ILE:HD11	2	0.12
(2,28)	1:87:A:GLU:HG2	1:87:A:GLU:HB3	4	0.12
(2,6)	1:72:A:ASN:HB2	1:126:A:GLY:HA2	7	0.12
(1,47)	1:103:A:MET:H	1:95:A:PHE:HB3	1	0.12
(1,47)	1:103:A:MET:H	1:95:A:PHE:HB3	10	0.12
(1,46)	1:108:A:LYS:HE3	1:59:A:MET:HA	7	0.12
(1,43)	1:132:A:ASP:HA	1:103:A:MET:HG2	7	0.12
(1,43)	1:132:A:ASP:HA	1:103:A:MET:HG2	10	0.12
(1,36)	1:85:A:ARG:HA	1:88:A:GLU:HB3	6	0.12
(1,23)	1:93:A:ILE:HG12	1:78:A:LYS:HG2	1	0.12
(1,23)	1:93:A:ILE:HG12	1:78:A:LYS:HG2	8	0.12
(2,1939)	1:127:A:GLY:H	1:122:A:ILE:HB	6	0.11
(2,1921)	1:86:A:ILE:H	1:85:A:ARG:HA	1	0.11
(2,1921)	1:86:A:ILE:H	1:85:A:ARG:HA	6	0.11
(2,1921)	1:86:A:ILE:H	1:85:A:ARG:HA	8	0.11
(2,1899)	1:74:A:SER:H	1:76:A:MET:HB3	3	0.11
(2,1892)	1:65:A:THR:H	1:128:A:VAL:HB	10	0.11
(2,1878)	1:58:A:GLU:H	1:90:A:GLY:HA2	5	0.11
(2,1852)	1:87:A:GLU:H	1:87:A:GLU:HB2	9	0.11
(2,1819)	1:136:A:LYS:H	1:58:A:GLU:HA	1	0.11
(2,1819)	1:136:A:LYS:H	1:58:A:GLU:HA	6	0.11
(2,1785)	1:103:A:MET:H	1:103:A:MET:HG2	1	0.11
(2,1659)	1:104:A:ILE:HG22	1:105:A:GLU:HA	10	0.11
(2,1649)	1:78:A:LYS:HD2	1:78:A:LYS:HA	6	0.11
(2,1618)	1:79:A:SER:HA	1:78:A:LYS:HB2	9	0.11
(2,1611)	1:104:A:ILE:HG12	1:82:A:PHE:HZ	1	0.11
(2,1593)	1:112:A:GLU:HB2	1:112:A:GLU:HA	8	0.11
(2,1557)	1:95:A:PHE:HE1	1:102:A:THR:HB	9	0.11
(2,1502)	1:133:A:SER:HB3	1:136:A:LYS:HB2	8	0.11
(2,1484)	1:122:A:ILE:HA	1:123:A:LEU:HA	5	0.11
(2,1408)	1:135:A:VAL:HG23	1:134:A:GLU:HA	1	0.11
(2,1403)	1:102:A:THR:HG23	1:74:A:SER:HA	3	0.11
(2,1391)	1:60:A:THR:HG23	1:61:A:ARG:HA	8	0.11
(2,1365)	1:89:A:LEU:HG	1:89:A:LEU:HD22	8	0.11
(2,1359)	1:119:A:LEU:HD21	1:115:A:MET:HG2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1349)	1:118:A:LEU:HG	1:118:A:LEU:HD23	9	0.11
(2,1349)	1:118:A:LEU:HG	1:118:A:LEU:HD22	10	0.11
(2,1329)	1:136:A:LYS:HG2	1:136:A:LYS:HD2	3	0.11
(2,1329)	1:136:A:LYS:HG2	1:136:A:LYS:HD2	9	0.11
(2,1323)	1:75:A:LYS:HG3	1:75:A:LYS:HE2	3	0.11
(2,1295)	1:106:A:LEU:HG	1:89:A:LEU:HB3	1	0.11
(2,1290)	1:118:A:LEU:HG	1:114:A:ASP:HB2	4	0.11
(2,1281)	1:93:A:ILE:HG13	1:87:A:GLU:HG3	2	0.11
(2,1240)	1:120:A:HIS:HB3	1:122:A:ILE:HG13	1	0.11
(2,1189)	1:115:A:MET:HG3	1:108:A:LYS:HG3	10	0.11
(2,1154)	1:72:A:ASN:HB2	1:73:A:PHE:HD1	9	0.11
(2,1088)	1:83:A:SER:H	1:82:A:PHE:HB2	8	0.11
(2,995)	1:125:A:ALA:H	1:126:A:GLY:HA2	2	0.11
(2,995)	1:125:A:ALA:H	1:126:A:GLY:HA2	6	0.11
(2,933)	1:60:A:THR:H	1:106:A:LEU:HB3	9	0.11
(2,817)	1:110:A:VAL:H	1:107:A:PRO:HG2	10	0.11
(2,794)	1:82:A:PHE:H	1:82:A:PHE:HD1	5	0.11
(2,723)	1:62:A:LEU:HB2	1:104:A:ILE:HB	6	0.11
(2,650)	1:126:A:GLY:HA3	1:123:A:LEU:HA	7	0.11
(2,634)	1:120:A:HIS:HD2	1:123:A:LEU:HD21	10	0.11
(2,625)	1:64:A:VAL:HG23	1:63:A:MET:HA	1	0.11
(2,608)	1:124:A:ALA:HB1	1:124:A:ALA:HA	4	0.11
(2,598)	1:66:A:GLU:HA	1:73:A:PHE:HD2	8	0.11
(2,579)	1:108:A:LYS:HA	1:108:A:LYS:HE3	8	0.11
(2,569)	1:95:A:PHE:HD1	1:94:A:SER:HA	2	0.11
(2,569)	1:95:A:PHE:HD1	1:94:A:SER:HA	3	0.11
(2,569)	1:95:A:PHE:HD1	1:94:A:SER:HA	6	0.11
(2,569)	1:95:A:PHE:HD1	1:94:A:SER:HA	7	0.11
(2,546)	1:119:A:LEU:HA	1:119:A:LEU:HB2	8	0.11
(2,546)	1:119:A:LEU:HA	1:119:A:LEU:HB2	9	0.11
(2,514)	1:115:A:MET:HG3	1:112:A:GLU:HA	5	0.11
(2,484)	1:86:A:ILE:HG13	1:86:A:ILE:HA	2	0.11
(2,479)	1:128:A:VAL:HG13	1:128:A:VAL:HA	8	0.11
(2,458)	1:74:A:SER:HA	1:74:A:SER:HB3	2	0.11
(2,458)	1:74:A:SER:HA	1:74:A:SER:HB3	3	0.11
(2,408)	1:122:A:ILE:HG13	1:122:A:ILE:HA	5	0.11
(2,371)	1:104:A:ILE:HD12	1:64:A:VAL:HG11	6	0.11
(2,364)	1:104:A:ILE:HD12	1:82:A:PHE:HE2	7	0.11
(2,326)	1:125:A:ALA:HB2	1:125:A:ALA:HA	5	0.11
(2,256)	1:89:A:LEU:HD23	1:89:A:LEU:HA	6	0.11
(2,202)	1:118:A:LEU:HD11	1:114:A:ASP:HB2	1	0.11
(2,186)	1:96:A:LEU:HG	1:103:A:MET:HG2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,180)	1:115:A:MET:HG3	1:119:A:LEU:HG	10	0.11
(2,177)	1:123:A:LEU:HG	1:122:A:ILE:HG22	1	0.11
(2,156)	1:107:A:PRO:HG2	1:107:A:PRO:HD3	1	0.11
(2,156)	1:107:A:PRO:HG2	1:107:A:PRO:HD3	4	0.11
(2,156)	1:107:A:PRO:HG2	1:107:A:PRO:HD3	6	0.11
(2,156)	1:107:A:PRO:HG2	1:107:A:PRO:HD3	7	0.11
(2,156)	1:107:A:PRO:HG2	1:107:A:PRO:HD3	8	0.11
(2,156)	1:107:A:PRO:HG2	1:107:A:PRO:HD3	10	0.11
(2,154)	1:107:A:PRO:HG3	1:106:A:LEU:HA	2	0.11
(2,48)	1:86:A:ILE:HB	1:86:A:ILE:HD13	5	0.11
(2,18)	1:122:A:ILE:HB	1:120:A:HIS:HA	5	0.11
(2,18)	1:122:A:ILE:HB	1:120:A:HIS:HA	6	0.11
(2,18)	1:122:A:ILE:HB	1:120:A:HIS:HA	9	0.11
(2,9)	1:105:A:GLU:HG2	1:61:A:ARG:HD2	8	0.11
(1,41)	1:105:A:GLU:HA	1:132:A:ASP:HB2	2	0.11
(1,23)	1:93:A:ILE:HG12	1:78:A:LYS:HG2	2	0.11
(2,1928)	1:83:A:SER:H	1:85:A:ARG:HB3	5	0.1
(2,1920)	1:120:A:HIS:H	1:119:A:LEU:HD23	7	0.1
(2,1905)	1:117:A:GLN:H	1:113:A:HIS:HA	3	0.1
(2,1856)	1:94:A:SER:H	1:93:A:ILE:HB	2	0.1
(2,1856)	1:94:A:SER:H	1:93:A:ILE:HB	8	0.1
(2,1800)	1:105:A:GLU:H	1:86:A:ILE:HG21	3	0.1
(2,1718)	1:85:A:ARG:HB3	1:85:A:ARG:HD3	1	0.1
(2,1662)	1:131:A:LEU:HA	1:61:A:ARG:HA	10	0.1
(2,1659)	1:104:A:ILE:HG22	1:105:A:GLU:HA	5	0.1
(2,1581)	1:104:A:ILE:HA	1:93:A:ILE:HG13	8	0.1
(2,1571)	1:82:A:PHE:HE2	1:102:A:THR:HB	8	0.1
(2,1553)	1:60:A:THR:HA	1:59:A:MET:HG2	2	0.1
(2,1484)	1:122:A:ILE:HA	1:123:A:LEU:HA	8	0.1
(2,1416)	1:64:A:VAL:HG23	1:73:A:PHE:HE2	7	0.1
(2,1230)	1:71:A:LYS:HB2	1:71:A:LYS:HE2	8	0.1
(2,1209)	1:110:A:VAL:HB	1:106:A:LEU:HG	3	0.1
(2,1176)	1:66:A:GLU:HG3	1:101:A:VAL:HG11	10	0.1
(2,1153)	1:72:A:ASN:HB3	1:76:A:MET:HG2	1	0.1
(2,1139)	1:109:A:THR:H	1:108:A:LYS:HG3	3	0.1
(2,1047)	1:79:A:SER:H	1:82:A:PHE:HD2	5	0.1
(2,1019)	1:117:A:GLN:H	1:116:A:ASP:HB2	4	0.1
(2,949)	1:118:A:LEU:H	1:117:A:GLN:HB2	1	0.1
(2,869)	1:87:A:GLU:H	1:86:A:ILE:HD13	7	0.1
(2,869)	1:87:A:GLU:H	1:86:A:ILE:HD11	10	0.1
(2,630)	1:77:A:ALA:HA	1:93:A:ILE:HG22	10	0.1
(2,569)	1:95:A:PHE:HD1	1:94:A:SER:HA	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,569)	1:95:A:PHE:HD1	1:94:A:SER:HA	5	0.1
(2,546)	1:119:A:LEU:HA	1:119:A:LEU:HB2	1	0.1
(2,546)	1:119:A:LEU:HA	1:119:A:LEU:HB2	4	0.1
(2,546)	1:119:A:LEU:HA	1:119:A:LEU:HB2	5	0.1
(2,546)	1:119:A:LEU:HA	1:119:A:LEU:HB2	6	0.1
(2,479)	1:128:A:VAL:HG13	1:128:A:VAL:HA	1	0.1
(2,479)	1:128:A:VAL:HG11	1:128:A:VAL:HA	4	0.1
(2,373)	1:104:A:ILE:HD13	1:122:A:ILE:HD11	4	0.1
(2,359)	1:122:A:ILE:HG22	1:64:A:VAL:HA	5	0.1
(2,299)	1:101:A:VAL:HG13	1:102:A:THR:HA	1	0.1
(2,293)	1:110:A:VAL:HG23	1:106:A:LEU:HG	1	0.1
(2,259)	1:97:A:THR:HG21	1:96:A:LEU:HA	10	0.1
(2,256)	1:89:A:LEU:HD23	1:89:A:LEU:HA	3	0.1
(2,177)	1:123:A:LEU:HG	1:122:A:ILE:HG21	4	0.1
(2,167)	1:61:A:ARG:HG2	1:105:A:GLU:HA	1	0.1
(2,156)	1:107:A:PRO:HG2	1:107:A:PRO:HD3	5	0.1
(2,156)	1:107:A:PRO:HG2	1:107:A:PRO:HD3	9	0.1
(2,154)	1:107:A:PRO:HG3	1:106:A:LEU:HA	3	0.1
(2,51)	1:103:A:MET:HB2	1:61:A:ARG:HG2	6	0.1
(2,48)	1:86:A:ILE:HB	1:86:A:ILE:HD13	7	0.1
(2,48)	1:86:A:ILE:HB	1:86:A:ILE:HD12	8	0.1
(2,18)	1:122:A:ILE:HB	1:120:A:HIS:HA	4	0.1
(2,13)	1:105:A:GLU:HG2	1:61:A:ARG:HG3	7	0.1
(1,41)	1:105:A:GLU:HA	1:132:A:ASP:HB2	9	0.1
(1,23)	1:93:A:ILE:HG12	1:78:A:LYS:HG2	3	0.1

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

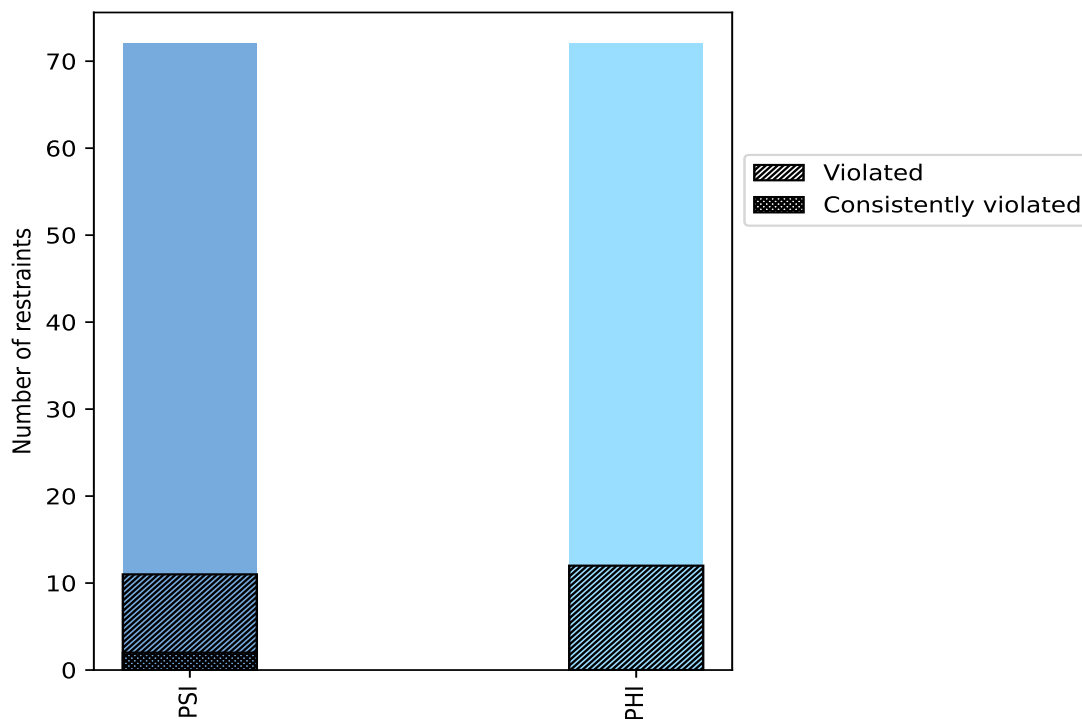
### 10.1 Summary of dihedral-angle violations [i](#)

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	72	50.0	11	15.3	7.6	2	2.8	1.4
PHI	72	50.0	12	16.7	8.3	0	0.0	0.0
Total	144	100.0	23	16.0	16.0	2	1.4	1.4

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

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



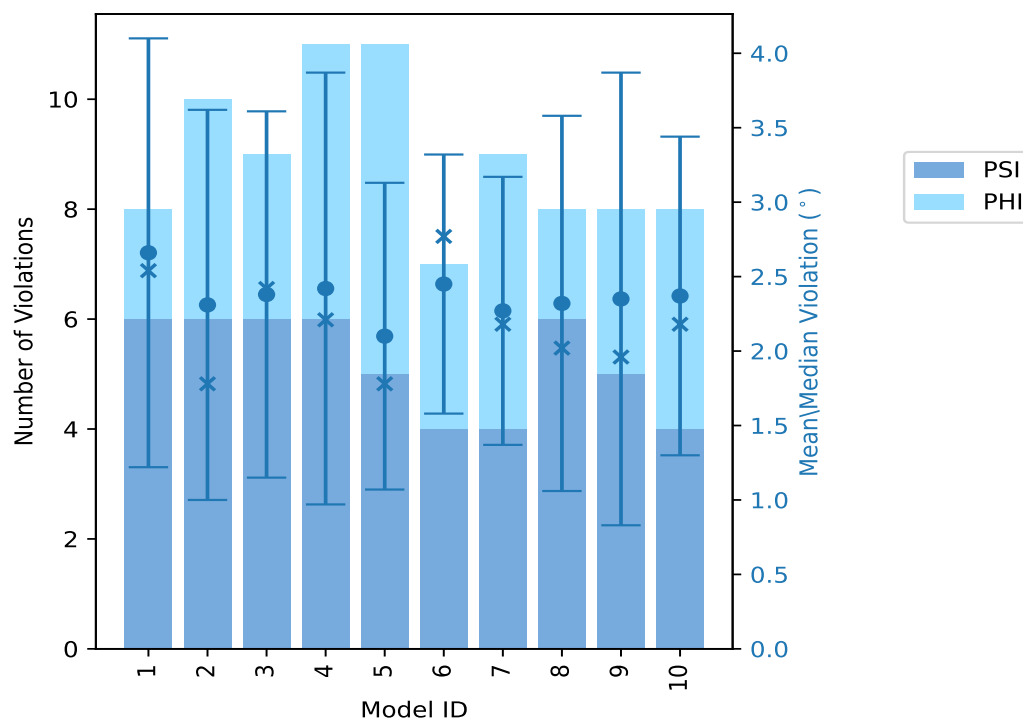
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	6	2	8	2.66	5.93	1.44	2.54
2	6	4	10	2.31	5.08	1.31	1.78
3	6	3	9	2.38	5.22	1.23	2.42
4	6	5	11	2.42	5.92	1.45	2.21
5	5	6	11	2.1	4.06	1.03	1.78
6	4	3	7	2.45	3.55	0.87	2.77
7	4	5	9	2.27	3.84	0.9	2.18
8	6	2	8	2.32	5.35	1.26	2.02
9	5	3	8	2.35	6.31	1.52	1.96
10	4	4	8	2.37	3.89	1.07	2.18

### 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

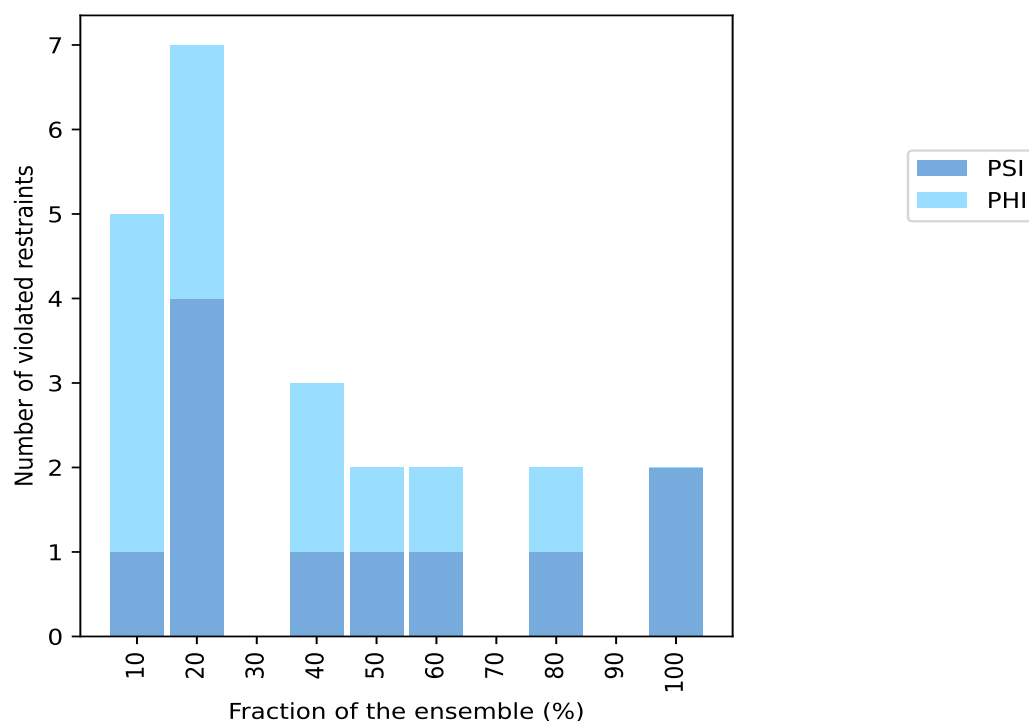
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

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

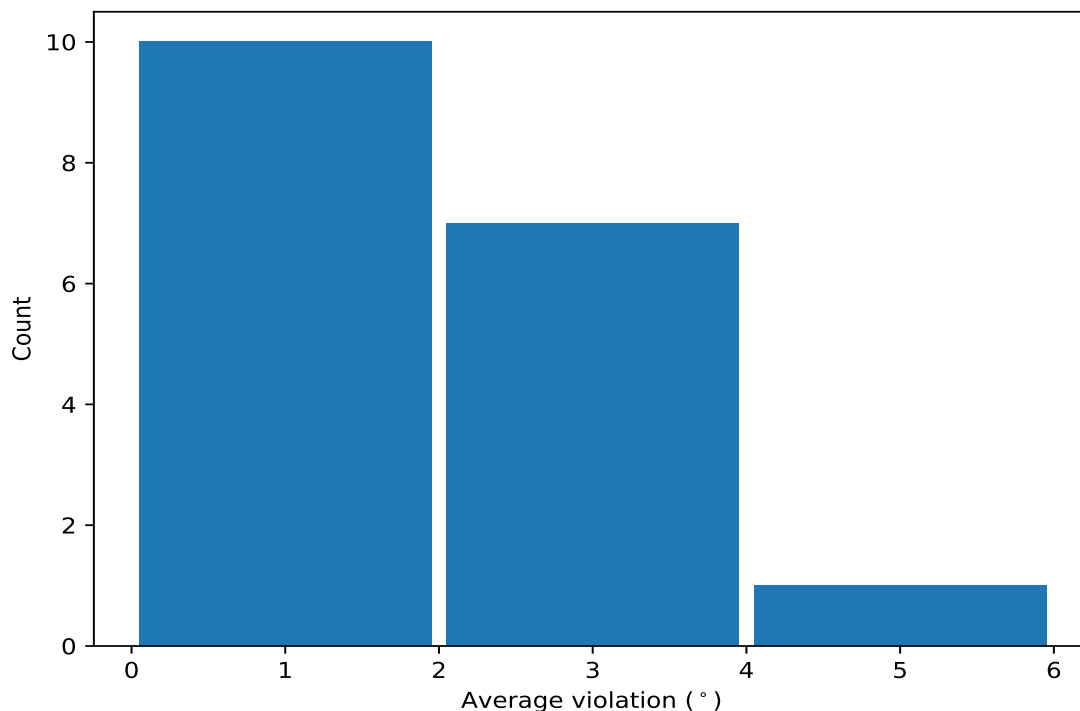
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



### 10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,46)	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	1:83:A:SER:N	10	3.46	0.94	3.42
(1,100)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:SER:N	10	2.52	1.06	2.46
(1,53)	1:85:A:ARG:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	8	2.84	0.54	2.77
(1,80)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:VAL:N	8	2.17	0.32	2.14
(1,144)	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	1:136:A:LYS:N	6	4.83	0.98	4.94
(1,49)	1:83:A:SER:C	1:84:A:THR:N	1:84:A:THR:CA	1:84:A:THR:C	6	2.16	1.89	1.21
(1,64)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:ILE:N	5	1.86	0.53	1.76
(1,61)	1:89:A:LEU:C	1:90:A:GLY:N	1:90:A:GLY:CA	1:90:A:GLY:C	5	1.53	0.46	1.22
(1,143)	1:134:A:GLU:C	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	4	2.51	0.81	2.37
(1,16)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:LYS:N	4	1.84	0.49	1.87
(1,31)	1:74:A:SER:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	4	1.63	0.34	1.46
(1,142)	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	1:135:A:VAL:N	2	2.43	0.34	2.43
(1,141)	1:133:A:SER:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	2	1.48	0.3	1.48

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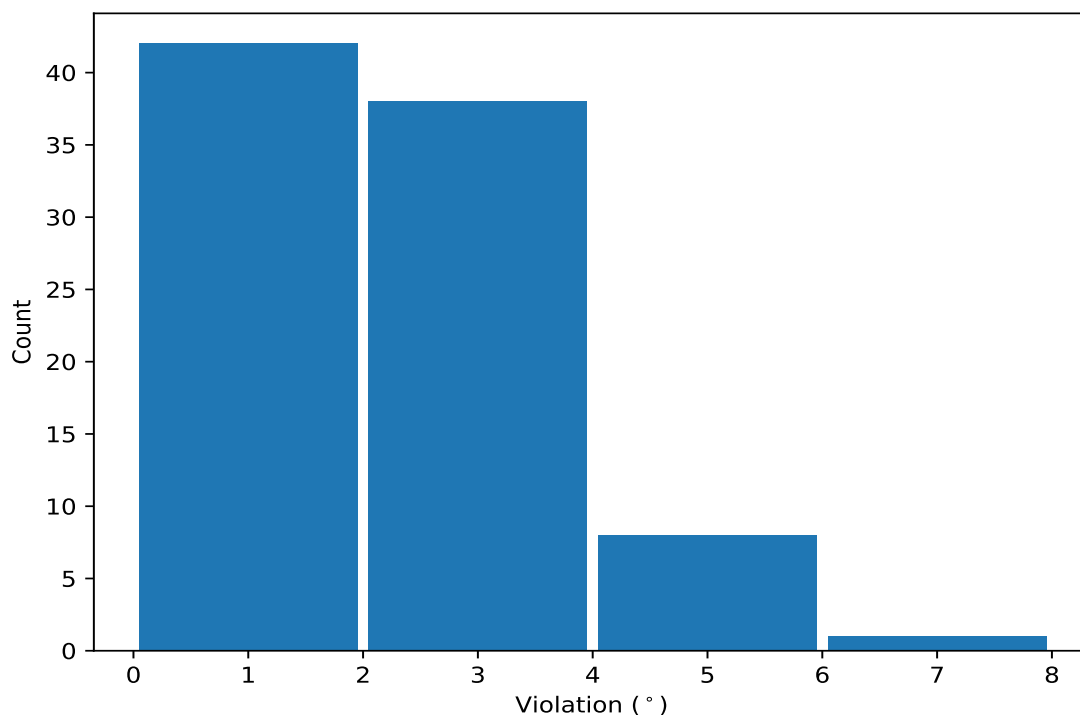
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,111)	1:115:A:MET:C	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	2	1.41	0.14	1.41
(1,32)	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	1:76:A:MET:N	2	1.34	0.06	1.34
(1,22)	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1:71:A:LYS:N	2	1.28	0.07	1.28
(1,81)	1:100:A:GLY:C	1:101:A:VAL:N	1:101:A:VAL:CA	1:101:A:VAL:C	2	1.2	0.03	1.2
(1,96)	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	1:109:A:THR:N	2	1.19	0.16	1.19

<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 (°)
(1,49)	1:83:A:SER:C	1:84:A:THR:N	1:84:A:THR:CA	1:84:A:THR:C	9	6.31
(1,144)	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	1:136:A:LYS:N	1	5.93

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,144)	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	1:136:A:LYS:N	4	5.92
(1,144)	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	1:136:A:LYS:N	8	5.35
(1,100)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:SER:N	3	5.22
(1,46)	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	1:83:A:SER:N	2	5.08
(1,144)	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	1:136:A:LYS:N	2	4.53
(1,46)	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	1:83:A:SER:N	4	4.38
(1,46)	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	1:83:A:SER:N	5	4.06
(1,53)	1:85:A:ARG:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	5	3.95
(1,144)	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	1:136:A:LYS:N	10	3.89
(1,46)	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	1:83:A:SER:N	7	3.84
(1,143)	1:134:A:GLU:C	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	10	3.77
(1,46)	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	1:83:A:SER:N	6	3.55
(1,144)	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	1:136:A:LYS:N	7	3.37
(1,46)	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	1:83:A:SER:N	1	3.3
(1,46)	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	1:83:A:SER:N	10	3.25
(1,46)	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	1:83:A:SER:N	3	3.22
(1,53)	1:85:A:ARG:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	6	3.17
(1,53)	1:85:A:ARG:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	7	3.07
(1,64)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:ILE:N	3	2.88
(1,100)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:SER:N	1	2.87
(1,53)	1:85:A:ARG:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	8	2.86
(1,100)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:SER:N	5	2.85
(1,100)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:SER:N	6	2.82
(1,142)	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	1:135:A:VAL:N	6	2.77
(1,100)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:SER:N	4	2.74
(1,53)	1:85:A:ARG:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	4	2.68
(1,80)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:VAL:N	1	2.57
(1,53)	1:85:A:ARG:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	1	2.52
(1,80)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:VAL:N	2	2.5
(1,80)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:VAL:N	6	2.48
(1,143)	1:134:A:GLU:C	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	3	2.45
(1,16)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:LYS:N	4	2.45
(1,53)	1:85:A:ARG:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	3	2.42
(1,46)	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	1:83:A:SER:N	8	2.35
(1,143)	1:134:A:GLU:C	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	7	2.29
(1,61)	1:89:A:LEU:C	1:90:A:GLY:N	1:90:A:GLY:CA	1:90:A:GLY:C	10	2.26
(1,31)	1:74:A:SER:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	4	2.21
(1,80)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:VAL:N	8	2.19
(1,100)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:SER:N	7	2.18
(1,49)	1:83:A:SER:C	1:84:A:THR:N	1:84:A:THR:CA	1:84:A:THR:C	5	2.16
(1,16)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:LYS:N	2	2.14
(1,80)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:VAL:N	10	2.1
(1,142)	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	1:135:A:VAL:N	9	2.09
(1,80)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:VAL:N	5	2.06
(1,53)	1:85:A:ARG:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	9	2.02
(1,80)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:VAL:N	9	1.98
(1,100)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:SER:N	9	1.93
(1,61)	1:89:A:LEU:C	1:90:A:GLY:N	1:90:A:GLY:CA	1:90:A:GLY:C	2	1.88
(1,100)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:SER:N	8	1.84
(1,141)	1:133:A:SER:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	5	1.78
(1,64)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:ILE:N	1	1.78

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:ILE:N	7	1.76
(1,100)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:SER:N	2	1.69
(1,46)	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	1:83:A:SER:N	9	1.59
(1,16)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:LYS:N	9	1.59
(1,111)	1:115:A:MET:C	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	10	1.55
(1,31)	1:74:A:SER:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	7	1.53
(1,143)	1:134:A:GLU:C	1:135:A:VAL:N	1:135:A:VAL:CA	1:135:A:VAL:C	4	1.52
(1,80)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:VAL:N	3	1.52
(1,64)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:ILE:N	5	1.49
(1,21)	1:69:A:GLU:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	2	1.45
(1,64)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:ILE:N	4	1.4
(1,32)	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	1:76:A:MET:N	8	1.4
(1,31)	1:74:A:SER:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	5	1.4
(1,31)	1:74:A:SER:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	2	1.38
(1,96)	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	1:109:A:THR:N	3	1.35
(1,22)	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1:71:A:LYS:N	8	1.35
(1,119)	1:119:A:LEU:C	1:120:A:HIS:N	1:120:A:HIS:CA	1:120:A:HIS:C	9	1.29
(1,32)	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	1:76:A:MET:N	1	1.28
(1,111)	1:115:A:MET:C	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	2	1.27
(1,49)	1:83:A:SER:C	1:84:A:THR:N	1:84:A:THR:CA	1:84:A:THR:C	7	1.25
(1,81)	1:100:A:GLY:C	1:101:A:VAL:N	1:101:A:VAL:CA	1:101:A:VAL:C	4	1.23
(1,61)	1:89:A:LEU:C	1:90:A:GLY:N	1:90:A:GLY:CA	1:90:A:GLY:C	8	1.22
(1,22)	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1:71:A:LYS:N	2	1.22
(1,16)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:LYS:N	3	1.19
(1,141)	1:133:A:SER:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	7	1.18
(1,81)	1:100:A:GLY:C	1:101:A:VAL:N	1:101:A:VAL:CA	1:101:A:VAL:C	3	1.18
(1,49)	1:83:A:SER:C	1:84:A:THR:N	1:84:A:THR:CA	1:84:A:THR:C	6	1.18
(1,61)	1:89:A:LEU:C	1:90:A:GLY:N	1:90:A:GLY:CA	1:90:A:GLY:C	6	1.16
(1,61)	1:89:A:LEU:C	1:90:A:GLY:N	1:90:A:GLY:CA	1:90:A:GLY:C	5	1.14
(1,57)	1:87:A:GLU:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	5	1.14
(1,135)	1:128:A:VAL:C	1:129:A:VAL:N	1:129:A:VAL:CA	1:129:A:VAL:C	4	1.11
(1,100)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:SER:N	10	1.1
(1,58)	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	1:89:A:LEU:N	5	1.06
(1,49)	1:83:A:SER:C	1:84:A:THR:N	1:84:A:THR:CA	1:84:A:THR:C	10	1.06
(1,96)	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	1:109:A:THR:N	4	1.03
(1,49)	1:83:A:SER:C	1:84:A:THR:N	1:84:A:THR:CA	1:84:A:THR:C	1	1.02