



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 04:49 PM EST

PDB ID : 2LNZ  
BMRB ID : 18186  
Title : Solution structure of the Get5 carboxyl domain from *S. cerevisiae*  
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Deposited on : 2012-01-08

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)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

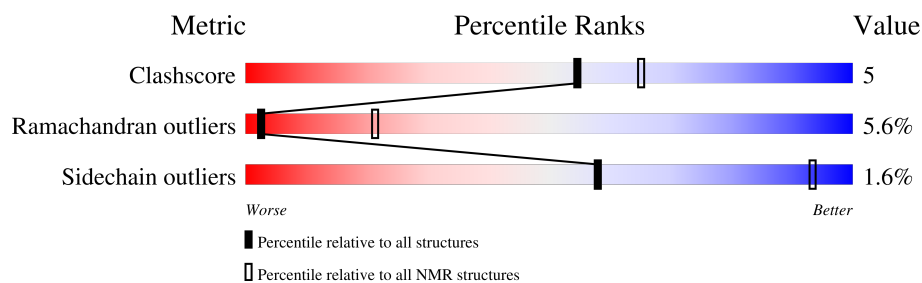
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 45%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	64	
1	B	64	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:176-A:211, B:176-B:212 (73)	0.19	1

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 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1308 atoms, of which 648 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin-like protein MDY2.

Mol	Chain	Residues	Atoms						Trace
1	A	40	Total	C	H	N	O	S	0
			654	207	324	58	64	1	
1	B	40	Total	C	H	N	O	S	0
			654	207	324	58	64	1	

There are 6 discrepancies between the modelled and reference sequences:

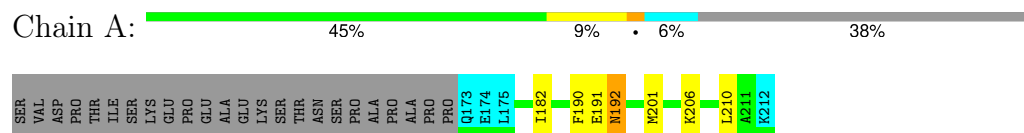
Chain	Residue	Modelled	Actual	Comment	Reference
A	149	SER	-	expression tag	UNP Q12285
A	150	VAL	-	expression tag	UNP Q12285
A	151	ASP	-	expression tag	UNP Q12285
B	149	SER	-	expression tag	UNP Q12285
B	150	VAL	-	expression tag	UNP Q12285
B	151	ASP	-	expression tag	UNP Q12285

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

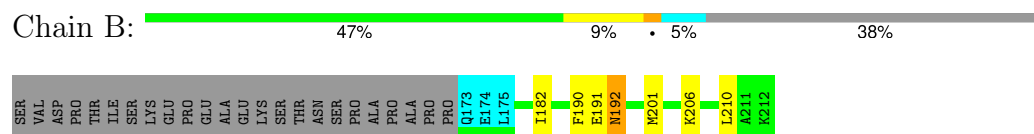
### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 1: Ubiquitin-like protein MDY2

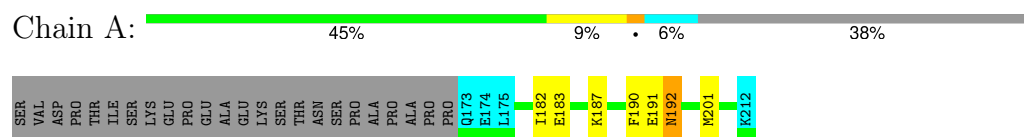


### 4.2 Scores per residue for each member of the ensemble

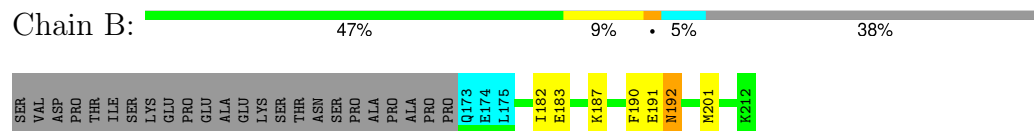
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Ubiquitin-like protein MDY2

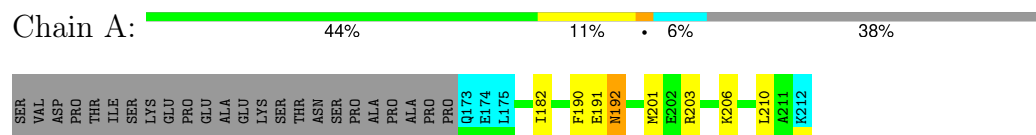


- Molecule 1: Ubiquitin-like protein MDY2

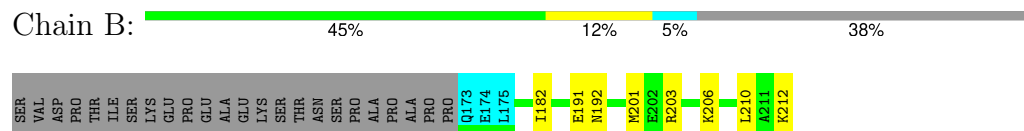


### 4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin-like protein MDY2

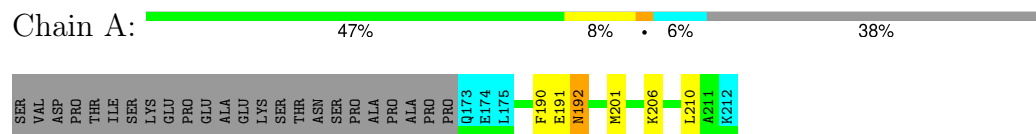


- Molecule 1: Ubiquitin-like protein MDY2

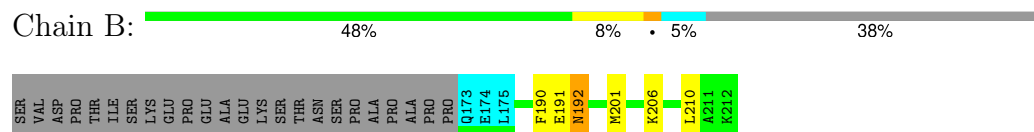


### 4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin-like protein MDY2

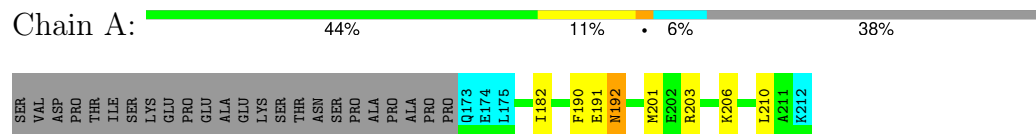


- Molecule 1: Ubiquitin-like protein MDY2

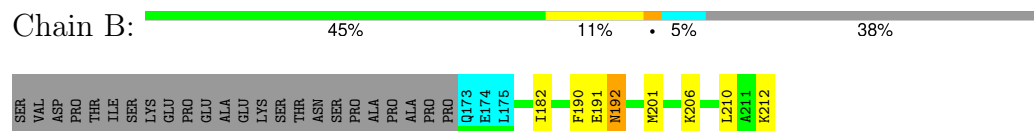


### 4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin-like protein MDY2

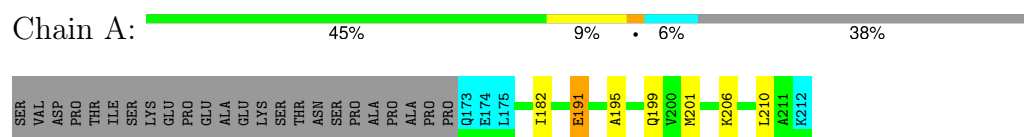


- Molecule 1: Ubiquitin-like protein MDY2

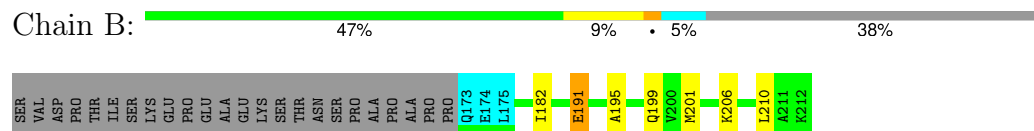


### 4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin-like protein MDY2

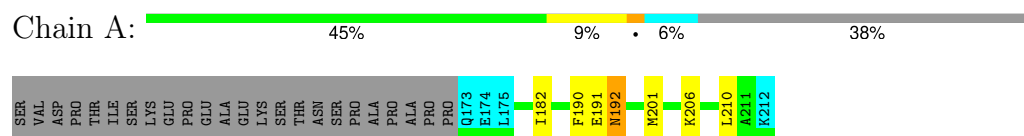


- Molecule 1: Ubiquitin-like protein MDY2

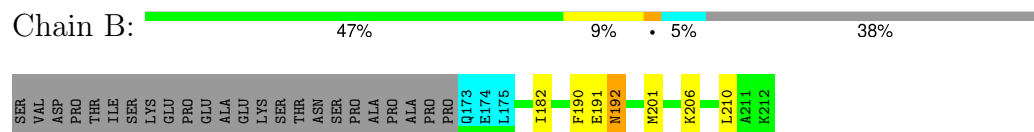


### 4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin-like protein MDY2

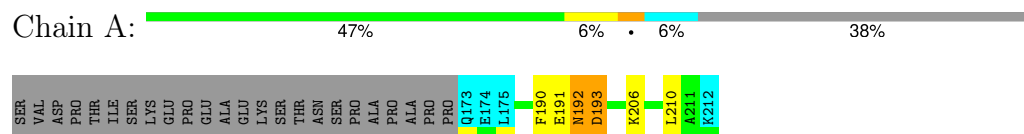


- Molecule 1: Ubiquitin-like protein MDY2

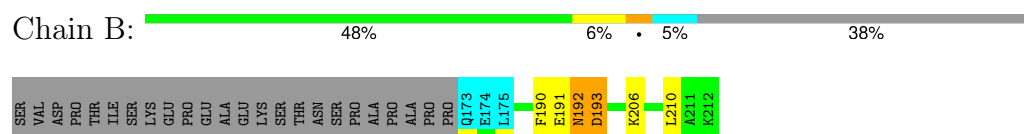


### 4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin-like protein MDY2

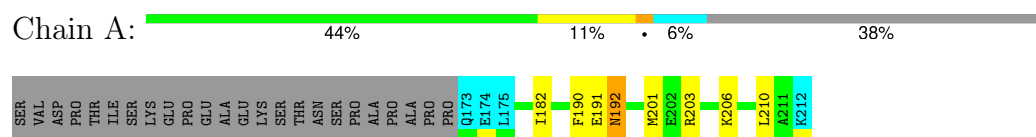


- Molecule 1: Ubiquitin-like protein MDY2

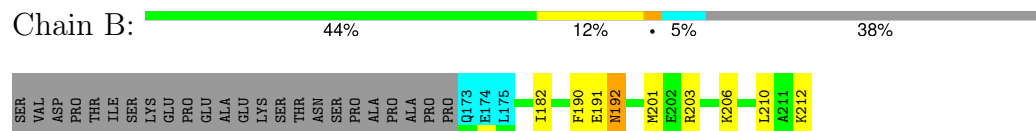


#### 4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin-like protein MDY2

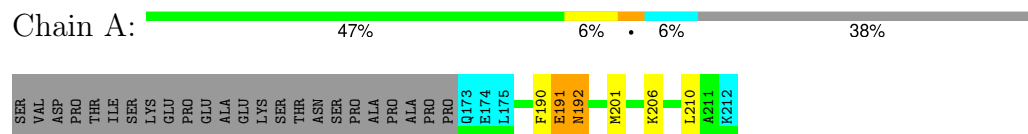


- Molecule 1: Ubiquitin-like protein MDY2

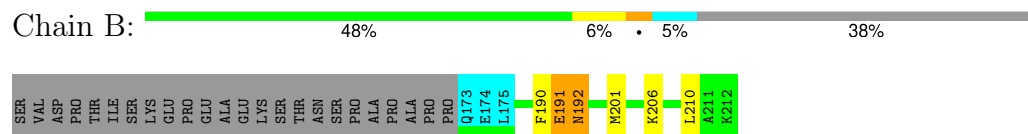


#### 4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin-like protein MDY2

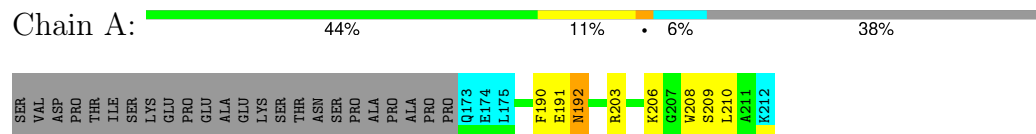


- Molecule 1: Ubiquitin-like protein MDY2

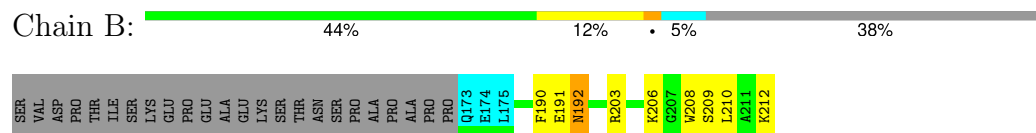


#### 4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin-like protein MDY2



- Molecule 1: Ubiquitin-like protein MDY2





## 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	2.3
CNS	refinement	1.21

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	762
Number of shifts mapped to atoms	518
Number of unparsed shifts	0
Number of shifts with mapping errors	244
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

## 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	294	286	286	3±1
1	B	304	299	299	3±1
All	All	5980	5850	5850	58

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:206:LYS:O	1:A:210:LEU:HG	0.54	2.03	4	9
1:B:206:LYS:O	1:B:210:LEU:HG	0.53	2.04	4	9
1:B:190:PHE:C	1:B:192:ASN:H	0.52	2.08	7	1
1:A:182:ILE:HG22	1:A:201:MET:SD	0.52	2.45	1	6
1:A:190:PHE:C	1:A:192:ASN:H	0.52	2.08	7	1
1:B:182:ILE:HG22	1:B:201:MET:SD	0.51	2.45	1	6
1:A:190:PHE:O	1:A:192:ASN:N	0.50	2.41	1	8
1:A:208:TRP:CZ3	1:B:203:ARG:HB3	0.49	2.41	10	1
1:A:203:ARG:HB3	1:B:208:TRP:CZ3	0.49	2.43	10	1
1:A:203:ARG:NH2	1:B:212:LYS:HG2	0.47	2.24	8	1
1:A:203:ARG:NH2	1:B:212:LYS:HA	0.45	2.27	10	1
1:B:190:PHE:O	1:B:192:ASN:N	0.45	2.42	6	7
1:A:203:ARG:CZ	1:B:212:LYS:HA	0.43	2.44	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:GLU:O	1:A:187:LYS:HB2	0.41	2.15	1	1
1:B:183:GLU:O	1:B:187:LYS:HB2	0.41	2.15	1	1
1:A:195:ALA:O	1:A:199:GLN:HG3	0.41	2.16	5	1
1:B:195:ALA:O	1:B:199:GLN:HG3	0.41	2.15	5	1
1:B:209:SER:O	1:B:212:LYS:HE3	0.40	2.16	10	1

## 6.3 Torsion angles [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	36/64 (56%)	32±0 (89±1%)	2±1 (5±2%)	2±0 (6±1%)	2	21
1	B	36/64 (56%)	32±0 (89±1%)	2±1 (5±2%)	2±0 (6±1%)	2	21
All	All	720/1280 (56%)	644 (89%)	36 (5%)	40 (6%)	2	21

All 6 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	191	GLU	10
1	B	191	GLU	10
1	A	192	ASN	9
1	B	192	ASN	9
1	A	193	ASP	1
1	B	193	ASP	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	31/56 (55%)	30±1 (98±2%)	0±1 (2±2%)	58	93
1	B	32/56 (57%)	32±1 (98±2%)	0±1 (2±2%)	58	93
All	All	630/1120 (56%)	620 (98%)	10 (2%)	58	93

All 6 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	201	MET	2
1	B	201	MET	2
1	A	191	GLU	2
1	B	191	GLU	2
1	A	193	ASP	1
1	B	193	ASP	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 6.7 Other polymers ⓘ

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 45% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

Total number of shifts	762
Number of shifts mapped to atoms	518
Number of unparsed shifts	0
Number of shifts with mapping errors	244
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 244 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	150	VAL	HA	4.188	0.001	1
1	A	150	VAL	HB	2.051	0	1
1	A	150	VAL	HG11	0.924	0	2
1	A	150	VAL	HG12	0.924	0	2
1	A	150	VAL	HG13	0.924	0	2
1	A	150	VAL	HG21	0.932	0	2
1	A	150	VAL	HG22	0.932	0	2
1	A	150	VAL	HG23	0.932	0	2
1	A	150	VAL	C	175.422	0	1
1	A	150	VAL	CA	62.042	0.067	1
1	A	150	VAL	CB	32.93	0.074	1
1	A	150	VAL	CG1	21.124	0	2
1	A	150	VAL	CG2	20.404	0.003	2
1	A	151	ASP	H	8.49	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	151	ASP	HA	4.908	0.001	1
1	A	151	ASP	HB2	2.558	0.007	2
1	A	151	ASP	HB3	2.818	0.002	2
1	A	151	ASP	CA	51.995	0.066	1
1	A	151	ASP	CB	41.174	0.026	1
1	A	151	ASP	N	126.293	0.026	1
1	A	152	PRO	HA	4.5	0.013	1
1	A	152	PRO	HB2	2.019	0	2
1	A	152	PRO	HB3	2.317	0	2
1	A	152	PRO	C	177.321	0	1
1	A	152	PRO	CA	63.537	0.05	1
1	A	152	PRO	CB	32.192	0.086	1
1	A	152	PRO	CG	26.992	0	1
1	A	152	PRO	CD	50.879	0	1
1	A	153	THR	H	8.423	0.002	1
1	A	153	THR	HA	4.259	0.002	1
1	A	153	THR	HB	4.205	0.005	1
1	A	153	THR	HG21	1.227	0.002	1
1	A	153	THR	HG22	1.227	0.002	1
1	A	153	THR	HG23	1.227	0.002	1
1	A	153	THR	C	174.81	0	1
1	A	153	THR	CA	62.769	0.072	1
1	A	153	THR	CB	69.533	0.054	1
1	A	153	THR	CG2	21.769	0.023	1
1	A	153	THR	N	113.744	0.028	1
1	A	154	ILE	H	7.822	0.001	1
1	A	154	ILE	HA	4.214	0.013	1
1	A	154	ILE	HB	1.912	0.007	1
1	A	154	ILE	HG12	1.2	0.002	2
1	A	154	ILE	HG13	1.468	0.002	2
1	A	154	ILE	HG21	0.913	0	1
1	A	154	ILE	HG22	0.913	0	1
1	A	154	ILE	HG23	0.913	0	1
1	A	154	ILE	HD11	0.876	0	1
1	A	154	ILE	HD12	0.876	0	1
1	A	154	ILE	HD13	0.876	0	1
1	A	154	ILE	C	176.15	0	1
1	A	154	ILE	CA	61.08	0.054	1
1	A	154	ILE	CB	38.714	0.052	1
1	A	154	ILE	CG1	27.227	0.033	1
1	A	154	ILE	CG2	17.419	0.017	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	154	ILE	CD1	12.916	0.054	1
1	A	154	ILE	N	122.501	0.018	1
1	A	155	SER	H	8.318	0.002	1
1	A	155	SER	HA	4.458	0.002	1
1	A	155	SER	HB2	3.844	0	1
1	A	155	SER	HB3	3.844	0	1
1	A	155	SER	C	174.203	0	1
1	A	155	SER	CA	58.168	0.08	1
1	A	155	SER	CB	63.742	0.043	1
1	A	155	SER	N	119.956	0.009	1
1	A	156	LYS	H	8.344	0.002	1
1	A	156	LYS	HA	4.384	0.007	1
1	A	156	LYS	HB2	1.735	0	2
1	A	156	LYS	HB3	1.847	0	2
1	A	156	LYS	HG2	1.443	0.004	1
1	A	156	LYS	HG3	1.443	0.004	1
1	A	156	LYS	HD2	1.693	0.003	1
1	A	156	LYS	HD3	1.693	0.003	1
1	A	156	LYS	HE2	2.996	0	1
1	A	156	LYS	HE3	2.996	0	1
1	A	156	LYS	C	176.183	0	1
1	A	156	LYS	CA	55.962	0.049	1
1	A	156	LYS	CB	33.242	0.07	1
1	A	156	LYS	CG	24.526	0.079	1
1	A	156	LYS	CD	28.962	0.082	1
1	A	156	LYS	CE	42.081	0	1
1	A	156	LYS	N	123.765	0.027	1
1	A	157	GLU	H	8.462	0.002	1
1	A	157	GLU	HA	4.555	0.008	1
1	A	157	GLU	HB2	1.878	0	2
1	A	157	GLU	HB3	2.076	0	2
1	A	157	GLU	HG2	2.33	0	1
1	A	157	GLU	HG3	2.33	0	1
1	A	157	GLU	CA	54.6	0.032	1
1	A	157	GLU	CB	29.502	0	1
1	A	157	GLU	N	123.909	0.024	1
1	A	158	PRO	HA	4.39	0.005	1
1	A	158	PRO	HB2	1.925	0	2
1	A	158	PRO	HB3	2.318	0	2
1	A	158	PRO	HG3	2.056	0	1
1	A	158	PRO	HD2	3.707	0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	158	PRO	HD3	3.821	0	2
1	A	158	PRO	C	177.12	0	1
1	A	158	PRO	CA	63.257	0.057	1
1	A	158	PRO	CB	32.063	0.085	1
1	A	158	PRO	CG	27.44	0.001	1
1	A	158	PRO	CD	50.624	0.003	1
1	A	159	GLU	H	8.543	0.001	1
1	A	159	GLU	HA	4.235	0	1
1	A	159	GLU	HB2	1.947	0	2
1	A	159	GLU	HB3	2.051	0	2
1	A	159	GLU	HG2	2.32	0	1
1	A	159	GLU	HG3	2.32	0	1
1	A	159	GLU	C	176.525	0	1
1	A	159	GLU	CA	56.604	0.066	1
1	A	159	GLU	CB	30.199	0.113	1
1	A	159	GLU	CG	36.293	0	1
1	A	159	GLU	N	121.225	0.023	1
1	A	160	ALA	H	8.325	0.002	1
1	A	160	ALA	HA	4.28	0.002	1
1	A	160	ALA	HB1	1.407	0.004	1
1	A	160	ALA	HB2	1.407	0.004	1
1	A	160	ALA	HB3	1.407	0.004	1
1	A	160	ALA	C	177.923	0	1
1	A	160	ALA	CA	52.758	0.105	1
1	A	160	ALA	CB	19.382	0.034	1
1	A	160	ALA	N	125.227	0.019	1
1	A	161	GLU	H	8.388	0.01	1
1	A	161	GLU	HA	4.229	0.012	1
1	A	161	GLU	HB2	2.051	0	2
1	A	161	GLU	HB3	1.96	0	2
1	A	161	GLU	HG2	2.306	0	1
1	A	161	GLU	HG3	2.306	0	1
1	A	161	GLU	C	176.613	0	1
1	A	161	GLU	CA	56.702	0.017	1
1	A	161	GLU	CB	30.11	0.097	1
1	A	161	GLU	CG	36.227	0	1
1	A	161	GLU	N	120.229	0.013	1
1	A	162	LYS	H	8.33	0.006	1
1	A	162	LYS	HA	4.373	0.002	1
1	A	162	LYS	HB2	1.869	0	2
1	A	162	LYS	HB3	1.731	0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	162	LYS	HG2	1.443	0.007	1
1	A	162	LYS	HG3	1.443	0.007	1
1	A	162	LYS	HD2	1.766	0	2
1	A	162	LYS	HD3	1.648	0	2
1	A	162	LYS	HE2	3.012	0.002	2
1	A	162	LYS	HE3	3.01	0	2
1	A	162	LYS	C	176.739	0	1
1	A	162	LYS	CA	56.252	0.086	1
1	A	162	LYS	CB	33.105	0.029	1
1	A	162	LYS	CG	24.754	0.054	1
1	A	162	LYS	CD	29.057	0.007	1
1	A	162	LYS	CE	42.125	0	1
1	A	162	LYS	N	122.474	0.048	1
1	A	163	SER	H	8.413	0.002	1
1	A	163	SER	HA	4.52	0.014	1
1	A	163	SER	HB2	3.892	0.001	2
1	A	163	SER	HB3	3.934	0	2
1	A	163	SER	C	174.994	0	1
1	A	163	SER	CA	58.346	0.064	1
1	A	163	SER	CB	63.753	0.029	1
1	A	163	SER	N	117.125	0.012	1
1	A	164	THR	H	8.246	0.001	1
1	A	164	THR	HA	4.378	0.003	1
1	A	164	THR	HB	4.283	0.001	1
1	A	164	THR	HG21	1.218	0.003	1
1	A	164	THR	HG22	1.218	0.003	1
1	A	164	THR	HG23	1.218	0.003	1
1	A	164	THR	C	174.356	0	1
1	A	164	THR	CA	61.834	0.074	1
1	A	164	THR	CB	69.706	0.026	1
1	A	164	THR	CG2	21.578	0.051	1
1	A	164	THR	N	115.57	0.011	1
1	A	165	ASN	H	8.409	0.002	1
1	A	165	ASN	HA	4.773	0	1
1	A	165	ASN	HB2	2.738	0.006	2
1	A	165	ASN	HB3	2.825	0.011	2
1	A	165	ASN	HD21	6.919	0	1
1	A	165	ASN	HD22	7.597	0	1
1	A	165	ASN	C	174.816	0	1
1	A	165	ASN	CA	53.141	0.055	1
1	A	165	ASN	CB	39.08	0.075	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	165	ASN	N	120.92	0.02	1
1	A	165	ASN	ND2	112.944	0	1
1	A	166	SER	H	8.271	0.002	1
1	A	166	SER	HA	4.762	0.008	1
1	A	166	SER	HB2	3.801	0.004	2
1	A	166	SER	HB3	3.881	0	2
1	A	166	SER	CA	56.442	0.103	1
1	A	166	SER	CB	63.237	0	1
1	A	166	SER	N	117.774	0.045	1
1	A	167	PRO	HA	4.387	0	1
1	A	167	PRO	HB2	1.879	0	2
1	A	167	PRO	HB3	2.263	0	2
1	A	167	PRO	C	176.325	0	1
1	A	167	PRO	CA	62.723	0.079	1
1	A	167	PRO	CB	31.989	0.06	1
1	A	167	PRO	CG	27.271	0	1
1	A	167	PRO	CD	50.403	0	1
1	A	168	ALA	H	8.372	0.002	1
1	A	168	ALA	HA	4.582	0.005	1
1	A	168	ALA	HB1	1.362	0.005	1
1	A	168	ALA	HB2	1.362	0.005	1
1	A	168	ALA	HB3	1.362	0.005	1
1	A	168	ALA	CA	50.374	0.048	1
1	A	168	ALA	CB	18.181	0.028	1
1	A	168	ALA	N	125.934	0.032	1
1	A	169	PRO	HA	4.42	0.016	1
1	A	169	PRO	HB2	1.916	0	2
1	A	169	PRO	HB3	2.275	0	2
1	A	169	PRO	HG3	2.035	0	1
1	A	169	PRO	HD2	3.643	0	2
1	A	169	PRO	HD3	3.819	0	2
1	A	169	PRO	C	176.344	0	1
1	A	169	PRO	CA	62.976	0.049	1
1	A	169	PRO	CB	32.02	0.067	1
1	A	169	PRO	CG	27.693	0	1
1	A	169	PRO	CD	50.668	0.009	1
1	A	170	ALA	H	8.407	0.002	1
1	A	170	ALA	HA	4.584	0.003	1
1	A	170	ALA	HB1	1.362	0.004	1
1	A	170	ALA	HB2	1.362	0.004	1
1	A	170	ALA	HB3	1.362	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	170	ALA	CA	50.424	0.034	1
1	A	170	ALA	CB	18.143	0.01	1
1	A	170	ALA	N	126.15	0.023	1
1	A	171	PRO	HA	4.713	0.003	1
1	A	171	PRO	HB2	1.92	0.001	2
1	A	171	PRO	HB3	2.366	0	2
1	A	171	PRO	HG3	2.046	0.004	1
1	A	171	PRO	HD2	3.826	0.002	2
1	A	171	PRO	HD3	3.647	0.001	2
1	A	171	PRO	CA	61.639	0.047	1
1	A	171	PRO	CB	31.95	0	1
1	A	171	PRO	CG	27.519	0	1
1	A	171	PRO	CD	50.679	0	1
1	A	172	PRO	HA	4.413	0.018	1
1	A	172	PRO	HB2	1.922	0.008	2
1	A	172	PRO	HB3	2.31	0.005	2
1	A	172	PRO	HG2	2.033	0	1
1	A	172	PRO	HG3	2.033	0	1
1	A	172	PRO	HD2	3.707	0.003	2
1	A	172	PRO	HD3	3.824	0.001	2
1	A	172	PRO	C	176.888	0	1
1	A	172	PRO	CA	62.937	0.059	1
1	A	172	PRO	CB	32.074	0.072	1
1	A	172	PRO	CG	27.369	0.002	1
1	A	172	PRO	CD	50.386	0.008	1

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	63	$-0.67 \pm 0.30$	Should be checked
$^{13}\text{C}_\beta$	62	$0.23 \pm 0.19$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	55	$-0.40 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	55	$-0.14 \pm 0.42$	None needed ( $< 0.5$ ppm)

### 7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 45%, i.e. 464 atoms were assigned a chemical shift out of a possible 1032. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	178/363 (49%)	72/146 (49%)	71/146 (49%)	35/71 (49%)
Sidechain	252/601 (42%)	170/386 (44%)	76/186 (41%)	6/29 (21%)
Aromatic	34/68 (50%)	17/34 (50%)	15/30 (50%)	2/4 (50%)
Overall	464/1032 (45%)	259/566 (46%)	162/362 (45%)	43/104 (41%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 45%, i.e. 518 atoms were assigned a chemical shift out of a possible 1140. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	197/398 (49%)	80/160 (50%)	78/160 (49%)	39/78 (50%)
Sidechain	287/674 (43%)	193/432 (45%)	87/210 (41%)	7/32 (22%)
Aromatic	34/68 (50%)	17/34 (50%)	15/30 (50%)	2/4 (50%)
Overall	518/1140 (45%)	290/626 (46%)	180/400 (45%)	48/114 (42%)

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

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

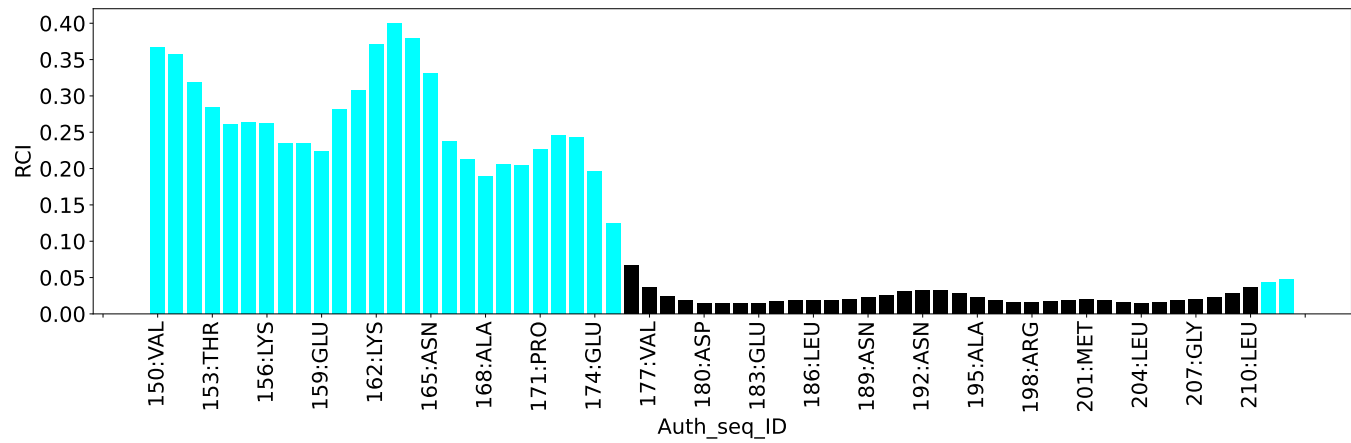
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	205	GLN	HG3	-0.05	0.91 – 3.68	-8.5
1	A	177	VAL	HG11	-0.99	-0.48 – 2.12	-7.0
1	A	177	VAL	HG12	-0.99	-0.48 – 2.12	-7.0
1	A	177	VAL	HG13	-0.99	-0.48 – 2.12	-7.0
1	A	203	ARG	HD2	1.57	1.97 – 4.26	-6.7
1	A	177	VAL	HB	0.16	0.43 – 3.54	-5.9
1	A	205	GLN	HE21	4.66	5.02 – 9.43	-5.8
1	A	177	VAL	HG21	-0.61	-0.58 – 2.19	-5.1
1	A	177	VAL	HG22	-0.61	-0.58 – 2.19	-5.1
1	A	177	VAL	HG23	-0.61	-0.58 – 2.19	-5.1

### 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	2976
Intra-residue ( $ i-j =0$ )	764
Sequential ( $ i-j =1$ )	508
Medium range ( $ i-j >1$ and $ i-j <5$ )	848
Long range ( $ i-j \geq 5$ )	358
Inter-chain	402
Hydrogen bond restraints	96
Disulfide bond restraints	0
Total dihedral-angle restraints	132
Number of unmapped restraints	0
Number of restraints per residue	24.3
Number of long range restraints per residue <sup>1</sup>	2.8

<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)	140.7	0.2
0.2-0.5 (Medium)	254.1	0.5
>0.5 (Large)	333.4	3.49

### 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)	5.9	7.53
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

### 9.1 Summary of distance violations ⓘ

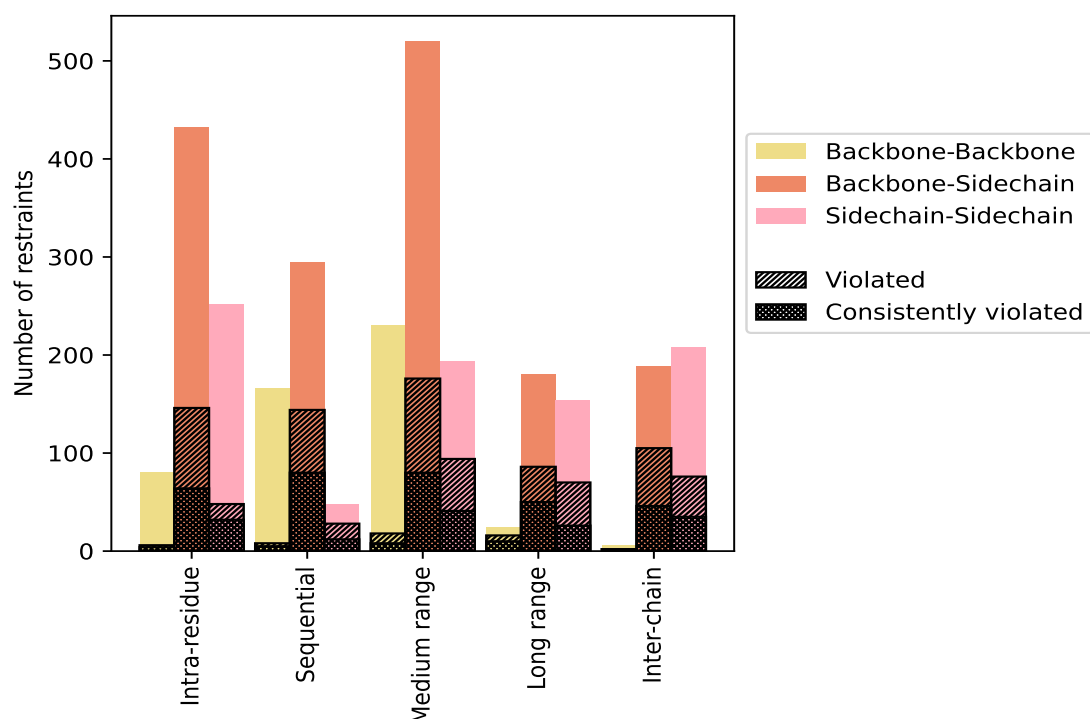
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

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>764</b>	<b>25.7</b>	<b>200</b>	<b>26.2</b>	<b>6.7</b>	<b>100</b>	<b>13.1</b>	<b>3.4</b>
Backbone-Backbone	80	2.7	6	7.5	0.2	4	5.0	0.1
Backbone-Sidechain	432	14.5	146	33.8	4.9	64	14.8	2.2
Sidechain-Sidechain	252	8.5	48	19.0	1.6	32	12.7	1.1
<b>Sequential (<math> i-j =1</math>)</b>	<b>508</b>	<b>17.1</b>	<b>180</b>	<b>35.4</b>	<b>6.0</b>	<b>97</b>	<b>19.1</b>	<b>3.3</b>
Backbone-Backbone	166	5.6	8	4.8	0.3	5	3.0	0.2
Backbone-Sidechain	294	9.9	144	49.0	4.8	80	27.2	2.7
Sidechain-Sidechain	48	1.6	28	58.3	0.9	12	25.0	0.4
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>848</b>	<b>28.5</b>	<b>288</b>	<b>34.0</b>	<b>9.7</b>	<b>129</b>	<b>15.2</b>	<b>4.3</b>
Backbone-Backbone	230	7.7	18	7.8	0.6	8	3.5	0.3
Backbone-Sidechain	424	14.2	176	41.5	5.9	80	18.9	2.7
Sidechain-Sidechain	194	6.5	94	48.5	3.2	41	21.1	1.4
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>358</b>	<b>12.0</b>	<b>172</b>	<b>48.0</b>	<b>5.8</b>	<b>86</b>	<b>24.0</b>	<b>2.9</b>
Backbone-Backbone	24	0.8	16	66.7	0.5	10	41.7	0.3
Backbone-Sidechain	180	6.0	86	47.8	2.9	50	27.8	1.7
Sidechain-Sidechain	154	5.2	70	45.5	2.4	26	16.9	0.9
<b>Inter-chain</b>	<b>402</b>	<b>13.5</b>	<b>183</b>	<b>45.5</b>	<b>6.1</b>	<b>83</b>	<b>20.6</b>	<b>2.8</b>
Backbone-Backbone	6	0.2	2	33.3	0.1	2	33.3	0.1
Backbone-Sidechain	188	6.3	105	55.9	3.5	46	24.5	1.5
Sidechain-Sidechain	208	7.0	76	36.5	2.6	35	16.8	1.2
<b>Hydrogen bond</b>	<b>96</b>	<b>3.2</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>2976</b>	<b>100.0</b>	<b>1023</b>	<b>34.4</b>	<b>34.4</b>	<b>495</b>	<b>16.6</b>	<b>16.6</b>
Backbone-Backbone	506	17.0	50	9.9	1.7	29	5.7	1.0
Backbone-Sidechain	1614	54.2	657	40.7	22.1	320	19.8	10.8
Sidechain-Sidechain	856	28.8	316	36.9	10.6	146	17.1	4.9

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

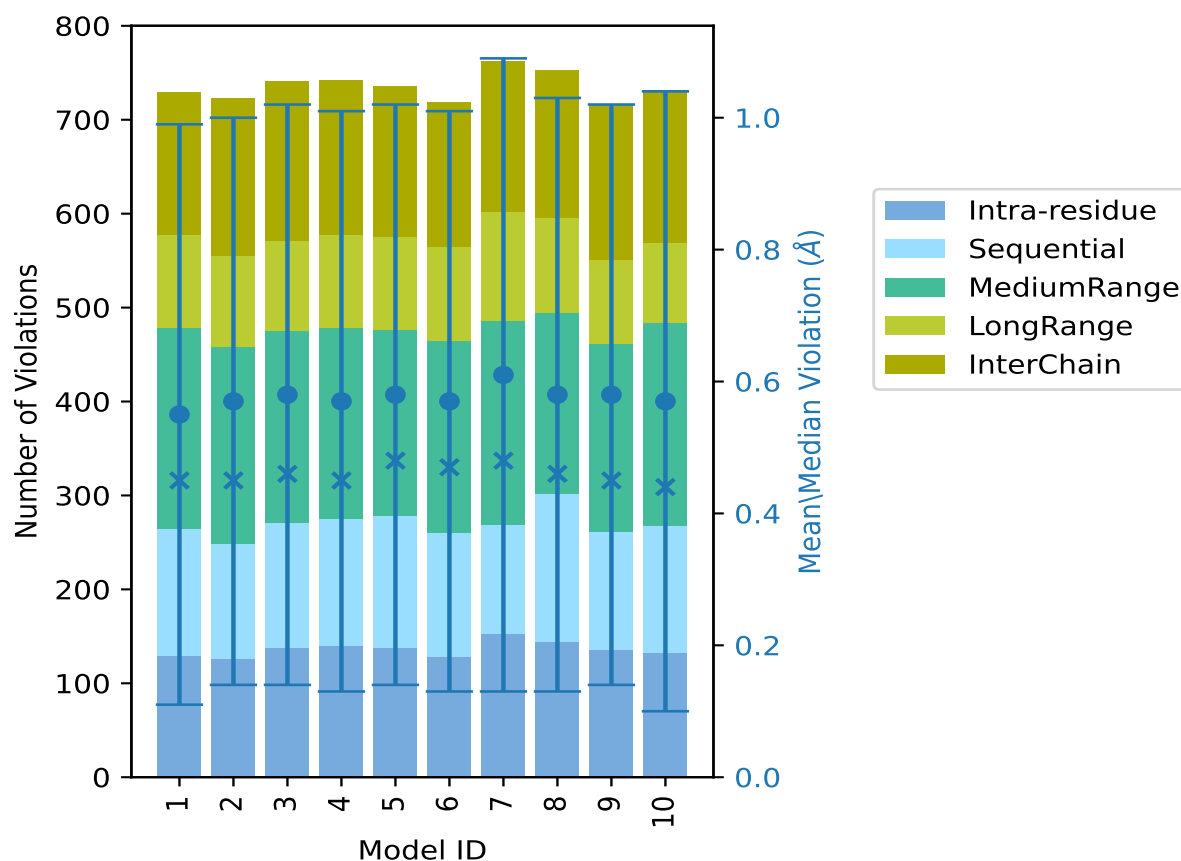
## 9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	129	135	215	98	152	729	0.55	3.49	0.44	0.45
2	126	123	210	96	168	723	0.57	2.16	0.43	0.45
3	138	133	205	95	170	741	0.58	2.26	0.44	0.46
4	140	135	204	98	165	742	0.57	2.48	0.44	0.45
5	138	140	198	100	160	736	0.58	2.42	0.44	0.48
6	128	132	204	101	154	719	0.57	3.45	0.44	0.47
7	153	116	217	116	160	762	0.61	3.45	0.48	0.48
8	144	158	192	102	157	753	0.58	3.25	0.45	0.46
9	136	125	200	90	164	715	0.58	2.49	0.44	0.45
10	132	136	216	85	162	731	0.57	2.54	0.47	0.44

<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, 1857(IR:564, SQ:328, MR:560, LR:186, IC:219) 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>	%
22	19	41	20	17	119	1	10.0
22	7	16	10	5	60	2	20.0
6	10	8	10	16	50	3	30.0

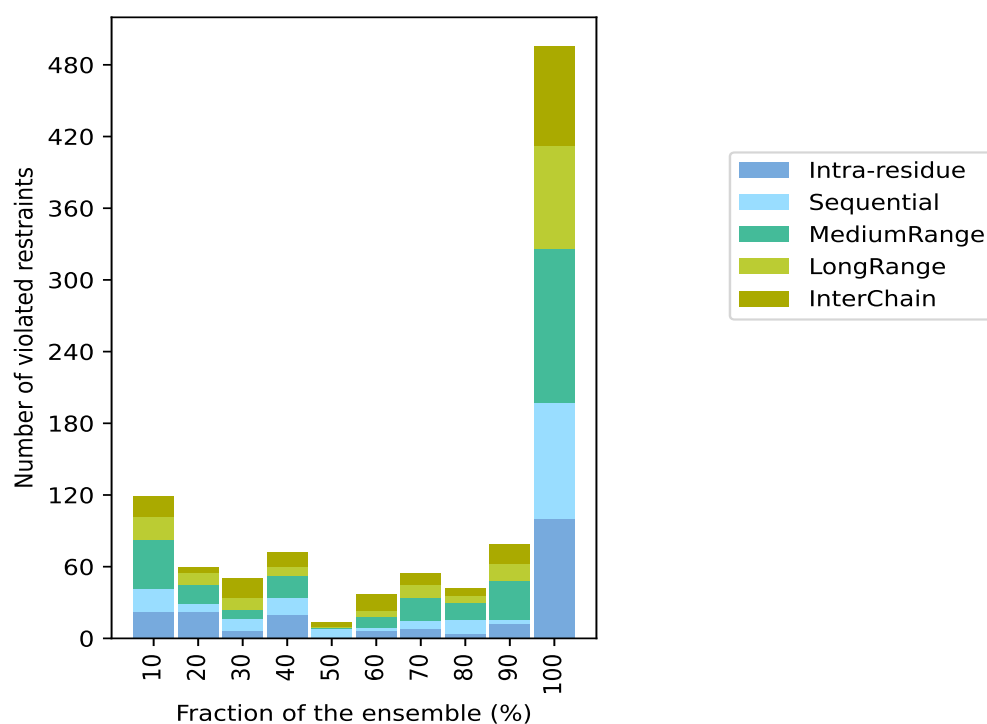
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
20	14	18	8	12	72	4	40.0
0	8	1	1	4	14	5	50.0
6	3	9	5	14	37	6	60.0
8	7	19	11	10	55	7	70.0
4	11	15	6	6	42	8	80.0
12	4	32	15	16	79	9	90.0
100	97	129	86	83	495	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 ⓘ

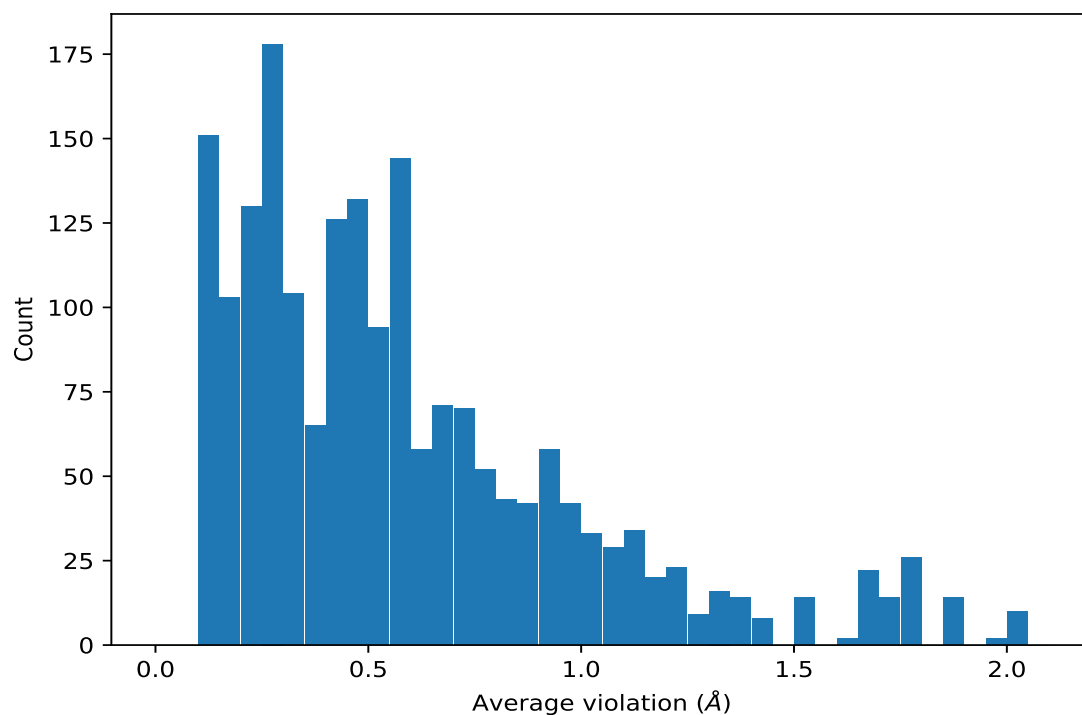


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2349)	1:197:A:VAL:H	1:187:A:LYS:HG2	10	2.02	0.16	2.02
(1,2349)	1:193:A:ASP:H	1:187:A:LYS:HG2	10	2.02	0.16	2.02
(1,2350)	1:197:B:VAL:H	1:187:B:LYS:HG2	10	2.02	0.16	2.01
(1,2350)	1:193:B:ASP:H	1:187:B:LYS:HG2	10	2.02	0.16	2.01
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	10	1.98	0.24	2.04
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	10	1.98	0.24	2.02
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD11	10	1.88	0.18	1.96
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD13	10	1.88	0.18	1.96
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD12	10	1.88	0.18	1.96
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD11	10	1.88	0.18	1.96
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD13	10	1.88	0.18	1.96
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD12	10	1.88	0.18	1.96
(1,2646)	1:188:B:ASN:HD22	1:185:B:LEU:HB3	10	1.86	0.47	2.06
(1,2646)	1:188:B:ASN:HD22	1:187:B:LYS:HG3	10	1.86	0.47	2.06
(1,2646)	1:188:B:ASN:HD22	1:178:A:PRO:HG2	10	1.86	0.47	2.06

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2645)	1:188:A:ASN:HD22	1:185:A:LEU:HB3	10	1.86	0.47	2.06
(1,2645)	1:188:A:ASN:HD22	1:187:A:LYS:HG3	10	1.86	0.47	2.06
(1,2645)	1:188:A:ASN:HD22	1:178:B:PRO:HG2	10	1.86	0.47	2.06
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG13	10	1.79	0.07	1.81
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG12	10	1.79	0.07	1.81
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG11	10	1.79	0.07	1.81
(1,2146)	1:199:B:GLN:HB3	1:200:B:VAL:HG23	10	1.79	0.07	1.81
(1,2146)	1:199:B:GLN:HB3	1:196:B:ALA:HB3	10	1.79	0.07	1.81
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG13	10	1.79	0.07	1.8
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG12	10	1.79	0.07	1.8
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG11	10	1.79	0.07	1.8
(1,2145)	1:199:A:GLN:HB3	1:200:A:VAL:HG23	10	1.79	0.07	1.8
(1,2145)	1:199:A:GLN:HB3	1:196:A:ALA:HB3	10	1.79	0.07	1.8
(1,2303)	1:188:A:ASN:HB2	1:187:A:LYS:HG3	10	1.76	0.26	1.83
(1,2303)	1:188:A:ASN:HB2	1:185:A:LEU:HB3	10	1.76	0.26	1.83
(1,2304)	1:188:B:ASN:HB2	1:187:B:LYS:HG3	10	1.76	0.26	1.83
(1,2304)	1:188:B:ASN:HB2	1:185:B:LEU:HB3	10	1.76	0.26	1.83
(1,2379)	1:182:A:ILE:HD11	1:185:B:LEU:H	10	1.76	0.12	1.72
(1,2379)	1:182:A:ILE:HD12	1:185:B:LEU:H	10	1.76	0.12	1.72
(1,2379)	1:182:A:ILE:HD13	1:185:B:LEU:H	10	1.76	0.12	1.72
(1,2380)	1:182:B:ILE:HD11	1:185:A:LEU:H	10	1.75	0.12	1.74
(1,2380)	1:182:B:ILE:HD12	1:185:A:LEU:H	10	1.75	0.12	1.74
(1,2380)	1:182:B:ILE:HD13	1:185:A:LEU:H	10	1.75	0.12	1.74
(1,2705)	1:189:A:ASN:HD22	1:181:B:ASP:HA	10	1.73	0.16	1.83
(1,2705)	1:189:A:ASN:HD22	1:188:A:ASN:HA	10	1.73	0.16	1.83
(1,2706)	1:189:B:ASN:HD22	1:181:A:ASP:HA	10	1.73	0.17	1.84
(1,2706)	1:189:B:ASN:HD22	1:188:B:ASN:HA	10	1.73	0.17	1.84
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB3	10	1.68	0.92	1.25
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB2	10	1.68	0.92	1.25
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB1	10	1.68	0.92	1.25
(1,2629)	1:173:A:GLN:HE21	1:195:B:ALA:HB1	10	1.68	0.92	1.25
(1,2629)	1:173:A:GLN:HE21	1:195:B:ALA:HB3	10	1.68	0.92	1.25
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB3	10	1.68	0.91	1.24
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB2	10	1.68	0.91	1.24
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB1	10	1.68	0.91	1.24
(1,2630)	1:173:B:GLN:HE21	1:195:A:ALA:HB1	10	1.68	0.91	1.24
(1,2630)	1:173:B:GLN:HE21	1:195:A:ALA:HB3	10	1.68	0.91	1.24
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB2	10	1.67	0.14	1.69
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB3	10	1.67	0.14	1.69
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB1	10	1.67	0.14	1.69
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB2	10	1.67	0.14	1.69
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB3	10	1.67	0.14	1.69

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB1	10	1.67	0.14	1.69
(1,2398)	1:195:B:ALA:HA	1:196:B:ALA:HB2	10	1.54	0.08	1.57
(1,2398)	1:195:B:ALA:HA	1:197:B:VAL:HG23	10	1.54	0.08	1.57
(1,2398)	1:195:B:ALA:HA	1:197:B:VAL:HG21	10	1.54	0.08	1.57
(1,2398)	1:195:B:ALA:HA	1:196:B:ALA:HB1	10	1.54	0.08	1.57
(1,2398)	1:195:B:ALA:HA	1:197:B:VAL:HG22	10	1.54	0.08	1.57
(1,2398)	1:195:B:ALA:HA	1:196:B:ALA:HB3	10	1.54	0.08	1.57
(1,2397)	1:195:A:ALA:HA	1:196:A:ALA:HB2	10	1.54	0.07	1.57
(1,2397)	1:195:A:ALA:HA	1:197:A:VAL:HG23	10	1.54	0.07	1.57
(1,2397)	1:195:A:ALA:HA	1:197:A:VAL:HG21	10	1.54	0.07	1.57
(1,2397)	1:195:A:ALA:HA	1:196:A:ALA:HB1	10	1.54	0.07	1.57
(1,2397)	1:195:A:ALA:HA	1:197:A:VAL:HG22	10	1.54	0.07	1.57
(1,2397)	1:195:A:ALA:HA	1:196:A:ALA:HB3	10	1.54	0.07	1.57
(1,887)	1:202:A:GLU:HG2	1:201:A:MET:HB2	10	1.54	0.72	1.02
(1,888)	1:202:B:GLU:HG2	1:201:B:MET:HB2	10	1.53	0.71	1.02
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD21	10	1.45	0.13	1.51
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD22	10	1.45	0.13	1.51
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD23	10	1.45	0.13	1.51
(1,1083)	1:199:A:GLN:HB3	1:198:A:ARG:H	10	1.45	0.04	1.44
(1,1084)	1:199:B:GLN:HB3	1:198:B:ARG:H	10	1.45	0.04	1.44
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD21	10	1.44	0.13	1.5
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD22	10	1.44	0.13	1.5
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD23	10	1.44	0.13	1.5
(1,2065)	1:201:A:MET:HE2	1:184:A:ALA:H	10	1.38	0.29	1.25
(1,2065)	1:201:A:MET:HE1	1:184:A:ALA:H	10	1.38	0.29	1.25
(1,2065)	1:201:A:MET:HE3	1:184:A:ALA:H	10	1.38	0.29	1.25
(1,2066)	1:201:B:MET:HE2	1:184:B:ALA:H	10	1.38	0.29	1.25
(1,2066)	1:201:B:MET:HE1	1:184:B:ALA:H	10	1.38	0.29	1.25
(1,2066)	1:201:B:MET:HE3	1:184:B:ALA:H	10	1.38	0.29	1.25
(1,951)	1:197:A:VAL:HG13	1:187:A:LYS:HG2	10	1.37	0.15	1.42
(1,951)	1:197:A:VAL:HG12	1:187:A:LYS:HG2	10	1.37	0.15	1.42
(1,951)	1:197:A:VAL:HG11	1:187:A:LYS:HG2	10	1.37	0.15	1.42
(1,952)	1:197:B:VAL:HG13	1:187:B:LYS:HG2	10	1.37	0.16	1.43
(1,952)	1:197:B:VAL:HG12	1:187:B:LYS:HG2	10	1.37	0.16	1.43
(1,952)	1:197:B:VAL:HG11	1:187:B:LYS:HG2	10	1.37	0.16	1.43
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD21	10	1.34	0.03	1.34
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD22	10	1.34	0.03	1.34
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD23	10	1.34	0.03	1.34
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD21	10	1.34	0.03	1.35
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD22	10	1.34	0.03	1.35
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD23	10	1.34	0.03	1.35
(1,892)	1:192:B:ASN:HB3	1:191:B:GLU:HB3	10	1.32	0.1	1.3

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,891)	1:192:A:ASN:HB3	1:191:A:GLU:HB3	10	1.32	0.1	1.3
(1,933)	1:197:A:VAL:HG23	1:187:A:LYS:HG2	10	1.31	0.15	1.33
(1,933)	1:197:A:VAL:HG22	1:187:A:LYS:HG2	10	1.31	0.15	1.33
(1,933)	1:197:A:VAL:HG21	1:187:A:LYS:HG2	10	1.31	0.15	1.33
(1,934)	1:197:B:VAL:HG23	1:187:B:LYS:HG2	10	1.31	0.15	1.33
(1,934)	1:197:B:VAL:HG22	1:187:B:LYS:HG2	10	1.31	0.15	1.33
(1,934)	1:197:B:VAL:HG21	1:187:B:LYS:HG2	10	1.31	0.15	1.33
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG23	10	1.28	0.14	1.27
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG21	10	1.28	0.14	1.27
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG23	10	1.27	0.14	1.27
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG21	10	1.27	0.14	1.27
(1,1259)	1:176:A:THR:HG22	1:177:A:VAL:HG11	10	1.24	0.07	1.26
(1,1259)	1:176:A:THR:HG22	1:177:A:VAL:HG13	10	1.24	0.07	1.26
(1,1259)	1:176:A:THR:HG21	1:177:A:VAL:HG13	10	1.24	0.07	1.26
(1,1259)	1:176:A:THR:HG23	1:177:A:VAL:HG13	10	1.24	0.07	1.26
(1,1259)	1:176:A:THR:HG21	1:177:A:VAL:HG11	10	1.24	0.07	1.26
(1,1260)	1:176:B:THR:HG22	1:177:B:VAL:HG11	10	1.23	0.07	1.26
(1,1260)	1:176:B:THR:HG22	1:177:B:VAL:HG13	10	1.23	0.07	1.26
(1,1260)	1:176:B:THR:HG21	1:177:B:VAL:HG13	10	1.23	0.07	1.26
(1,1260)	1:176:B:THR:HG23	1:177:B:VAL:HG13	10	1.23	0.07	1.26
(1,1260)	1:176:B:THR:HG21	1:177:B:VAL:HG11	10	1.23	0.07	1.26
(1,2079)	1:175:A:LEU:HD21	1:196:B:ALA:H	10	1.23	0.12	1.27
(1,2079)	1:175:A:LEU:HD22	1:208:A:TRP:HZ2	10	1.23	0.12	1.27
(1,2079)	1:175:A:LEU:HD22	1:196:B:ALA:H	10	1.23	0.12	1.27
(1,2079)	1:175:A:LEU:HD23	1:196:B:ALA:H	10	1.23	0.12	1.27
(1,2080)	1:175:B:LEU:HD21	1:196:A:ALA:H	10	1.22	0.12	1.25
(1,2080)	1:175:B:LEU:HD22	1:208:B:TRP:HZ2	10	1.22	0.12	1.25
(1,2080)	1:175:B:LEU:HD22	1:196:A:ALA:H	10	1.22	0.12	1.25
(1,2080)	1:175:B:LEU:HD23	1:196:A:ALA:H	10	1.22	0.12	1.25
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD21	10	1.2	0.09	1.23
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD22	10	1.2	0.09	1.23
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD23	10	1.2	0.09	1.23
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD21	10	1.2	0.09	1.21
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD22	10	1.2	0.09	1.21
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD23	10	1.2	0.09	1.21
(1,945)	1:175:A:LEU:HD22	1:199:B:GLN:HB3	10	1.19	0.62	0.92
(1,945)	1:175:A:LEU:HD23	1:199:B:GLN:HB3	10	1.19	0.62	0.92
(1,945)	1:175:A:LEU:HD21	1:199:B:GLN:HB3	10	1.19	0.62	0.92
(1,946)	1:175:B:LEU:HD22	1:199:A:GLN:HB3	10	1.19	0.63	0.94
(1,946)	1:175:B:LEU:HD23	1:199:A:GLN:HB3	10	1.19	0.63	0.94
(1,946)	1:175:B:LEU:HD21	1:199:A:GLN:HB3	10	1.19	0.63	0.94
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG22	10	1.17	0.07	1.19

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG23	10	1.17	0.07	1.19
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG21	10	1.17	0.07	1.19
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG22	10	1.17	0.07	1.19
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG23	10	1.17	0.07	1.19
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG21	10	1.17	0.07	1.19
(1,281)	1:185:A:LEU:HD12	1:185:A:LEU:HB3	10	1.14	0.01	1.14
(1,281)	1:185:A:LEU:HD11	1:185:A:LEU:HB3	10	1.14	0.01	1.14
(1,281)	1:185:A:LEU:HD13	1:185:A:LEU:HB3	10	1.14	0.01	1.14
(1,282)	1:185:B:LEU:HD12	1:185:B:LEU:HB3	10	1.14	0.01	1.14
(1,282)	1:185:B:LEU:HD11	1:185:B:LEU:HB3	10	1.14	0.01	1.14
(1,282)	1:185:B:LEU:HD13	1:185:B:LEU:HB3	10	1.14	0.01	1.14
(1,197)	1:201:A:MET:HE3	1:177:A:VAL:HG11	10	1.13	0.42	1.0
(1,197)	1:201:A:MET:HE3	1:177:A:VAL:HG13	10	1.13	0.42	1.0
(1,197)	1:201:A:MET:HE2	1:177:A:VAL:HG13	10	1.13	0.42	1.0
(1,197)	1:201:A:MET:HE2	1:177:A:VAL:HG11	10	1.13	0.42	1.0
(1,197)	1:201:A:MET:HE1	1:177:A:VAL:HG13	10	1.13	0.42	1.0
(1,197)	1:201:A:MET:HE1	1:177:A:VAL:HG11	10	1.13	0.42	1.0
(1,198)	1:201:B:MET:HE3	1:177:B:VAL:HG11	10	1.13	0.42	1.0
(1,198)	1:201:B:MET:HE3	1:177:B:VAL:HG13	10	1.13	0.42	1.0
(1,198)	1:201:B:MET:HE2	1:177:B:VAL:HG13	10	1.13	0.42	1.0
(1,198)	1:201:B:MET:HE2	1:177:B:VAL:HG11	10	1.13	0.42	1.0
(1,198)	1:201:B:MET:HE1	1:177:B:VAL:HG13	10	1.13	0.42	1.0
(1,198)	1:201:B:MET:HE1	1:177:B:VAL:HG11	10	1.13	0.42	1.0
(1,940)	1:175:B:LEU:HD21	1:175:B:LEU:HB2	10	1.12	0.02	1.12
(1,940)	1:175:B:LEU:HD22	1:175:B:LEU:HB2	10	1.12	0.02	1.12
(1,940)	1:175:B:LEU:HD23	1:175:B:LEU:HB2	10	1.12	0.02	1.12
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD11	10	1.12	0.05	1.14
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD13	10	1.12	0.05	1.14
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD12	10	1.12	0.05	1.14
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD11	10	1.12	0.05	1.14
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD13	10	1.12	0.05	1.14
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD12	10	1.12	0.05	1.14
(1,939)	1:175:A:LEU:HD21	1:175:A:LEU:HB2	10	1.12	0.02	1.12
(1,939)	1:175:A:LEU:HD22	1:175:A:LEU:HB2	10	1.12	0.02	1.12
(1,939)	1:175:A:LEU:HD23	1:175:A:LEU:HB2	10	1.12	0.02	1.12
(1,2115)	1:182:A:ILE:HD11	1:178:A:PRO:HB2	10	1.09	0.09	1.1
(1,2115)	1:182:A:ILE:HD13	1:178:A:PRO:HB2	10	1.09	0.09	1.1
(1,2115)	1:182:A:ILE:HD13	1:204:B:LEU:HG	10	1.09	0.09	1.1
(1,2116)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	10	1.09	0.09	1.1
(1,2116)	1:182:B:ILE:HD13	1:178:B:PRO:HB2	10	1.09	0.09	1.1
(1,2116)	1:182:B:ILE:HD13	1:204:A:LEU:HG	10	1.09	0.09	1.1
(1,2071)	1:211:A:ALA:HB3	1:208:B:TRP:H	10	1.09	0.08	1.08

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2071)	1:211:A:ALA:HB1	1:208:B:TRP:H	10	1.09	0.08	1.08
(1,2071)	1:208:A:TRP:H	1:211:A:ALA:HB1	10	1.09	0.08	1.08
(1,2071)	1:211:A:ALA:HB2	1:208:B:TRP:H	10	1.09	0.08	1.08
(1,157)	1:182:A:ILE:HD11	1:178:A:PRO:HD3	10	1.08	0.16	1.01
(1,157)	1:182:A:ILE:HD12	1:178:A:PRO:HD3	10	1.08	0.16	1.01
(1,157)	1:182:A:ILE:HD13	1:178:A:PRO:HD3	10	1.08	0.16	1.01
(1,158)	1:182:B:ILE:HD11	1:178:B:PRO:HD3	10	1.08	0.17	1.01
(1,158)	1:182:B:ILE:HD12	1:178:B:PRO:HD3	10	1.08	0.17	1.01
(1,158)	1:182:B:ILE:HD13	1:178:B:PRO:HD3	10	1.08	0.17	1.01
(1,2072)	1:211:B:ALA:HB3	1:208:A:TRP:H	10	1.08	0.08	1.06
(1,2072)	1:211:B:ALA:HB1	1:208:A:TRP:H	10	1.08	0.08	1.06
(1,2072)	1:211:B:ALA:HB2	1:208:A:TRP:H	10	1.08	0.08	1.06
(1,1257)	1:176:A:THR:HG22	1:177:A:VAL:HG23	10	1.06	0.09	1.06
(1,1257)	1:176:A:THR:HG21	1:177:A:VAL:HG22	10	1.06	0.09	1.06
(1,1257)	1:176:A:THR:HG23	1:177:A:VAL:HG23	10	1.06	0.09	1.06
(1,1257)	1:176:A:THR:HG22	1:177:A:VAL:HG21	10	1.06	0.09	1.06
(1,1257)	1:176:A:THR:HG21	1:177:A:VAL:HG21	10	1.06	0.09	1.06
(1,1258)	1:176:B:THR:HG22	1:177:B:VAL:HG23	10	1.06	0.09	1.06
(1,1258)	1:176:B:THR:HG21	1:177:B:VAL:HG22	10	1.06	0.09	1.06
(1,1258)	1:176:B:THR:HG23	1:177:B:VAL:HG23	10	1.06	0.09	1.06
(1,1258)	1:176:B:THR:HG22	1:177:B:VAL:HG21	10	1.06	0.09	1.06
(1,1258)	1:176:B:THR:HG21	1:177:B:VAL:HG21	10	1.06	0.09	1.06
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB1	10	1.03	0.03	1.04
(1,2260)	1:190:B:PHE:HA	1:197:B:VAL:HG21	10	1.03	0.03	1.04
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB2	10	1.03	0.03	1.04
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB3	10	1.03	0.03	1.04
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB1	10	1.03	0.03	1.04
(1,2259)	1:190:A:PHE:HA	1:197:A:VAL:HG21	10	1.03	0.03	1.04
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB2	10	1.03	0.03	1.04
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB3	10	1.03	0.03	1.04
(1,1721)	1:196:A:ALA:H	1:198:A:ARG:HG2	10	1.02	0.13	1.04
(1,2103)	1:204:A:LEU:HD23	1:179:B:TRP:HE3	10	1.02	0.1	0.99
(1,2103)	1:204:A:LEU:HD22	1:179:B:TRP:HE3	10	1.02	0.1	0.99
(1,2103)	1:204:A:LEU:HD21	1:179:B:TRP:HE3	10	1.02	0.1	0.99
(1,1722)	1:196:B:ALA:H	1:198:B:ARG:HG2	10	1.02	0.13	1.04
(1,2104)	1:204:B:LEU:HD23	1:179:A:TRP:HE3	10	1.02	0.1	1.0
(1,2104)	1:204:B:LEU:HD22	1:179:A:TRP:HE3	10	1.02	0.1	1.0
(1,2104)	1:204:B:LEU:HD21	1:179:A:TRP:HE3	10	1.02	0.1	1.0
(1,1245)	1:175:A:LEU:HD11	1:177:A:VAL:HG23	10	1.01	0.24	0.92
(1,1245)	1:175:A:LEU:HD12	1:177:A:VAL:HG23	10	1.01	0.24	0.92
(1,1245)	1:175:A:LEU:HD11	1:177:A:VAL:HG22	10	1.01	0.24	0.92
(1,1245)	1:175:A:LEU:HD13	1:177:A:VAL:HG23	10	1.01	0.24	0.92

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1245)	1:175:A:LEU:HD11	1:177:A:VAL:HG21	10	1.01	0.24	0.92
(1,1245)	1:175:A:LEU:HD13	1:177:A:VAL:HG22	10	1.01	0.24	0.92
(1,1246)	1:175:B:LEU:HD11	1:177:B:VAL:HG23	10	1.01	0.24	0.92
(1,1246)	1:175:B:LEU:HD12	1:177:B:VAL:HG23	10	1.01	0.24	0.92
(1,1246)	1:175:B:LEU:HD11	1:177:B:VAL:HG22	10	1.01	0.24	0.92
(1,1246)	1:175:B:LEU:HD13	1:177:B:VAL:HG23	10	1.01	0.24	0.92
(1,1246)	1:175:B:LEU:HD11	1:177:B:VAL:HG21	10	1.01	0.24	0.92
(1,1246)	1:175:B:LEU:HD13	1:177:B:VAL:HG22	10	1.01	0.24	0.92
(1,2120)	1:177:B:VAL:HG12	1:182:B:ILE:HG22	10	0.99	0.08	0.96
(1,2120)	1:177:B:VAL:HG11	1:182:B:ILE:HG23	10	0.99	0.08	0.96
(1,2120)	1:177:B:VAL:HG11	1:182:B:ILE:HG21	10	0.99	0.08	0.96
(1,2120)	1:177:B:VAL:HG11	1:182:B:ILE:HG22	10	0.99	0.08	0.96
(1,2120)	1:177:B:VAL:HG12	1:182:B:ILE:HG23	10	0.99	0.08	0.96
(1,2119)	1:177:A:VAL:HG12	1:182:A:ILE:HG22	10	0.99	0.08	0.96
(1,2119)	1:177:A:VAL:HG11	1:182:A:ILE:HG23	10	0.99	0.08	0.96
(1,2119)	1:177:A:VAL:HG11	1:182:A:ILE:HG21	10	0.99	0.08	0.96
(1,2119)	1:177:A:VAL:HG11	1:182:A:ILE:HG22	10	0.99	0.08	0.96
(1,2119)	1:177:A:VAL:HG12	1:182:A:ILE:HG23	10	0.99	0.08	0.96
(1,689)	1:199:A:GLN:HB3	1:196:A:ALA:HA	10	0.99	0.1	0.98
(1,690)	1:199:B:GLN:HB3	1:196:B:ALA:HA	10	0.99	0.1	0.98
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG13	10	0.98	0.05	0.98
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG12	10	0.98	0.05	0.98
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG13	10	0.98	0.04	0.98
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG12	10	0.98	0.04	0.98
(1,1646)	1:201:B:MET:H	1:175:A:LEU:HB2	10	0.98	0.08	1.0
(1,1645)	1:201:A:MET:H	1:175:B:LEU:HB2	10	0.97	0.07	1.0
(1,57)	1:211:A:ALA:HB1	1:206:B:LYS:H	10	0.97	0.11	1.0
(1,57)	1:211:A:ALA:HB2	1:206:B:LYS:H	10	0.97	0.11	1.0
(1,57)	1:211:A:ALA:HB3	1:206:B:LYS:H	10	0.97	0.11	1.0
(1,58)	1:211:B:ALA:HB1	1:206:A:LYS:H	10	0.96	0.09	1.0
(1,58)	1:211:B:ALA:HB2	1:206:A:LYS:H	10	0.96	0.09	1.0
(1,58)	1:211:B:ALA:HB3	1:206:A:LYS:H	10	0.96	0.09	1.0
(1,2148)	1:183:B:GLU:HB2	1:197:B:VAL:HG12	10	0.96	0.09	0.99
(1,2148)	1:183:B:GLU:HB2	1:197:B:VAL:HG11	10	0.96	0.09	0.99
(1,2148)	1:194:B:GLN:HB2	1:197:B:VAL:HG22	10	0.96	0.09	0.99
(1,2148)	1:183:B:GLU:HB2	1:197:B:VAL:HG13	10	0.96	0.09	0.99
(1,2147)	1:183:A:GLU:HB2	1:197:A:VAL:HG12	10	0.96	0.09	0.99
(1,2147)	1:183:A:GLU:HB2	1:197:A:VAL:HG11	10	0.96	0.09	0.99
(1,2147)	1:194:A:GLN:HB2	1:197:A:VAL:HG22	10	0.96	0.09	0.99
(1,2147)	1:183:A:GLU:HB2	1:197:A:VAL:HG13	10	0.96	0.09	0.99
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB3	10	0.95	0.08	0.92
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB1	10	0.95	0.08	0.92

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB2	10	0.95	0.08	0.92
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB3	10	0.95	0.08	0.94
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB1	10	0.95	0.08	0.94
(1,2592)	1:208:B:TRP:H	1:211:B:ALA:HB1	10	0.95	0.08	0.94
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB2	10	0.95	0.08	0.94
(1,1220)	1:185:B:LEU:HD22	1:177:A:VAL:HG13	10	0.95	0.11	0.92
(1,1220)	1:185:B:LEU:HD22	1:177:A:VAL:HG12	10	0.95	0.11	0.92
(1,1220)	1:185:B:LEU:HD23	1:177:A:VAL:HG12	10	0.95	0.11	0.92
(1,1220)	1:185:B:LEU:HD21	1:177:A:VAL:HG13	10	0.95	0.11	0.92
(1,1219)	1:185:A:LEU:HD22	1:177:B:VAL:HG13	10	0.95	0.12	0.9
(1,1219)	1:185:A:LEU:HD22	1:177:B:VAL:HG12	10	0.95	0.12	0.9
(1,1219)	1:185:A:LEU:HD23	1:177:B:VAL:HG12	10	0.95	0.12	0.9
(1,1219)	1:185:A:LEU:HD21	1:177:B:VAL:HG13	10	0.95	0.12	0.9
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG23	10	0.95	0.05	0.96
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG21	10	0.95	0.05	0.96
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG22	10	0.95	0.05	0.96
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG23	10	0.94	0.05	0.95
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG21	10	0.94	0.05	0.95
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG22	10	0.94	0.05	0.95
(1,2373)	1:176:A:THR:HG22	1:190:B:PHE:HZ	10	0.93	0.15	0.96
(1,2373)	1:176:A:THR:HG21	1:190:B:PHE:HZ	10	0.93	0.15	0.96
(1,2373)	1:176:A:THR:HG23	1:190:B:PHE:HZ	10	0.93	0.15	0.96
(1,170)	1:182:B:ILE:HD11	1:177:B:VAL:HG21	10	0.93	0.1	0.92
(1,170)	1:182:B:ILE:HD12	1:177:B:VAL:HG21	10	0.93	0.1	0.92
(1,170)	1:182:B:ILE:HD12	1:177:B:VAL:HG23	10	0.93	0.1	0.92
(1,170)	1:182:B:ILE:HD12	1:177:B:VAL:HG22	10	0.93	0.1	0.92
(1,170)	1:182:B:ILE:HD11	1:177:B:VAL:HG23	10	0.93	0.1	0.92
(1,170)	1:182:B:ILE:HD13	1:177:B:VAL:HG22	10	0.93	0.1	0.92
(1,169)	1:182:A:ILE:HD11	1:177:A:VAL:HG21	10	0.93	0.1	0.92
(1,169)	1:182:A:ILE:HD12	1:177:A:VAL:HG21	10	0.93	0.1	0.92
(1,169)	1:182:A:ILE:HD12	1:177:A:VAL:HG23	10	0.93	0.1	0.92
(1,169)	1:182:A:ILE:HD12	1:177:A:VAL:HG22	10	0.93	0.1	0.92
(1,169)	1:182:A:ILE:HD11	1:177:A:VAL:HG23	10	0.93	0.1	0.92
(1,169)	1:182:A:ILE:HD13	1:177:A:VAL:HG22	10	0.93	0.1	0.92
(1,2374)	1:176:B:THR:HG22	1:190:A:PHE:HZ	10	0.93	0.14	0.96
(1,2374)	1:176:B:THR:HG21	1:190:A:PHE:HZ	10	0.93	0.14	0.96
(1,2374)	1:176:B:THR:HG23	1:190:A:PHE:HZ	10	0.93	0.14	0.96
(1,2871)	1:209:A:SER:H	1:204:B:LEU:HG	10	0.92	0.05	0.92
(1,2872)	1:209:B:SER:H	1:204:A:LEU:HG	10	0.91	0.06	0.92
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB3	10	0.91	0.04	0.91
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB1	10	0.91	0.04	0.91
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB2	10	0.91	0.04	0.91

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB3	10	0.91	0.04	0.9
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB1	10	0.91	0.04	0.9
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB2	10	0.91	0.04	0.9
(1,2331)	1:212:A:LYS:HB3	1:211:A:ALA:H	10	0.9	0.61	0.61
(1,2332)	1:212:B:LYS:HB3	1:211:B:ALA:H	10	0.9	0.6	0.61
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB2	10	0.89	0.12	0.9
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB3	10	0.89	0.12	0.9
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB1	10	0.89	0.12	0.9
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB2	10	0.89	0.12	0.9
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB3	10	0.89	0.12	0.9
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB1	10	0.89	0.12	0.9
(1,2073)	1:211:A:ALA:HB2	1:208:A:TRP:HE3	10	0.89	0.07	0.88
(1,2073)	1:211:A:ALA:HB3	1:208:A:TRP:HE3	10	0.89	0.07	0.88
(1,2073)	1:211:A:ALA:HB1	1:208:A:TRP:HE3	10	0.89	0.07	0.88
(1,2074)	1:211:B:ALA:HB2	1:208:B:TRP:HE3	10	0.89	0.08	0.88
(1,2074)	1:211:B:ALA:HB3	1:208:B:TRP:HE3	10	0.89	0.08	0.88
(1,2074)	1:211:B:ALA:HB1	1:208:B:TRP:HE3	10	0.89	0.08	0.88
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG12	10	0.89	0.07	0.88
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG11	10	0.89	0.07	0.88
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG13	10	0.89	0.07	0.88
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG12	10	0.89	0.07	0.87
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG11	10	0.89	0.07	0.87
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG13	10	0.89	0.07	0.87
(1,2061)	1:177:A:VAL:HG13	1:182:A:ILE:HG12	10	0.89	0.06	0.88
(1,2061)	1:177:A:VAL:HG12	1:182:A:ILE:HG12	10	0.89	0.06	0.88
(1,2062)	1:177:B:VAL:HG13	1:182:B:ILE:HG12	10	0.89	0.06	0.88
(1,2062)	1:177:B:VAL:HG12	1:182:B:ILE:HG12	10	0.89	0.06	0.88
(1,706)	1:195:B:ALA:HA	1:198:B:ARG:HG2	10	0.89	0.19	0.96
(1,705)	1:195:A:ALA:HA	1:198:A:ARG:HG2	10	0.89	0.18	0.96
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG21	10	0.88	0.11	0.88
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG22	10	0.88	0.11	0.88
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG23	10	0.88	0.11	0.88
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG21	10	0.88	0.1	0.88
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG22	10	0.88	0.1	0.88
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG23	10	0.88	0.1	0.88
(1,1818)	1:192:B:ASN:H	1:187:B:LYS:HG2	10	0.88	0.23	0.88
(1,1817)	1:192:A:ASN:H	1:187:A:LYS:HG2	10	0.87	0.23	0.88
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD11	10	0.83	0.12	0.8
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD12	10	0.83	0.12	0.8
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD13	10	0.83	0.12	0.8
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD11	10	0.83	0.12	0.82
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD12	10	0.83	0.12	0.82

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD13	10	0.83	0.12	0.82
(1,749)	1:185:A:LEU:HD23	1:185:A:LEU:HA	10	0.83	0.01	0.82
(1,749)	1:185:A:LEU:HD21	1:185:A:LEU:HA	10	0.83	0.01	0.82
(1,749)	1:185:A:LEU:HD22	1:185:A:LEU:HA	10	0.83	0.01	0.82
(1,750)	1:185:B:LEU:HD23	1:185:B:LEU:HA	10	0.82	0.01	0.82
(1,750)	1:185:B:LEU:HD21	1:185:B:LEU:HA	10	0.82	0.01	0.82
(1,750)	1:185:B:LEU:HD22	1:185:B:LEU:HA	10	0.82	0.01	0.82
(1,2301)	1:188:A:ASN:HB3	1:185:A:LEU:HB3	10	0.82	0.57	0.66
(1,2302)	1:188:B:ASN:HB3	1:185:B:LEU:HB3	10	0.82	0.57	0.66
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG22	10	0.82	0.02	0.82
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG23	10	0.82	0.02	0.82
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG22	10	0.82	0.01	0.82
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG23	10	0.82	0.01	0.82
(1,1553)	1:173:A:GLN:HE21	1:175:A:LEU:HB3	10	0.81	0.48	0.8
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB1	10	0.8	0.03	0.79
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB2	10	0.8	0.03	0.79
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB3	10	0.8	0.03	0.79
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB1	10	0.8	0.03	0.79
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB2	10	0.8	0.03	0.79
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB3	10	0.8	0.03	0.79
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG11	10	0.8	0.09	0.8
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG13	10	0.8	0.09	0.8
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG12	10	0.8	0.09	0.8
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG11	10	0.8	0.09	0.8
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG13	10	0.8	0.09	0.8
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG12	10	0.8	0.09	0.8
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD13	10	0.79	0.04	0.78
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD11	10	0.79	0.04	0.78
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD12	10	0.79	0.04	0.78
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD13	10	0.78	0.05	0.78
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD11	10	0.78	0.05	0.78
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD12	10	0.78	0.05	0.78
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD11	10	0.78	0.13	0.76
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD13	10	0.78	0.13	0.76
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD12	10	0.78	0.13	0.76
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD11	10	0.78	0.13	0.76
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD13	10	0.78	0.13	0.76
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD12	10	0.78	0.13	0.76
(1,1658)	1:200:B:VAL:H	1:199:B:GLN:HB3	10	0.78	0.04	0.76
(1,1657)	1:200:A:VAL:H	1:199:A:GLN:HB3	10	0.78	0.04	0.77
(1,1123)	1:211:A:ALA:HB2	1:204:B:LEU:H	10	0.78	0.08	0.8
(1,1123)	1:211:A:ALA:HB3	1:204:B:LEU:H	10	0.78	0.08	0.8

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1123)	1:211:A:ALA:HB1	1:204:B:LEU:H	10	0.78	0.08	0.8
(1,1124)	1:211:B:ALA:HB2	1:204:A:LEU:H	10	0.77	0.06	0.78
(1,1124)	1:211:B:ALA:HB3	1:204:A:LEU:H	10	0.77	0.06	0.78
(1,1124)	1:211:B:ALA:HB1	1:204:A:LEU:H	10	0.77	0.06	0.78
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD13	10	0.77	0.04	0.78
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD11	10	0.77	0.04	0.78
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD12	10	0.77	0.04	0.78
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD23	10	0.77	0.1	0.78
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD22	10	0.77	0.1	0.78
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD21	10	0.77	0.1	0.78
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD23	10	0.77	0.1	0.78
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD22	10	0.77	0.1	0.78
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD21	10	0.77	0.1	0.78
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD13	10	0.77	0.04	0.78
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD11	10	0.77	0.04	0.78
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD12	10	0.77	0.04	0.78
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG21	10	0.75	0.17	0.84
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG23	10	0.75	0.17	0.84
(1,2746)	1:195:B:ALA:H	1:196:B:ALA:HB2	10	0.75	0.17	0.84
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG22	10	0.75	0.17	0.84
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG21	10	0.75	0.17	0.84
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG23	10	0.75	0.17	0.84
(1,2745)	1:195:A:ALA:H	1:196:A:ALA:HB2	10	0.75	0.17	0.84
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG22	10	0.75	0.17	0.84
(1,2234)	1:200:B:VAL:HA	1:190:B:PHE:HE2	10	0.75	0.05	0.76
(1,2233)	1:200:A:VAL:HA	1:190:A:PHE:HE2	10	0.75	0.05	0.76
(1,2836)	1:179:B:TRP:H	1:183:B:GLU:HA	10	0.74	0.06	0.72
(1,2835)	1:179:A:TRP:H	1:183:A:GLU:HA	10	0.74	0.06	0.72
(1,1010)	1:208:B:TRP:HB3	1:208:B:TRP:HE3	10	0.74	0.01	0.74
(1,1009)	1:208:A:TRP:HB3	1:208:A:TRP:HE3	10	0.74	0.01	0.74
(1,159)	1:182:A:ILE:HD11	1:177:A:VAL:HA	10	0.73	0.11	0.7
(1,159)	1:182:A:ILE:HD12	1:177:A:VAL:HA	10	0.73	0.11	0.7
(1,159)	1:182:A:ILE:HD13	1:177:A:VAL:HA	10	0.73	0.11	0.7
(1,160)	1:182:B:ILE:HD11	1:177:B:VAL:HA	10	0.73	0.11	0.71
(1,160)	1:182:B:ILE:HD12	1:177:B:VAL:HA	10	0.73	0.11	0.71
(1,160)	1:182:B:ILE:HD13	1:177:B:VAL:HA	10	0.73	0.11	0.71
(1,2323)	1:204:A:LEU:HD12	1:200:A:VAL:HA	10	0.73	0.09	0.68
(1,2323)	1:204:A:LEU:HD11	1:200:A:VAL:HA	10	0.73	0.09	0.68
(1,2323)	1:204:A:LEU:HD13	1:200:A:VAL:HA	10	0.73	0.09	0.68
(1,2324)	1:204:B:LEU:HD12	1:200:B:VAL:HA	10	0.73	0.09	0.68
(1,2324)	1:204:B:LEU:HD11	1:200:B:VAL:HA	10	0.73	0.09	0.68
(1,2324)	1:204:B:LEU:HD13	1:200:B:VAL:HA	10	0.73	0.09	0.68

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB3	10	0.73	0.15	0.74
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB2	10	0.73	0.15	0.74
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB1	10	0.73	0.15	0.74
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB3	10	0.73	0.15	0.74
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB2	10	0.73	0.15	0.74
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB1	10	0.73	0.15	0.74
(1,2121)	1:182:A:ILE:HG22	1:182:A:ILE:HG13	10	0.73	0.01	0.73
(1,2121)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	10	0.73	0.01	0.73
(1,2121)	1:182:A:ILE:HG21	1:182:A:ILE:HG13	10	0.73	0.01	0.73
(1,2122)	1:182:B:ILE:HG22	1:182:B:ILE:HG13	10	0.73	0.01	0.73
(1,2122)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	10	0.73	0.01	0.73
(1,2122)	1:182:B:ILE:HG21	1:182:B:ILE:HG13	10	0.73	0.01	0.73
(1,1769)	1:175:A:LEU:H	1:175:A:LEU:HB3	10	0.73	0.1	0.68
(1,1770)	1:175:B:LEU:H	1:175:B:LEU:HB3	10	0.73	0.1	0.68
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE3	10	0.72	0.2	0.76
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE2	10	0.72	0.2	0.76
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE1	10	0.72	0.2	0.76
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE3	10	0.72	0.2	0.76
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE2	10	0.72	0.2	0.76
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE1	10	0.72	0.2	0.76
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB1	10	0.72	0.09	0.72
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB2	10	0.72	0.09	0.72
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB3	10	0.72	0.09	0.72
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB1	10	0.72	0.09	0.72
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB2	10	0.72	0.09	0.72
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB3	10	0.72	0.09	0.72
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD13	10	0.72	0.04	0.72
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD11	10	0.72	0.04	0.72
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD12	10	0.72	0.04	0.72
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD13	10	0.72	0.04	0.72
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD11	10	0.72	0.04	0.72
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD12	10	0.72	0.04	0.72
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG21	10	0.72	0.07	0.74
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG22	10	0.72	0.07	0.74
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG23	10	0.72	0.07	0.74
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG21	10	0.72	0.07	0.74
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG22	10	0.72	0.07	0.74
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG23	10	0.72	0.07	0.74
(1,2361)	1:196:A:ALA:H	1:194:A:GLN:HB3	10	0.71	0.05	0.71
(1,2362)	1:196:B:ALA:H	1:194:B:GLN:HB3	10	0.71	0.06	0.71
(1,2188)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	10	0.7	0.11	0.73
(1,2188)	1:193:B:ASP:H	1:192:B:ASN:HB2	10	0.7	0.11	0.73

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2187)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	10	0.7	0.11	0.72
(1,2187)	1:193:A:ASP:H	1:192:A:ASN:HB2	10	0.7	0.11	0.72
(1,106)	1:185:B:LEU:HD21	1:183:A:GLU:H	10	0.69	0.06	0.68
(1,106)	1:185:B:LEU:HD22	1:183:A:GLU:H	10	0.69	0.06	0.68
(1,106)	1:185:B:LEU:HD23	1:183:A:GLU:H	10	0.69	0.06	0.68
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG12	10	0.69	0.04	0.71
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG11	10	0.69	0.04	0.71
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG13	10	0.69	0.04	0.71
(1,105)	1:185:A:LEU:HD21	1:183:B:GLU:H	10	0.69	0.06	0.67
(1,105)	1:185:A:LEU:HD22	1:183:B:GLU:H	10	0.69	0.06	0.67
(1,105)	1:185:A:LEU:HD23	1:183:B:GLU:H	10	0.69	0.06	0.67
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG12	10	0.69	0.04	0.7
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG11	10	0.69	0.04	0.7
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG13	10	0.69	0.04	0.7
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD21	10	0.69	0.01	0.69
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD23	10	0.69	0.01	0.69
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD22	10	0.69	0.01	0.69
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD21	10	0.69	0.01	0.69
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD23	10	0.69	0.01	0.69
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD22	10	0.69	0.01	0.69
(1,193)	1:201:A:MET:HE3	1:182:A:ILE:HD13	10	0.68	0.65	0.44
(1,193)	1:201:A:MET:HE3	1:182:A:ILE:HD11	10	0.68	0.65	0.44
(1,193)	1:201:A:MET:HE2	1:182:A:ILE:HD11	10	0.68	0.65	0.44
(1,193)	1:201:A:MET:HE2	1:182:A:ILE:HD13	10	0.68	0.65	0.44
(1,193)	1:201:A:MET:HE1	1:182:A:ILE:HD13	10	0.68	0.65	0.44
(1,193)	1:201:A:MET:HE1	1:182:A:ILE:HD12	10	0.68	0.65	0.44
(1,194)	1:201:B:MET:HE3	1:182:B:ILE:HD13	10	0.68	0.65	0.44
(1,194)	1:201:B:MET:HE3	1:182:B:ILE:HD11	10	0.68	0.65	0.44
(1,194)	1:201:B:MET:HE2	1:182:B:ILE:HD11	10	0.68	0.65	0.44
(1,194)	1:201:B:MET:HE2	1:182:B:ILE:HD13	10	0.68	0.65	0.44
(1,194)	1:201:B:MET:HE1	1:182:B:ILE:HD13	10	0.68	0.65	0.44
(1,194)	1:201:B:MET:HE1	1:182:B:ILE:HD12	10	0.68	0.65	0.44
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG13	10	0.67	0.21	0.58
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG12	10	0.67	0.21	0.58
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG11	10	0.67	0.21	0.58
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG13	10	0.67	0.22	0.57
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG12	10	0.67	0.22	0.57
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG11	10	0.67	0.22	0.57
(1,2414)	1:192:B:ASN:HB2	1:191:B:GLU:HA	10	0.66	0.06	0.68
(1,2413)	1:192:A:ASN:HB2	1:191:A:GLU:HA	10	0.66	0.06	0.68
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG12	10	0.66	0.04	0.65
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG11	10	0.66	0.04	0.65

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG13	10	0.66	0.04	0.65
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG12	10	0.66	0.04	0.65
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG11	10	0.66	0.04	0.65
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG13	10	0.66	0.04	0.65
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD22	10	0.65	0.04	0.66
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD23	10	0.65	0.04	0.66
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD21	10	0.65	0.04	0.66
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD22	10	0.65	0.04	0.65
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD23	10	0.65	0.04	0.65
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD21	10	0.65	0.04	0.65
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD13	10	0.64	0.52	0.58
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD12	10	0.64	0.52	0.58
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD11	10	0.64	0.52	0.58
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD13	10	0.64	0.52	0.57
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD12	10	0.64	0.52	0.57
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD11	10	0.64	0.52	0.57
(1,1122)	1:184:B:ALA:HB2	1:182:B:ILE:H	10	0.64	0.04	0.64
(1,1122)	1:184:B:ALA:HB3	1:182:B:ILE:H	10	0.64	0.04	0.64
(1,1122)	1:184:B:ALA:HB1	1:182:B:ILE:H	10	0.64	0.04	0.64
(1,1121)	1:184:A:ALA:HB2	1:182:A:ILE:H	10	0.64	0.04	0.64
(1,1121)	1:184:A:ALA:HB3	1:182:A:ILE:H	10	0.64	0.04	0.64
(1,1121)	1:184:A:ALA:HB1	1:182:A:ILE:H	10	0.64	0.04	0.64
(1,2368)	1:185:B:LEU:HG	1:185:B:LEU:H	10	0.63	0.0	0.63
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD21	10	0.63	0.09	0.68
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD22	10	0.63	0.09	0.68
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD23	10	0.63	0.09	0.68
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD21	10	0.63	0.09	0.67
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD22	10	0.63	0.09	0.67
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD23	10	0.63	0.09	0.67
(1,2367)	1:185:A:LEU:HG	1:185:A:LEU:H	10	0.63	0.0	0.63
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG22	10	0.63	0.05	0.64
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG21	10	0.63	0.05	0.64
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG23	10	0.63	0.05	0.64
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG22	10	0.62	0.05	0.64
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG21	10	0.62	0.05	0.64
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG23	10	0.62	0.05	0.64
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG23	10	0.61	0.04	0.62
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG21	10	0.61	0.04	0.62
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG23	10	0.61	0.04	0.62
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG21	10	0.61	0.04	0.62
(1,2406)	1:179:B:TRP:HA	1:182:B:ILE:HG12	10	0.59	0.06	0.6
(1,2405)	1:179:A:TRP:HA	1:182:A:ILE:HG12	10	0.59	0.06	0.6

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB2	10	0.59	0.17	0.65
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB3	10	0.59	0.17	0.65
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB1	10	0.59	0.17	0.65
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD21	10	0.59	0.08	0.56
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD22	10	0.59	0.08	0.56
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD23	10	0.59	0.08	0.56
(1,2313)	1:182:A:ILE:HG22	1:182:A:ILE:HG13	10	0.59	0.01	0.59
(1,2313)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	10	0.59	0.01	0.59
(1,2313)	1:182:A:ILE:HG21	1:182:A:ILE:HG13	10	0.59	0.01	0.59
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG21	10	0.59	0.04	0.58
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG22	10	0.59	0.04	0.58
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG23	10	0.59	0.04	0.58
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD21	10	0.59	0.08	0.57
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD22	10	0.59	0.08	0.57
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD23	10	0.59	0.08	0.57
(1,2314)	1:182:B:ILE:HG22	1:182:B:ILE:HG13	10	0.59	0.01	0.58
(1,2314)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	10	0.59	0.01	0.58
(1,2314)	1:182:B:ILE:HG21	1:182:B:ILE:HG13	10	0.59	0.01	0.58
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG21	10	0.59	0.04	0.58
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG22	10	0.59	0.04	0.58
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG23	10	0.59	0.04	0.58
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB2	10	0.58	0.17	0.64
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB3	10	0.58	0.17	0.64
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB1	10	0.58	0.17	0.64
(1,2239)	1:187:A:LYS:HA	1:197:A:VAL:H	10	0.58	0.04	0.6
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD23	10	0.58	0.06	0.58
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD22	10	0.58	0.06	0.58
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD21	10	0.58	0.06	0.58
(1,2240)	1:187:B:LYS:HA	1:197:B:VAL:H	10	0.58	0.04	0.6
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB3	10	0.58	0.05	0.56
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB2	10	0.58	0.05	0.56
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB1	10	0.58	0.05	0.56
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD23	10	0.57	0.06	0.58
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD22	10	0.57	0.06	0.58
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD21	10	0.57	0.06	0.58
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD12	10	0.57	0.03	0.58
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD11	10	0.57	0.03	0.58
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD13	10	0.57	0.03	0.58
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB3	10	0.57	0.04	0.56
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB2	10	0.57	0.04	0.56
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB1	10	0.57	0.04	0.56
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD12	10	0.57	0.03	0.58

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD11	10	0.57	0.03	0.58
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD13	10	0.57	0.03	0.58
(1,971)	1:204:A:LEU:HD22	1:182:B:ILE:HD12	10	0.57	0.18	0.61
(1,971)	1:204:A:LEU:HD21	1:182:B:ILE:HD13	10	0.57	0.18	0.61
(1,971)	1:204:A:LEU:HD23	1:182:B:ILE:HD13	10	0.57	0.18	0.61
(1,971)	1:204:A:LEU:HD21	1:182:B:ILE:HD12	10	0.57	0.18	0.61
(1,971)	1:204:A:LEU:HD22	1:182:B:ILE:HD13	10	0.57	0.18	0.61
(1,971)	1:204:A:LEU:HD23	1:182:B:ILE:HD12	10	0.57	0.18	0.61
(1,971)	1:204:A:LEU:HD22	1:182:B:ILE:HD11	10	0.57	0.18	0.61
(1,2543)	1:185:A:LEU:H	1:185:B:LEU:HD23	10	0.57	0.07	0.56
(1,2543)	1:185:A:LEU:H	1:185:A:LEU:HD23	10	0.57	0.07	0.56
(1,2543)	1:185:A:LEU:H	1:185:B:LEU:HD22	10	0.57	0.07	0.56
(1,2544)	1:185:B:LEU:H	1:185:A:LEU:HD23	10	0.57	0.07	0.56
(1,2544)	1:185:B:LEU:H	1:185:B:LEU:HD23	10	0.57	0.07	0.56
(1,2544)	1:185:B:LEU:H	1:185:A:LEU:HD22	10	0.57	0.07	0.56
(1,972)	1:204:B:LEU:HD22	1:182:A:ILE:HD12	10	0.57	0.18	0.62
(1,972)	1:204:B:LEU:HD21	1:182:A:ILE:HD13	10	0.57	0.18	0.62
(1,972)	1:204:B:LEU:HD23	1:182:A:ILE:HD13	10	0.57	0.18	0.62
(1,972)	1:204:B:LEU:HD21	1:182:A:ILE:HD12	10	0.57	0.18	0.62
(1,972)	1:204:B:LEU:HD22	1:182:A:ILE:HD13	10	0.57	0.18	0.62
(1,972)	1:204:B:LEU:HD23	1:182:A:ILE:HD12	10	0.57	0.18	0.62
(1,972)	1:204:B:LEU:HD22	1:182:A:ILE:HD11	10	0.57	0.18	0.62
(1,2485)	1:180:A:ASP:H	1:183:A:GLU:HB3	10	0.57	0.2	0.57
(1,2485)	1:180:A:ASP:H	1:201:A:MET:HE2	10	0.57	0.2	0.57
(1,2485)	1:180:A:ASP:H	1:201:A:MET:HE1	10	0.57	0.2	0.57
(1,2486)	1:180:B:ASP:H	1:183:B:GLU:HB3	10	0.57	0.2	0.56
(1,2486)	1:180:B:ASP:H	1:201:B:MET:HE2	10	0.57	0.2	0.56
(1,2486)	1:180:B:ASP:H	1:201:B:MET:HE1	10	0.57	0.2	0.56
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD11	10	0.57	0.02	0.56
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD12	10	0.57	0.02	0.56
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD13	10	0.57	0.02	0.56
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD11	10	0.56	0.02	0.56
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD12	10	0.56	0.02	0.56
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD13	10	0.56	0.02	0.56
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD23	10	0.56	0.34	0.58
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD21	10	0.56	0.34	0.58
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD22	10	0.56	0.34	0.58
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD23	10	0.55	0.34	0.57
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD21	10	0.55	0.34	0.57
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD22	10	0.55	0.34	0.57
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG11	10	0.55	0.08	0.56
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG13	10	0.55	0.08	0.56

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG12	10	0.55	0.08	0.56
(1,2507)	1:176:A:THR:H	1:176:A:THR:HG21	10	0.55	0.08	0.56
(1,2227)	1:208:A:TRP:HA	1:179:A:TRP:HH2	10	0.55	0.12	0.53
(1,2227)	1:208:A:TRP:HA	1:212:A:LYS:H	10	0.55	0.12	0.53
(1,2228)	1:208:B:TRP:HA	1:179:B:TRP:HH2	10	0.55	0.12	0.53
(1,2228)	1:208:B:TRP:HA	1:212:B:LYS:H	10	0.55	0.12	0.53
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG11	10	0.55	0.07	0.55
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG13	10	0.55	0.07	0.55
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG12	10	0.55	0.07	0.55
(1,2508)	1:176:B:THR:H	1:176:B:THR:HG21	10	0.55	0.07	0.55
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD11	10	0.55	0.06	0.53
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD13	10	0.55	0.06	0.53
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD12	10	0.55	0.06	0.53
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD11	10	0.55	0.07	0.54
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD13	10	0.55	0.07	0.54
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD12	10	0.55	0.07	0.54
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD11	10	0.54	0.09	0.56
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD12	10	0.54	0.09	0.56
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD13	10	0.54	0.09	0.56
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD11	10	0.54	0.09	0.56
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD12	10	0.54	0.09	0.56
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD13	10	0.54	0.09	0.56
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB2	10	0.53	0.11	0.55
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB1	10	0.53	0.11	0.55
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB3	10	0.53	0.11	0.55
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB2	10	0.53	0.11	0.55
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB1	10	0.53	0.11	0.55
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB3	10	0.53	0.11	0.55
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD22	10	0.53	0.02	0.52
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD21	10	0.53	0.02	0.52
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD23	10	0.53	0.02	0.52
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD22	10	0.52	0.03	0.52
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD21	10	0.52	0.03	0.52
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD23	10	0.52	0.03	0.52
(1,1813)	1:192:A:ASN:H	1:191:A:GLU:HB3	10	0.52	0.02	0.53
(1,1814)	1:192:B:ASN:H	1:191:B:GLU:HB3	10	0.52	0.02	0.53
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB1	10	0.52	0.15	0.48
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB2	10	0.52	0.15	0.48
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB3	10	0.52	0.15	0.48
(1,2778)	1:193:B:ASP:H	1:197:B:VAL:HG22	10	0.52	0.15	0.48
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB1	10	0.52	0.15	0.48
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB2	10	0.52	0.15	0.48

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB3	10	0.52	0.15	0.48
(1,2777)	1:193:A:ASP:H	1:197:A:VAL:HG22	10	0.52	0.15	0.48
(1,1471)	1:208:A:TRP:HE1	1:208:A:TRP:HB2	10	0.52	0.01	0.52
(1,54)	1:195:B:ALA:HB2	1:199:B:GLN:H	10	0.52	0.07	0.53
(1,54)	1:195:B:ALA:HB1	1:199:B:GLN:H	10	0.52	0.07	0.53
(1,54)	1:195:B:ALA:HB3	1:199:B:GLN:H	10	0.52	0.07	0.53
(1,53)	1:195:A:ALA:HB2	1:199:A:GLN:H	10	0.52	0.07	0.53
(1,53)	1:195:A:ALA:HB1	1:199:A:GLN:H	10	0.52	0.07	0.53
(1,53)	1:195:A:ALA:HB3	1:199:A:GLN:H	10	0.52	0.07	0.53
(1,393)	1:176:A:THR:H	1:175:A:LEU:HB2	10	0.51	0.09	0.52
(1,1472)	1:208:B:TRP:HE1	1:208:B:TRP:HB2	10	0.51	0.01	0.52
(1,394)	1:176:B:THR:H	1:175:B:LEU:HB2	10	0.51	0.09	0.52
(1,2581)	1:179:A:TRP:HE1	1:204:B:LEU:HG	10	0.51	0.11	0.52
(1,2582)	1:179:B:TRP:HE1	1:204:A:LEU:HG	10	0.51	0.11	0.52
(1,2053)	1:199:A:GLN:H	1:199:A:GLN:HB3	10	0.5	0.01	0.5
(1,2054)	1:199:B:GLN:H	1:199:B:GLN:HB3	10	0.5	0.01	0.5
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD23	10	0.5	0.07	0.47
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD22	10	0.5	0.07	0.47
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD21	10	0.5	0.07	0.47
(1,2129)	1:185:A:LEU:HD23	1:185:A:LEU:HA	10	0.5	0.01	0.5
(1,2129)	1:185:A:LEU:HD21	1:185:A:LEU:HA	10	0.5	0.01	0.5
(1,2129)	1:185:A:LEU:HD22	1:185:A:LEU:HA	10	0.5	0.01	0.5
(1,2130)	1:185:B:LEU:HD23	1:185:B:LEU:HA	10	0.5	0.01	0.5
(1,2130)	1:185:B:LEU:HD21	1:185:B:LEU:HA	10	0.5	0.01	0.5
(1,2130)	1:185:B:LEU:HD22	1:185:B:LEU:HA	10	0.5	0.01	0.5
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD23	10	0.5	0.07	0.46
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD22	10	0.5	0.07	0.46
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD21	10	0.5	0.07	0.46
(1,2297)	1:200:A:VAL:HG12	1:197:A:VAL:HA	10	0.5	0.07	0.48
(1,2297)	1:200:A:VAL:HG11	1:197:A:VAL:HA	10	0.5	0.07	0.48
(1,2297)	1:200:A:VAL:HG13	1:197:A:VAL:HA	10	0.5	0.07	0.48
(1,2297)	1:197:A:VAL:HA	1:186:A:LEU:HB2	10	0.5	0.07	0.48
(1,2298)	1:200:B:VAL:HG12	1:197:B:VAL:HA	10	0.5	0.07	0.48
(1,2298)	1:200:B:VAL:HG11	1:197:B:VAL:HA	10	0.5	0.07	0.48
(1,2298)	1:200:B:VAL:HG13	1:197:B:VAL:HA	10	0.5	0.07	0.48
(1,2298)	1:197:B:VAL:HA	1:186:B:LEU:HB2	10	0.5	0.07	0.48
(1,122)	1:199:B:GLN:H	1:198:B:ARG:HG2	10	0.5	0.04	0.51
(1,121)	1:199:A:GLN:H	1:198:A:ARG:HG2	10	0.5	0.03	0.5
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD11	10	0.49	0.06	0.51
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD12	10	0.49	0.06	0.51
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD13	10	0.49	0.06	0.51
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD11	10	0.49	0.06	0.51

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD12	10	0.49	0.06	0.51
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD13	10	0.49	0.06	0.51
(1,2128)	1:185:B:LEU:HD11	1:178:A:PRO:HB2	10	0.49	0.08	0.48
(1,2128)	1:185:B:LEU:HD13	1:178:A:PRO:HB2	10	0.49	0.08	0.48
(1,2128)	1:185:B:LEU:HD12	1:178:A:PRO:HB2	10	0.49	0.08	0.48
(1,2128)	1:185:B:LEU:HD13	1:189:B:ASN:HB2	10	0.49	0.08	0.48
(1,2128)	1:185:B:LEU:HD12	1:189:B:ASN:HB2	10	0.49	0.08	0.48
(1,51)	1:195:A:ALA:HB3	1:194:A:GLN:H	10	0.48	0.05	0.48
(1,51)	1:195:A:ALA:HB2	1:194:A:GLN:H	10	0.48	0.05	0.48
(1,51)	1:195:A:ALA:HB1	1:194:A:GLN:H	10	0.48	0.05	0.48
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG23	10	0.48	0.14	0.48
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG22	10	0.48	0.14	0.48
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG21	10	0.48	0.14	0.48
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG23	10	0.48	0.15	0.48
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG22	10	0.48	0.15	0.48
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG21	10	0.48	0.15	0.48
(1,2127)	1:185:A:LEU:HD11	1:178:B:PRO:HB2	10	0.48	0.09	0.49
(1,2127)	1:185:A:LEU:HD13	1:178:B:PRO:HB2	10	0.48	0.09	0.49
(1,2127)	1:185:A:LEU:HD12	1:178:B:PRO:HB2	10	0.48	0.09	0.49
(1,2127)	1:185:A:LEU:HD13	1:189:A:ASN:HB2	10	0.48	0.09	0.49
(1,2127)	1:185:A:LEU:HD12	1:189:A:ASN:HB2	10	0.48	0.09	0.49
(1,52)	1:195:B:ALA:HB3	1:194:B:GLN:H	10	0.48	0.05	0.48
(1,52)	1:195:B:ALA:HB2	1:194:B:GLN:H	10	0.48	0.05	0.48
(1,52)	1:195:B:ALA:HB1	1:194:B:GLN:H	10	0.48	0.05	0.48
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG13	10	0.47	0.12	0.46
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG12	10	0.47	0.12	0.46
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG11	10	0.47	0.12	0.46
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG13	10	0.47	0.12	0.47
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG12	10	0.47	0.12	0.47
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG11	10	0.47	0.12	0.47
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD13	10	0.47	0.04	0.46
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD11	10	0.47	0.04	0.46
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD12	10	0.47	0.04	0.46
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD13	10	0.46	0.05	0.46
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD11	10	0.46	0.05	0.46
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD12	10	0.46	0.05	0.46
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD21	10	0.46	0.15	0.52
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD22	10	0.46	0.15	0.52
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD13	10	0.46	0.15	0.52
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG21	10	0.46	0.03	0.46
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG22	10	0.46	0.03	0.46
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG23	10	0.46	0.03	0.46

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG21	10	0.46	0.03	0.46
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG22	10	0.46	0.03	0.46
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG23	10	0.46	0.03	0.46
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD11	10	0.46	0.07	0.46
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD13	10	0.46	0.07	0.46
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD12	10	0.46	0.07	0.46
(1,2740)	1:196:B:ALA:H	1:197:B:VAL:HB	10	0.46	0.04	0.48
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG12	10	0.46	0.04	0.46
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG11	10	0.46	0.04	0.46
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG13	10	0.46	0.04	0.46
(1,2739)	1:196:A:ALA:H	1:197:A:VAL:HB	10	0.46	0.04	0.46
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG12	10	0.46	0.04	0.46
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG11	10	0.46	0.04	0.46
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG13	10	0.46	0.04	0.46
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD11	10	0.46	0.07	0.45
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD13	10	0.46	0.07	0.45
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD12	10	0.46	0.07	0.45
(1,2561)	1:209:A:SER:H	1:206:A:LYS:HG3	10	0.46	0.08	0.48
(1,2561)	1:209:A:SER:H	1:211:A:ALA:HB1	10	0.46	0.08	0.48
(1,2562)	1:209:B:SER:H	1:206:B:LYS:HG3	10	0.45	0.08	0.48
(1,2562)	1:209:B:SER:H	1:211:B:ALA:HB1	10	0.45	0.08	0.48
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD21	10	0.45	0.15	0.5
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD22	10	0.45	0.15	0.5
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD13	10	0.45	0.15	0.5
(1,296)	1:185:B:LEU:HD22	1:182:A:ILE:HD11	10	0.45	0.05	0.46
(1,296)	1:185:B:LEU:HD22	1:182:A:ILE:HD12	10	0.45	0.05	0.46
(1,296)	1:185:B:LEU:HD23	1:182:A:ILE:HD11	10	0.45	0.05	0.46
(1,296)	1:185:B:LEU:HD23	1:182:A:ILE:HD12	10	0.45	0.05	0.46
(1,296)	1:185:B:LEU:HD22	1:182:A:ILE:HD13	10	0.45	0.05	0.46
(1,296)	1:185:B:LEU:HD21	1:182:A:ILE:HD11	10	0.45	0.05	0.46
(1,2126)	1:186:B:LEU:HD11	1:178:A:PRO:HG2	10	0.45	0.09	0.44
(1,2126)	1:186:B:LEU:HD13	1:178:A:PRO:HG2	10	0.45	0.09	0.44
(1,2126)	1:186:B:LEU:HD12	1:178:A:PRO:HG2	10	0.45	0.09	0.44
(1,2125)	1:186:A:LEU:HD11	1:178:B:PRO:HG2	10	0.45	0.09	0.45
(1,2125)	1:186:A:LEU:HD13	1:178:B:PRO:HG2	10	0.45	0.09	0.45
(1,2125)	1:186:A:LEU:HD12	1:178:B:PRO:HG2	10	0.45	0.09	0.45
(1,295)	1:185:A:LEU:HD22	1:182:B:ILE:HD11	10	0.45	0.06	0.45
(1,295)	1:185:A:LEU:HD22	1:182:B:ILE:HD12	10	0.45	0.06	0.45
(1,295)	1:185:A:LEU:HD23	1:182:B:ILE:HD11	10	0.45	0.06	0.45
(1,295)	1:185:A:LEU:HD23	1:182:B:ILE:HD12	10	0.45	0.06	0.45
(1,295)	1:185:A:LEU:HD22	1:182:B:ILE:HD13	10	0.45	0.06	0.45
(1,295)	1:185:A:LEU:HD21	1:182:B:ILE:HD11	10	0.45	0.06	0.45

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG21	10	0.45	0.01	0.45
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG22	10	0.45	0.01	0.45
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG21	10	0.45	0.0	0.45
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG22	10	0.45	0.0	0.45
(1,261)	1:175:A:LEU:HD13	1:199:B:GLN:HG3	10	0.45	0.11	0.5
(1,261)	1:175:A:LEU:HD11	1:199:B:GLN:HG3	10	0.45	0.11	0.5
(1,261)	1:175:A:LEU:HD12	1:199:B:GLN:HG3	10	0.45	0.11	0.5
(1,262)	1:175:B:LEU:HD13	1:199:A:GLN:HG3	10	0.44	0.12	0.48
(1,262)	1:175:B:LEU:HD11	1:199:A:GLN:HG3	10	0.44	0.12	0.48
(1,262)	1:175:B:LEU:HD12	1:199:A:GLN:HG3	10	0.44	0.12	0.48
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD22	10	0.44	0.0	0.44
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD21	10	0.44	0.0	0.44
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD23	10	0.44	0.0	0.44
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD22	10	0.44	0.0	0.44
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD21	10	0.44	0.0	0.44
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD23	10	0.44	0.0	0.44
(1,347)	1:202:A:GLU:H	1:202:A:GLU:HG2	10	0.44	0.05	0.43
(1,348)	1:202:B:GLU:H	1:202:B:GLU:HG2	10	0.44	0.05	0.42
(1,2166)	1:189:B:ASN:HB3	1:185:B:LEU:HG	10	0.43	0.06	0.44
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD11	10	0.43	0.11	0.45
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD13	10	0.43	0.11	0.45
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD12	10	0.43	0.11	0.45
(1,352)	1:203:B:ARG:H	1:202:B:GLU:HG2	10	0.43	0.02	0.42
(1,110)	1:210:B:LEU:HD11	1:212:A:LYS:H	10	0.43	0.09	0.44
(1,110)	1:210:B:LEU:HD12	1:212:A:LYS:H	10	0.43	0.09	0.44
(1,110)	1:210:B:LEU:HD13	1:212:A:LYS:H	10	0.43	0.09	0.44
(1,351)	1:203:A:ARG:H	1:202:A:GLU:HG2	10	0.43	0.02	0.42
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD11	10	0.43	0.11	0.46
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD13	10	0.43	0.11	0.46
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD12	10	0.43	0.11	0.46
(1,2165)	1:189:A:ASN:HB3	1:185:A:LEU:HG	10	0.43	0.06	0.43
(1,109)	1:210:A:LEU:HD11	1:212:B:LYS:H	10	0.42	0.09	0.44
(1,109)	1:210:A:LEU:HD12	1:212:B:LYS:H	10	0.42	0.09	0.44
(1,109)	1:210:A:LEU:HD13	1:212:B:LYS:H	10	0.42	0.09	0.44
(1,832)	1:182:B:ILE:HG22	1:179:B:TRP:HA	10	0.42	0.1	0.43
(1,832)	1:182:B:ILE:HG23	1:179:B:TRP:HA	10	0.42	0.1	0.43
(1,832)	1:182:B:ILE:HG21	1:179:B:TRP:HA	10	0.42	0.1	0.43
(1,831)	1:182:A:ILE:HG22	1:179:A:TRP:HA	10	0.42	0.1	0.42
(1,831)	1:182:A:ILE:HG23	1:179:A:TRP:HA	10	0.42	0.1	0.42
(1,831)	1:182:A:ILE:HG21	1:179:A:TRP:HA	10	0.42	0.1	0.42
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG11	10	0.42	0.12	0.4
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG13	10	0.42	0.12	0.4

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG12	10	0.42	0.12	0.4
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG11	10	0.42	0.12	0.4
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG13	10	0.42	0.12	0.4
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG12	10	0.42	0.12	0.4
(1,2231)	1:187:A:LYS:H	1:197:A:VAL:HA	10	0.42	0.06	0.42
(1,398)	1:175:B:LEU:HB2	1:190:A:PHE:HZ	10	0.42	0.18	0.44
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG21	10	0.42	0.06	0.4
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG22	10	0.42	0.06	0.4
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG23	10	0.42	0.06	0.4
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG21	10	0.42	0.06	0.4
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG22	10	0.42	0.06	0.4
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG23	10	0.42	0.06	0.4
(1,2232)	1:187:B:LYS:H	1:197:B:VAL:HA	10	0.42	0.06	0.42
(1,2473)	1:190:A:PHE:H	1:193:A:ASP:H	10	0.42	0.15	0.36
(1,2473)	1:197:A:VAL:H	1:190:A:PHE:H	10	0.42	0.15	0.36
(1,2474)	1:190:B:PHE:H	1:193:B:ASP:H	10	0.42	0.15	0.36
(1,2474)	1:197:B:VAL:H	1:190:B:PHE:H	10	0.42	0.15	0.36
(1,2407)	1:197:A:VAL:HA	1:194:A:GLN:HA	10	0.42	0.04	0.43
(1,2407)	1:197:A:VAL:HA	1:196:A:ALA:HA	10	0.42	0.04	0.43
(1,2408)	1:197:B:VAL:HA	1:194:B:GLN:HA	10	0.42	0.04	0.43
(1,2408)	1:197:B:VAL:HA	1:196:B:ALA:HA	10	0.42	0.04	0.43
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD11	10	0.41	0.05	0.42
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD12	10	0.41	0.05	0.42
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD13	10	0.41	0.05	0.42
(1,2416)	1:189:B:ASN:HA	1:186:B:LEU:HA	10	0.41	0.07	0.38
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD11	10	0.41	0.05	0.42
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD12	10	0.41	0.05	0.42
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD13	10	0.41	0.05	0.42
(1,2415)	1:189:A:ASN:HA	1:186:A:LEU:HA	10	0.41	0.07	0.38
(1,179)	1:196:A:ALA:HB1	1:197:A:VAL:HA	10	0.41	0.04	0.42
(1,179)	1:196:A:ALA:HB2	1:197:A:VAL:HA	10	0.41	0.04	0.42
(1,179)	1:196:A:ALA:HB3	1:197:A:VAL:HA	10	0.41	0.04	0.42
(1,180)	1:196:B:ALA:HB1	1:197:B:VAL:HA	10	0.41	0.04	0.42
(1,180)	1:196:B:ALA:HB2	1:197:B:VAL:HA	10	0.41	0.04	0.42
(1,180)	1:196:B:ALA:HB3	1:197:B:VAL:HA	10	0.41	0.04	0.42
(1,2372)	1:186:B:LEU:HD13	1:177:A:VAL:H	10	0.4	0.09	0.41
(1,2372)	1:186:B:LEU:HD12	1:177:A:VAL:H	10	0.4	0.09	0.41
(1,2372)	1:186:B:LEU:HD11	1:177:A:VAL:H	10	0.4	0.09	0.41
(1,2093)	1:185:A:LEU:HD21	1:181:B:ASP:H	10	0.4	0.05	0.4
(1,2093)	1:185:A:LEU:HD22	1:181:B:ASP:H	10	0.4	0.05	0.4
(1,2093)	1:185:A:LEU:HD23	1:181:B:ASP:H	10	0.4	0.05	0.4
(1,2094)	1:185:B:LEU:HD21	1:181:A:ASP:H	10	0.4	0.05	0.4

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2094)	1:185:B:LEU:HD22	1:181:A:ASP:H	10	0.4	0.05	0.4
(1,2094)	1:185:B:LEU:HD23	1:181:A:ASP:H	10	0.4	0.05	0.4
(1,2333)	1:208:A:TRP:HB2	1:208:A:TRP:HD1	10	0.4	0.01	0.4
(1,2334)	1:208:B:TRP:HB2	1:208:B:TRP:HD1	10	0.4	0.01	0.4
(1,2371)	1:186:A:LEU:HD13	1:177:B:VAL:H	10	0.4	0.08	0.42
(1,2371)	1:186:A:LEU:HD12	1:177:B:VAL:H	10	0.4	0.08	0.42
(1,2371)	1:186:A:LEU:HD11	1:177:B:VAL:H	10	0.4	0.08	0.42
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD13	10	0.38	0.04	0.38
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD12	10	0.38	0.04	0.38
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD11	10	0.38	0.04	0.38
(1,2445)	1:187:A:LYS:H	1:187:A:LYS:HG2	10	0.38	0.02	0.38
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD13	10	0.38	0.04	0.38
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD12	10	0.38	0.04	0.38
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD11	10	0.38	0.04	0.38
(1,2446)	1:187:B:LYS:H	1:187:B:LYS:HG2	10	0.38	0.02	0.39
(1,2685)	1:203:A:ARG:H	1:203:A:ARG:HG3	10	0.37	0.09	0.4
(1,2686)	1:203:B:ARG:H	1:203:B:ARG:HG3	10	0.37	0.09	0.4
(1,2075)	1:210:A:LEU:HD11	1:211:B:ALA:H	10	0.37	0.07	0.39
(1,2075)	1:210:A:LEU:HD12	1:211:B:ALA:H	10	0.37	0.07	0.39
(1,2075)	1:210:A:LEU:HD13	1:211:B:ALA:H	10	0.37	0.07	0.39
(1,2076)	1:210:B:LEU:HD11	1:211:A:ALA:H	10	0.37	0.06	0.39
(1,2076)	1:210:B:LEU:HD12	1:211:A:ALA:H	10	0.37	0.06	0.39
(1,2076)	1:210:B:LEU:HD13	1:211:A:ALA:H	10	0.37	0.06	0.39
(1,841)	1:177:A:VAL:HG13	1:178:A:PRO:HD3	10	0.37	0.02	0.37
(1,841)	1:177:A:VAL:HG12	1:178:A:PRO:HD3	10	0.37	0.02	0.37
(1,842)	1:177:B:VAL:HG13	1:178:B:PRO:HD3	10	0.37	0.02	0.37
(1,842)	1:177:B:VAL:HG12	1:178:B:PRO:HD3	10	0.37	0.02	0.37
(1,1737)	1:195:A:ALA:H	1:194:A:GLN:HB3	10	0.36	0.15	0.3
(1,1738)	1:195:B:ALA:H	1:194:B:GLN:HB3	10	0.36	0.15	0.29
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD23	10	0.36	0.06	0.36
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD21	10	0.36	0.06	0.36
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD22	10	0.36	0.06	0.36
(1,777)	1:206:A:LYS:HA	1:206:A:LYS:HB3	10	0.36	0.0	0.36
(1,778)	1:206:B:LYS:HA	1:206:B:LYS:HB3	10	0.36	0.0	0.36
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD23	10	0.36	0.07	0.36
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD21	10	0.36	0.07	0.36
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD22	10	0.36	0.07	0.36
(1,2623)	1:206:A:LYS:H	1:206:A:LYS:HG3	10	0.36	0.01	0.36
(1,2624)	1:206:B:LYS:H	1:206:B:LYS:HG3	10	0.36	0.01	0.36
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG11	10	0.35	0.08	0.34
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG13	10	0.35	0.08	0.34
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG12	10	0.35	0.08	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG11	10	0.35	0.08	0.34
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG13	10	0.35	0.08	0.34
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG12	10	0.35	0.08	0.34
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG21	10	0.35	0.06	0.36
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG23	10	0.35	0.06	0.36
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG22	10	0.35	0.06	0.36
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG21	10	0.35	0.06	0.36
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG23	10	0.35	0.06	0.36
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG22	10	0.35	0.06	0.36
(1,407)	1:185:A:LEU:HB2	1:186:A:LEU:H	10	0.35	0.02	0.34
(1,860)	1:200:B:VAL:HA	1:175:A:LEU:HB3	10	0.35	0.28	0.22
(1,408)	1:185:B:LEU:HB2	1:186:B:LEU:H	10	0.35	0.02	0.34
(1,859)	1:200:A:VAL:HA	1:175:B:LEU:HB3	10	0.34	0.28	0.2
(1,1793)	1:193:A:ASP:H	1:188:A:ASN:HA	10	0.34	0.15	0.32
(1,1794)	1:193:B:ASP:H	1:188:B:ASN:HA	10	0.34	0.14	0.32
(1,2281)	1:202:A:GLU:HB2	1:199:A:GLN:HA	10	0.33	0.08	0.31
(1,2281)	1:199:A:GLN:HA	1:199:A:GLN:HB2	10	0.33	0.08	0.31
(1,2282)	1:202:B:GLU:HB2	1:199:B:GLN:HA	10	0.33	0.08	0.3
(1,2282)	1:199:B:GLN:HA	1:199:B:GLN:HB2	10	0.33	0.08	0.3
(1,2555)	1:209:A:SER:H	1:204:A:LEU:HA	10	0.33	0.05	0.32
(1,2556)	1:209:B:SER:H	1:204:B:LEU:HA	10	0.33	0.04	0.32
(1,1336)	1:188:B:ASN:H	1:187:B:LYS:HG3	10	0.33	0.06	0.32
(1,521)	1:190:A:PHE:H	1:191:A:GLU:HA	10	0.33	0.05	0.32
(1,522)	1:190:B:PHE:H	1:191:B:GLU:HA	10	0.33	0.06	0.32
(1,905)	1:186:A:LEU:HD22	1:186:A:LEU:HB3	10	0.32	0.01	0.32
(1,905)	1:186:A:LEU:HD21	1:186:A:LEU:HB3	10	0.32	0.01	0.32
(1,905)	1:186:A:LEU:HD23	1:186:A:LEU:HB3	10	0.32	0.01	0.32
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG11	10	0.32	0.02	0.32
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG13	10	0.32	0.02	0.32
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG11	10	0.32	0.03	0.32
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG13	10	0.32	0.03	0.32
(1,906)	1:186:B:LEU:HD22	1:186:B:LEU:HB3	10	0.32	0.01	0.32
(1,906)	1:186:B:LEU:HD21	1:186:B:LEU:HB3	10	0.32	0.01	0.32
(1,906)	1:186:B:LEU:HD23	1:186:B:LEU:HB3	10	0.32	0.01	0.32
(1,1335)	1:188:A:ASN:H	1:187:A:LYS:HG3	10	0.32	0.06	0.32
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD23	10	0.32	0.11	0.3
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD22	10	0.32	0.11	0.3
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD21	10	0.32	0.11	0.3
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD23	10	0.32	0.11	0.3
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD22	10	0.32	0.11	0.3
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD21	10	0.32	0.11	0.3
(1,2179)	1:186:A:LEU:HB2	1:190:A:PHE:HD2	10	0.32	0.02	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,959)	1:200:A:VAL:HG11	1:200:A:VAL:HG23	10	0.32	0.02	0.33
(1,959)	1:200:A:VAL:HG11	1:200:A:VAL:HG21	10	0.32	0.02	0.33
(1,959)	1:200:A:VAL:HG13	1:200:A:VAL:HG23	10	0.32	0.02	0.33
(1,959)	1:200:A:VAL:HG12	1:200:A:VAL:HG23	10	0.32	0.02	0.33
(1,959)	1:200:A:VAL:HG12	1:200:A:VAL:HG21	10	0.32	0.02	0.33
(1,960)	1:200:B:VAL:HG11	1:200:B:VAL:HG23	10	0.32	0.02	0.33
(1,960)	1:200:B:VAL:HG11	1:200:B:VAL:HG21	10	0.32	0.02	0.33
(1,960)	1:200:B:VAL:HG13	1:200:B:VAL:HG23	10	0.32	0.02	0.33
(1,960)	1:200:B:VAL:HG12	1:200:B:VAL:HG23	10	0.32	0.02	0.33
(1,960)	1:200:B:VAL:HG12	1:200:B:VAL:HG21	10	0.32	0.02	0.33
(1,2180)	1:186:B:LEU:HB2	1:190:B:PHE:HD2	10	0.32	0.02	0.32
(1,1455)	1:209:A:SER:H	1:208:A:TRP:HB2	10	0.32	0.03	0.31
(1,1456)	1:209:B:SER:H	1:208:B:TRP:HB2	10	0.31	0.03	0.31
(1,1071)	1:175:A:LEU:HD11	1:201:B:MET:H	10	0.31	0.19	0.26
(1,1071)	1:175:A:LEU:HD12	1:201:B:MET:H	10	0.31	0.19	0.26
(1,1071)	1:175:A:LEU:HD13	1:201:B:MET:H	10	0.31	0.19	0.26
(1,1072)	1:175:B:LEU:HD11	1:201:A:MET:H	10	0.31	0.2	0.24
(1,1072)	1:175:B:LEU:HD12	1:201:A:MET:H	10	0.31	0.2	0.24
(1,1072)	1:175:B:LEU:HD13	1:201:A:MET:H	10	0.31	0.2	0.24
(1,1173)	1:203:A:ARG:HA	1:203:A:ARG:HD3	10	0.31	0.03	0.32
(1,1174)	1:203:B:ARG:HA	1:203:B:ARG:HD3	10	0.3	0.03	0.31
(1,2395)	1:207:A:GLY:HA3	1:206:A:LYS:HG2	10	0.3	0.1	0.28
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG12	10	0.3	0.05	0.3
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG11	10	0.3	0.05	0.3
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG13	10	0.3	0.05	0.3
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG12	10	0.3	0.05	0.3
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG11	10	0.3	0.05	0.3
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG13	10	0.3	0.05	0.3
(1,2396)	1:207:B:GLY:HA3	1:206:B:LYS:HG2	10	0.29	0.09	0.27
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG21	10	0.29	0.05	0.29
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG22	10	0.29	0.05	0.29
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG21	10	0.29	0.05	0.29
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG22	10	0.29	0.05	0.29
(1,882)	1:192:B:ASN:HB3	1:191:B:GLU:HA	10	0.29	0.06	0.27
(1,881)	1:192:A:ASN:HB3	1:191:A:GLU:HA	10	0.29	0.06	0.27
(1,2687)	1:202:A:GLU:H	1:197:A:VAL:HA	10	0.29	0.05	0.29
(1,2688)	1:202:B:GLU:H	1:197:B:VAL:HA	10	0.29	0.05	0.29
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB2	10	0.29	0.03	0.3
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB3	10	0.29	0.03	0.3
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB1	10	0.29	0.03	0.3
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB2	10	0.29	0.02	0.29
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB3	10	0.29	0.02	0.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB1	10	0.29	0.02	0.29
(1,619)	1:200:A:VAL:HA	1:199:A:GLN:H	10	0.29	0.02	0.28
(1,620)	1:200:B:VAL:HA	1:199:B:GLN:H	10	0.28	0.02	0.29
(1,2101)	1:204:A:LEU:HD11	1:179:A:TRP:HZ3	10	0.28	0.17	0.22
(1,2101)	1:204:A:LEU:HD13	1:179:A:TRP:HZ3	10	0.28	0.17	0.22
(1,2101)	1:204:A:LEU:HD12	1:179:A:TRP:HZ3	10	0.28	0.17	0.22
(1,2102)	1:204:B:LEU:HD11	1:179:B:TRP:HZ3	10	0.28	0.17	0.22
(1,2102)	1:204:B:LEU:HD13	1:179:B:TRP:HZ3	10	0.28	0.17	0.22
(1,2102)	1:204:B:LEU:HD12	1:179:B:TRP:HZ3	10	0.28	0.17	0.22
(1,755)	1:185:A:LEU:HB3	1:185:A:LEU:HA	10	0.28	0.0	0.28
(1,756)	1:185:B:LEU:HB3	1:185:B:LEU:HA	10	0.28	0.0	0.28
(1,2366)	1:189:B:ASN:H	1:185:B:LEU:HG	10	0.28	0.03	0.28
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG23	10	0.28	0.08	0.26
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG22	10	0.28	0.08	0.26
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG21	10	0.28	0.08	0.26
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG23	10	0.27	0.07	0.26
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG22	10	0.27	0.07	0.26
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG21	10	0.27	0.07	0.26
(1,2365)	1:189:A:ASN:H	1:185:A:LEU:HG	10	0.27	0.03	0.28
(1,225)	1:177:A:VAL:HG21	1:200:B:VAL:HG11	10	0.27	0.09	0.3
(1,225)	1:177:A:VAL:HG23	1:200:B:VAL:HG13	10	0.27	0.09	0.3
(1,225)	1:177:A:VAL:HG21	1:200:B:VAL:HG13	10	0.27	0.09	0.3
(1,225)	1:177:A:VAL:HG22	1:200:B:VAL:HG12	10	0.27	0.09	0.3
(1,225)	1:177:A:VAL:HG22	1:200:B:VAL:HG11	10	0.27	0.09	0.3
(1,225)	1:177:A:VAL:HG21	1:200:B:VAL:HG12	10	0.27	0.09	0.3
(1,226)	1:177:B:VAL:HG21	1:200:A:VAL:HG11	10	0.27	0.08	0.28
(1,226)	1:177:B:VAL:HG23	1:200:A:VAL:HG13	10	0.27	0.08	0.28
(1,226)	1:177:B:VAL:HG21	1:200:A:VAL:HG13	10	0.27	0.08	0.28
(1,226)	1:177:B:VAL:HG22	1:200:A:VAL:HG12	10	0.27	0.08	0.28
(1,226)	1:177:B:VAL:HG22	1:200:A:VAL:HG11	10	0.27	0.08	0.28
(1,226)	1:177:B:VAL:HG21	1:200:A:VAL:HG12	10	0.27	0.08	0.28
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG21	10	0.26	0.03	0.27
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG22	10	0.26	0.03	0.27
(1,78)	1:200:B:VAL:HG13	1:208:A:TRP:HZ3	10	0.26	0.06	0.25
(1,78)	1:200:B:VAL:HG12	1:208:A:TRP:HZ3	10	0.26	0.06	0.25
(1,78)	1:200:B:VAL:HG11	1:208:A:TRP:HZ3	10	0.26	0.06	0.25
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG21	10	0.26	0.03	0.27
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG22	10	0.26	0.03	0.27
(1,697)	1:184:A:ALA:HA	1:183:A:GLU:HB3	10	0.26	0.05	0.28
(1,698)	1:184:B:ALA:HA	1:183:B:GLU:HB3	10	0.26	0.05	0.28
(1,77)	1:200:A:VAL:HG13	1:208:B:TRP:HZ3	10	0.26	0.06	0.24
(1,77)	1:200:A:VAL:HG12	1:208:B:TRP:HZ3	10	0.26	0.06	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,77)	1:200:A:VAL:HG11	1:208:B:TRP:HZ3	10	0.26	0.06	0.24
(1,2673)	1:202:A:GLU:H	1:179:A:TRP:HE3	10	0.26	0.13	0.24
(1,2674)	1:202:B:GLU:H	1:179:B:TRP:HE3	10	0.26	0.14	0.23
(1,234)	1:200:B:VAL:HG11	1:177:A:VAL:HG21	10	0.26	0.09	0.28
(1,234)	1:200:B:VAL:HG13	1:177:A:VAL:HG23	10	0.26	0.09	0.28
(1,234)	1:200:B:VAL:HG13	1:177:A:VAL:HG21	10	0.26	0.09	0.28
(1,234)	1:200:B:VAL:HG12	1:177:A:VAL:HG22	10	0.26	0.09	0.28
(1,234)	1:200:B:VAL:HG11	1:177:A:VAL:HG22	10	0.26	0.09	0.28
(1,234)	1:200:B:VAL:HG12	1:177:A:VAL:HG21	10	0.26	0.09	0.28
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD21	10	0.25	0.04	0.26
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD22	10	0.25	0.04	0.26
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD23	10	0.25	0.04	0.26
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB3	10	0.25	0.03	0.24
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB2	10	0.25	0.03	0.24
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB1	10	0.25	0.03	0.24
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB3	10	0.25	0.04	0.24
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB2	10	0.25	0.04	0.24
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB1	10	0.25	0.04	0.24
(1,2172)	1:210:B:LEU:H	1:210:B:LEU:HB3	10	0.25	0.0	0.25
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD21	10	0.25	0.02	0.25
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD23	10	0.25	0.02	0.25
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD22	10	0.25	0.02	0.25
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD21	10	0.25	0.02	0.25
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD23	10	0.25	0.02	0.25
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD22	10	0.25	0.02	0.25
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD21	10	0.25	0.05	0.25
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD22	10	0.25	0.05	0.25
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD23	10	0.25	0.05	0.25
(1,233)	1:200:A:VAL:HG11	1:177:B:VAL:HG21	10	0.25	0.09	0.26
(1,233)	1:200:A:VAL:HG13	1:177:B:VAL:HG23	10	0.25	0.09	0.26
(1,233)	1:200:A:VAL:HG13	1:177:B:VAL:HG21	10	0.25	0.09	0.26
(1,233)	1:200:A:VAL:HG12	1:177:B:VAL:HG22	10	0.25	0.09	0.26
(1,233)	1:200:A:VAL:HG11	1:177:B:VAL:HG22	10	0.25	0.09	0.26
(1,233)	1:200:A:VAL:HG12	1:177:B:VAL:HG21	10	0.25	0.09	0.26
(1,2171)	1:210:A:LEU:H	1:210:A:LEU:HB3	10	0.25	0.0	0.25
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG11	10	0.24	0.06	0.24
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG13	10	0.24	0.06	0.24
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG11	10	0.24	0.06	0.24
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG13	10	0.24	0.06	0.24
(1,2487)	1:180:A:ASP:H	1:178:A:PRO:HG2	10	0.24	0.08	0.2
(1,2789)	1:189:A:ASN:H	1:191:A:GLU:HA	10	0.24	0.12	0.2
(1,2488)	1:180:B:ASP:H	1:178:B:PRO:HG2	10	0.24	0.08	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2790)	1:189:B:ASN:H	1:191:B:GLU:HA	10	0.24	0.12	0.19
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG12	10	0.23	0.03	0.24
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG11	10	0.23	0.03	0.24
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG13	10	0.23	0.03	0.24
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD23	10	0.23	0.07	0.22
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD21	10	0.23	0.07	0.22
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD22	10	0.23	0.07	0.22
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG12	10	0.23	0.03	0.24
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG11	10	0.23	0.03	0.24
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG13	10	0.23	0.03	0.24
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD23	10	0.22	0.07	0.21
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD21	10	0.22	0.07	0.21
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD22	10	0.22	0.07	0.21
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD12	10	0.22	0.03	0.23
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD11	10	0.22	0.03	0.23
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD13	10	0.22	0.03	0.23
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD12	10	0.22	0.04	0.23
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD11	10	0.22	0.04	0.23
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD13	10	0.22	0.04	0.23
(1,2589)	1:208:A:TRP:H	1:203:B:ARG:HG2	10	0.22	0.05	0.2
(1,2589)	1:208:A:TRP:H	1:206:A:LYS:HG2	10	0.22	0.05	0.2
(1,2590)	1:208:B:TRP:H	1:203:A:ARG:HG2	10	0.22	0.05	0.2
(1,2590)	1:208:B:TRP:H	1:206:B:LYS:HG2	10	0.22	0.05	0.2
(1,851)	1:182:A:ILE:HA	1:185:A:LEU:HB2	10	0.22	0.03	0.22
(1,852)	1:182:B:ILE:HA	1:185:B:LEU:HB2	10	0.22	0.03	0.22
(1,1433)	1:210:A:LEU:H	1:208:A:TRP:HB2	10	0.21	0.03	0.21
(1,1434)	1:210:B:LEU:H	1:208:B:TRP:HB2	10	0.21	0.03	0.2
(1,4)	1:177:B:VAL:HG11	1:179:B:TRP:HE3	10	0.21	0.07	0.2
(1,4)	1:177:B:VAL:HG13	1:179:B:TRP:HE3	10	0.21	0.07	0.2
(1,3)	1:177:A:VAL:HG11	1:179:A:TRP:HE3	10	0.21	0.07	0.2
(1,3)	1:177:A:VAL:HG13	1:179:A:TRP:HE3	10	0.21	0.07	0.2
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB2	10	0.2	0.0	0.2
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB3	10	0.2	0.0	0.2
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB1	10	0.2	0.0	0.2
(1,685)	1:192:A:ASN:HA	1:192:A:ASN:HB3	10	0.2	0.0	0.2
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB2	10	0.2	0.01	0.2
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB3	10	0.2	0.01	0.2
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB1	10	0.2	0.01	0.2
(1,686)	1:192:B:ASN:HA	1:192:B:ASN:HB3	10	0.2	0.0	0.2
(1,479)	1:192:A:ASN:H	1:192:A:ASN:HA	10	0.2	0.02	0.2
(1,480)	1:192:B:ASN:H	1:192:B:ASN:HA	10	0.2	0.02	0.2
(1,2276)	1:202:B:GLU:HA	1:202:B:GLU:HB2	10	0.2	0.0	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2275)	1:202:A:GLU:HA	1:202:A:GLU:HB2	10	0.2	0.0	0.2
(1,2280)	1:194:B:GLN:HA	1:197:B:VAL:HB	10	0.2	0.07	0.18
(1,2279)	1:194:A:GLN:HA	1:197:A:VAL:HB	10	0.2	0.07	0.18
(1,523)	1:191:A:GLU:H	1:191:A:GLU:HA	10	0.2	0.04	0.18
(1,1093)	1:191:A:GLU:HB2	1:191:A:GLU:H	10	0.2	0.01	0.2
(1,1094)	1:191:B:GLU:HB2	1:191:B:GLU:H	10	0.2	0.01	0.2
(1,524)	1:191:B:GLU:H	1:191:B:GLU:HA	10	0.19	0.04	0.18
(1,2319)	1:210:A:LEU:HD11	1:210:A:LEU:HB2	10	0.19	0.01	0.18
(1,2319)	1:210:A:LEU:HD12	1:210:A:LEU:HB2	10	0.19	0.01	0.18
(1,2319)	1:210:A:LEU:HD13	1:210:A:LEU:HB2	10	0.19	0.01	0.18
(1,2285)	1:183:A:GLU:HB3	1:183:A:GLU:HA	10	0.19	0.0	0.19
(1,2285)	1:201:A:MET:HE3	1:183:A:GLU:HA	10	0.19	0.0	0.19
(1,2286)	1:183:B:GLU:HB3	1:183:B:GLU:HA	10	0.19	0.0	0.19
(1,2286)	1:201:B:MET:HE3	1:183:B:GLU:HA	10	0.19	0.0	0.19
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD13	10	0.19	0.04	0.18
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD11	10	0.19	0.04	0.18
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD12	10	0.19	0.04	0.18
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD13	10	0.19	0.04	0.18
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD11	10	0.19	0.04	0.18
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD12	10	0.19	0.04	0.18
(1,2320)	1:210:B:LEU:HD11	1:210:B:LEU:HB2	10	0.19	0.01	0.18
(1,2320)	1:210:B:LEU:HD12	1:210:B:LEU:HB2	10	0.19	0.01	0.18
(1,2320)	1:210:B:LEU:HD13	1:210:B:LEU:HB2	10	0.19	0.01	0.18
(1,437)	1:188:A:ASN:HD22	1:188:A:ASN:HB3	10	0.18	0.17	0.13
(1,438)	1:188:B:ASN:HD22	1:188:B:ASN:HB3	10	0.18	0.17	0.13
(1,1529)	1:207:A:GLY:H	1:206:A:LYS:HB2	10	0.18	0.02	0.18
(1,1530)	1:207:B:GLY:H	1:206:B:LYS:HB2	10	0.18	0.02	0.18
(1,2383)	1:202:A:GLU:HG3	1:203:A:ARG:H	10	0.18	0.03	0.18
(1,2384)	1:202:B:GLU:HG3	1:203:B:ARG:H	10	0.18	0.03	0.18
(1,729)	1:186:A:LEU:HA	1:186:A:LEU:HG	10	0.17	0.0	0.17
(1,730)	1:186:B:LEU:HA	1:186:B:LEU:HG	10	0.17	0.0	0.17
(1,1000)	1:199:B:GLN:HE22	1:199:B:GLN:HG2	10	0.17	0.0	0.17
(1,999)	1:199:A:GLN:HE22	1:199:A:GLN:HG2	10	0.17	0.0	0.17
(1,360)	1:188:B:ASN:H	1:189:B:ASN:HB2	10	0.17	0.04	0.18
(1,1002)	1:199:B:GLN:H	1:197:B:VAL:HB	10	0.16	0.03	0.16
(1,359)	1:188:A:ASN:H	1:189:A:ASN:HB2	10	0.16	0.03	0.18
(1,1001)	1:199:A:GLN:H	1:197:A:VAL:HB	10	0.16	0.04	0.16
(1,2222)	1:208:B:TRP:HA	1:207:A:GLY:H	10	0.16	0.04	0.16
(1,2605)	1:207:A:GLY:H	1:205:A:GLN:HA	10	0.15	0.03	0.16
(1,2606)	1:207:B:GLY:H	1:205:B:GLN:HA	10	0.15	0.03	0.16
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB1	10	0.15	0.03	0.15
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB2	10	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB3	10	0.15	0.03	0.15
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB1	10	0.15	0.03	0.15
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB2	10	0.15	0.03	0.15
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB3	10	0.15	0.03	0.15
(1,713)	1:175:A:LEU:HB2	1:175:A:LEU:HA	10	0.15	0.0	0.15
(1,714)	1:175:B:LEU:HB2	1:175:B:LEU:HA	10	0.15	0.0	0.15
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD12	10	0.14	0.02	0.15
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD11	10	0.14	0.02	0.15
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD13	10	0.14	0.02	0.15
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD12	10	0.14	0.02	0.15
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD11	10	0.14	0.02	0.15
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD13	10	0.14	0.02	0.15
(1,1082)	1:206:B:LYS:H	1:206:B:LYS:HG3	10	0.14	0.01	0.14
(1,1081)	1:206:A:LYS:H	1:206:A:LYS:HG3	10	0.14	0.01	0.14
(1,947)	1:197:A:VAL:HG12	1:197:A:VAL:HB	10	0.13	0.0	0.13
(1,947)	1:197:A:VAL:HG13	1:197:A:VAL:HB	10	0.13	0.0	0.13
(1,947)	1:197:A:VAL:HG11	1:197:A:VAL:HB	10	0.13	0.0	0.13
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB2	10	0.13	0.01	0.14
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB3	10	0.13	0.01	0.14
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB1	10	0.13	0.01	0.14
(1,948)	1:197:B:VAL:HG12	1:197:B:VAL:HB	10	0.13	0.0	0.13
(1,948)	1:197:B:VAL:HG11	1:197:B:VAL:HB	10	0.13	0.0	0.13
(1,948)	1:197:B:VAL:HG13	1:197:B:VAL:HB	10	0.13	0.0	0.13
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB2	10	0.13	0.01	0.13
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB3	10	0.13	0.01	0.13
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB1	10	0.13	0.01	0.13
(1,957)	1:204:A:LEU:HD13	1:204:A:LEU:HD23	10	0.11	0.0	0.11
(1,957)	1:204:A:LEU:HD12	1:204:A:LEU:HD22	10	0.11	0.0	0.11
(1,957)	1:204:A:LEU:HD11	1:204:A:LEU:HD21	10	0.11	0.0	0.11
(1,957)	1:204:A:LEU:HD11	1:204:A:LEU:HD22	10	0.11	0.0	0.11
(1,957)	1:204:A:LEU:HD11	1:204:A:LEU:HD23	10	0.11	0.0	0.11
(1,957)	1:204:A:LEU:HD12	1:204:A:LEU:HD23	10	0.11	0.0	0.11
(1,957)	1:204:A:LEU:HD13	1:204:A:LEU:HD21	10	0.11	0.0	0.11
(1,216)	1:176:B:THR:HG22	1:176:B:THR:HB	10	0.11	0.0	0.11
(1,216)	1:176:B:THR:HG21	1:176:B:THR:HB	10	0.11	0.0	0.11
(1,216)	1:176:B:THR:HG23	1:176:B:THR:HB	10	0.11	0.0	0.11
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG22	9	2.04	0.13	1.99
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG21	9	2.04	0.13	1.99
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG23	9	2.04	0.13	1.99
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG22	9	2.04	0.13	1.98
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG21	9	2.04	0.13	1.98
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG23	9	2.04	0.13	1.98

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1466)	1:208:B:TRP:HE1	1:173:B:GLN:H	9	1.87	0.94	2.0
(1,1465)	1:208:A:TRP:HE1	1:173:A:GLN:H	9	1.86	0.94	1.99
(1,2661)	1:173:A:GLN:HE21	1:196:B:ALA:HA	9	1.66	0.55	1.82
(1,2661)	1:192:A:ASN:HD22	1:194:A:GLN:HA	9	1.66	0.55	1.82
(1,2662)	1:173:B:GLN:HE21	1:196:A:ALA:HA	9	1.64	0.56	1.79
(1,2662)	1:192:B:ASN:HD22	1:194:B:GLN:HA	9	1.64	0.56	1.79
(1,2643)	1:188:A:ASN:HD22	1:185:A:LEU:HB2	9	1.34	0.18	1.37
(1,2644)	1:188:B:ASN:HD22	1:185:B:LEU:HB2	9	1.34	0.18	1.38
(1,1291)	1:191:A:GLU:H	1:193:A:ASP:HB3	9	1.24	0.35	1.32
(1,1292)	1:191:B:GLU:H	1:193:B:ASP:HB3	9	1.23	0.35	1.32
(1,2650)	1:188:B:ASN:HD22	1:178:A:PRO:HG3	9	1.0	0.34	1.1
(1,2649)	1:188:A:ASN:HD22	1:178:B:PRO:HG3	9	0.99	0.35	1.05
(1,2569)	1:208:A:TRP:HE1	1:204:B:LEU:HG	9	0.96	0.07	0.95
(1,2570)	1:208:B:TRP:HE1	1:204:A:LEU:HG	9	0.96	0.08	0.93
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB2	9	0.91	0.14	0.91
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB3	9	0.91	0.14	0.91
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB1	9	0.91	0.14	0.91
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB2	9	0.91	0.14	0.88
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB3	9	0.91	0.14	0.88
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB1	9	0.91	0.14	0.88
(1,1554)	1:173:B:GLN:HE21	1:175:B:LEU:HB3	9	0.88	0.44	0.79
(1,173)	1:211:A:ALA:HB2	1:203:B:ARG:HD3	9	0.88	0.14	0.88
(1,173)	1:211:A:ALA:HB3	1:203:B:ARG:HD3	9	0.88	0.14	0.88
(1,173)	1:211:A:ALA:HB1	1:203:B:ARG:HD3	9	0.88	0.14	0.88
(1,174)	1:211:B:ALA:HB2	1:203:A:ARG:HD3	9	0.87	0.14	0.84
(1,174)	1:211:B:ALA:HB3	1:203:A:ARG:HD3	9	0.87	0.14	0.84
(1,174)	1:211:B:ALA:HB1	1:203:A:ARG:HD3	9	0.87	0.14	0.84
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG13	9	0.85	0.18	0.91
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG12	9	0.85	0.18	0.91
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG11	9	0.85	0.18	0.91
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG13	9	0.84	0.18	0.89
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG12	9	0.84	0.18	0.89
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG11	9	0.84	0.18	0.89
(1,1580)	1:188:B:ASN:HD22	1:185:B:LEU:HA	9	0.81	0.15	0.81
(1,1579)	1:188:A:ASN:HD22	1:185:A:LEU:HA	9	0.81	0.15	0.82
(1,2020)	1:205:B:GLN:HE22	1:179:B:TRP:HD1	9	0.66	0.25	0.59
(1,2019)	1:205:A:GLN:HE22	1:179:A:TRP:HD1	9	0.65	0.26	0.57
(1,419)	1:193:A:ASP:H	1:193:A:ASP:HB3	9	0.61	0.04	0.59
(1,420)	1:193:B:ASP:H	1:193:B:ASP:HB3	9	0.61	0.04	0.59
(1,421)	1:196:A:ALA:H	1:193:A:ASP:HB2	9	0.57	0.37	0.41
(1,422)	1:196:B:ALA:H	1:193:B:ASP:HB2	9	0.57	0.37	0.41
(1,1073)	1:192:A:ASN:H	1:187:A:LYS:HG3	9	0.57	0.3	0.42

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1074)	1:192:B:ASN:H	1:187:B:LYS:HG3	9	0.57	0.29	0.42
(1,648)	1:195:B:ALA:HB2	1:198:B:ARG:HD3	9	0.57	0.64	0.26
(1,648)	1:195:B:ALA:HB1	1:198:B:ARG:HD3	9	0.57	0.64	0.26
(1,648)	1:195:B:ALA:HB3	1:198:B:ARG:HD3	9	0.57	0.64	0.26
(1,647)	1:195:A:ALA:HB2	1:198:A:ARG:HD3	9	0.56	0.64	0.26
(1,647)	1:195:A:ALA:HB1	1:198:A:ARG:HD3	9	0.56	0.64	0.26
(1,647)	1:195:A:ALA:HB3	1:198:A:ARG:HD3	9	0.56	0.64	0.26
(1,2402)	1:208:B:TRP:HA	1:203:A:ARG:HB3	9	0.54	0.05	0.51
(1,2401)	1:208:A:TRP:HA	1:203:B:ARG:HB3	9	0.54	0.05	0.52
(1,1105)	1:176:A:THR:HG21	1:179:A:TRP:HD1	9	0.53	0.18	0.51
(1,1105)	1:176:A:THR:HG23	1:179:A:TRP:HD1	9	0.53	0.18	0.51
(1,1105)	1:176:A:THR:HG22	1:179:A:TRP:HD1	9	0.53	0.18	0.51
(1,1106)	1:176:B:THR:HG21	1:179:B:TRP:HD1	9	0.53	0.18	0.51
(1,1106)	1:176:B:THR:HG23	1:179:B:TRP:HD1	9	0.53	0.18	0.51
(1,1106)	1:176:B:THR:HG22	1:179:B:TRP:HD1	9	0.53	0.18	0.51
(1,2573)	1:208:A:TRP:HE1	1:212:A:LYS:HB3	9	0.52	0.12	0.52
(1,2573)	1:208:A:TRP:HE1	1:203:B:ARG:HD2	9	0.52	0.12	0.52
(1,2574)	1:208:B:TRP:HE1	1:212:B:LYS:HB3	9	0.51	0.11	0.54
(1,2574)	1:208:B:TRP:HE1	1:203:A:ARG:HD2	9	0.51	0.11	0.54
(1,2511)	1:176:A:THR:H	1:174:A:GLU:HB3	9	0.46	0.41	0.31
(1,2511)	1:176:A:THR:H	1:173:A:GLN:HB3	9	0.46	0.41	0.31
(1,2512)	1:176:B:THR:H	1:174:B:GLU:HB3	9	0.46	0.42	0.31
(1,2512)	1:176:B:THR:H	1:173:B:GLN:HB3	9	0.46	0.42	0.31
(1,2670)	1:202:B:GLU:H	1:179:B:TRP:HZ3	9	0.46	0.11	0.46
(1,397)	1:175:A:LEU:HB2	1:190:B:PHE:HZ	9	0.46	0.17	0.51
(1,2669)	1:202:A:GLU:H	1:179:A:TRP:HZ3	9	0.46	0.11	0.46
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG21	9	0.44	0.12	0.49
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG23	9	0.44	0.12	0.49
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG22	9	0.44	0.12	0.49
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG21	9	0.44	0.12	0.49
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG23	9	0.44	0.12	0.49
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG22	9	0.44	0.12	0.49
(1,1571)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	9	0.43	0.08	0.46
(1,1572)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	9	0.43	0.08	0.46
(1,2360)	1:200:B:VAL:HG13	1:175:A:LEU:H	9	0.41	0.12	0.34
(1,2360)	1:200:B:VAL:HG12	1:175:A:LEU:H	9	0.41	0.12	0.34
(1,2360)	1:200:B:VAL:HG11	1:175:A:LEU:H	9	0.41	0.12	0.34
(1,2359)	1:200:A:VAL:HG13	1:175:B:LEU:H	9	0.41	0.12	0.35
(1,2359)	1:200:A:VAL:HG12	1:175:B:LEU:H	9	0.41	0.12	0.35
(1,2359)	1:200:A:VAL:HG11	1:175:B:LEU:H	9	0.41	0.12	0.35
(1,2382)	1:182:B:ILE:HD11	1:186:A:LEU:H	9	0.31	0.1	0.28
(1,2382)	1:182:B:ILE:HD12	1:186:A:LEU:H	9	0.31	0.1	0.28

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2382)	1:182:B:ILE:HD13	1:186:A:LEU:H	9	0.31	0.1	0.28
(1,2381)	1:182:A:ILE:HD11	1:186:B:LEU:H	9	0.31	0.11	0.26
(1,2381)	1:182:A:ILE:HD12	1:186:B:LEU:H	9	0.31	0.11	0.26
(1,2381)	1:182:A:ILE:HD13	1:186:B:LEU:H	9	0.31	0.11	0.26
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD11	9	0.3	0.16	0.31
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD12	9	0.3	0.16	0.31
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD13	9	0.3	0.16	0.31
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD11	9	0.3	0.16	0.3
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD12	9	0.3	0.16	0.3
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD13	9	0.3	0.16	0.3
(1,2174)	1:203:B:ARG:HD2	1:208:A:TRP:HZ3	9	0.28	0.1	0.24
(1,2173)	1:203:A:ARG:HD2	1:208:B:TRP:HZ3	9	0.27	0.09	0.26
(1,2330)	1:199:B:GLN:HG3	1:196:B:ALA:H	9	0.27	0.08	0.29
(1,2330)	1:194:B:GLN:HG3	1:193:B:ASP:H	9	0.27	0.08	0.29
(1,2329)	1:199:A:GLN:HG3	1:196:A:ALA:H	9	0.27	0.08	0.29
(1,2329)	1:194:A:GLN:HG3	1:193:A:ASP:H	9	0.27	0.08	0.29
(1,1135)	1:188:A:ASN:HD22	1:188:A:ASN:HA	9	0.26	0.05	0.24
(1,2772)	1:175:B:LEU:H	1:190:A:PHE:HZ	9	0.26	0.15	0.2
(1,1136)	1:188:B:ASN:HD22	1:188:B:ASN:HA	9	0.26	0.05	0.23
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG13	9	0.25	0.12	0.17
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG12	9	0.25	0.12	0.17
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG11	9	0.25	0.12	0.17
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG13	9	0.24	0.12	0.19
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG12	9	0.24	0.12	0.19
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG11	9	0.24	0.12	0.19
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG21	9	0.22	0.06	0.24
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG22	9	0.22	0.06	0.24
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG23	9	0.22	0.06	0.24
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG21	9	0.22	0.06	0.24
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG22	9	0.22	0.06	0.24
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG23	9	0.22	0.06	0.24
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD12	9	0.19	0.08	0.16
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD11	9	0.19	0.08	0.16
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD13	9	0.19	0.08	0.16
(1,2225)	1:208:A:TRP:HA	1:208:A:TRP:HE3	9	0.17	0.04	0.17
(1,2226)	1:208:B:TRP:HA	1:208:B:TRP:HE3	9	0.17	0.04	0.17
(1,721)	1:190:A:PHE:HA	1:189:A:ASN:HB3	9	0.17	0.03	0.18
(1,2221)	1:208:A:TRP:HA	1:207:B:GLY:H	9	0.17	0.04	0.17
(1,722)	1:190:B:PHE:HA	1:189:B:ASN:HB3	9	0.17	0.03	0.18
(1,2483)	1:180:A:ASP:H	1:178:A:PRO:HD2	9	0.17	0.05	0.16
(1,2483)	1:180:A:ASP:H	1:182:A:ILE:HA	9	0.17	0.05	0.16
(1,775)	1:173:A:GLN:HB2	1:173:A:GLN:HA	9	0.16	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)
(1,776)	1:173:B:GLN:HB2	1:173:B:GLN:HA	9	0.16	0.01	0.17
(1,2737)	1:197:A:VAL:H	1:187:A:LYS:H	9	0.16	0.03	0.15
(1,2738)	1:197:B:VAL:H	1:187:B:LYS:H	9	0.15	0.02	0.15
(1,2516)	1:205:B:GLN:H	1:204:B:LEU:HB3	9	0.13	0.02	0.14
(1,958)	1:204:B:LEU:HD13	1:204:B:LEU:HD23	9	0.11	0.0	0.11
(1,958)	1:204:B:LEU:HD12	1:204:B:LEU:HD22	9	0.11	0.0	0.11
(1,958)	1:204:B:LEU:HD11	1:204:B:LEU:HD21	9	0.11	0.0	0.11
(1,958)	1:204:B:LEU:HD11	1:204:B:LEU:HD22	9	0.11	0.0	0.11
(1,958)	1:204:B:LEU:HD11	1:204:B:LEU:HD23	9	0.11	0.0	0.11
(1,958)	1:204:B:LEU:HD12	1:204:B:LEU:HD23	9	0.11	0.0	0.11
(1,958)	1:204:B:LEU:HD13	1:204:B:LEU:HD21	9	0.11	0.0	0.11
(1,215)	1:176:A:THR:HG22	1:176:A:THR:HB	9	0.11	0.0	0.11
(1,215)	1:176:A:THR:HG21	1:176:A:THR:HB	9	0.11	0.0	0.11
(1,215)	1:176:A:THR:HG23	1:176:A:THR:HB	9	0.11	0.0	0.11
(1,2854)	1:176:B:THR:H	1:189:A:ASN:HB3	8	1.74	0.18	1.68
(1,2854)	1:176:B:THR:H	1:173:B:GLN:HG3	8	1.74	0.18	1.68
(1,2853)	1:176:A:THR:H	1:189:B:ASN:HB3	8	1.74	0.18	1.66
(1,2853)	1:176:A:THR:H	1:173:A:GLN:HG3	8	1.74	0.18	1.66
(1,2576)	1:208:B:TRP:HE1	1:211:B:ALA:HB2	8	1.71	0.27	1.77
(1,2576)	1:208:B:TRP:HE1	1:211:B:ALA:HB3	8	1.71	0.27	1.77
(1,2576)	1:208:B:TRP:HE1	1:211:B:ALA:HB1	8	1.71	0.27	1.77
(1,2575)	1:208:A:TRP:HE1	1:211:A:ALA:HB2	8	1.71	0.27	1.78
(1,2575)	1:208:A:TRP:HE1	1:211:A:ALA:HB3	8	1.71	0.27	1.78
(1,2575)	1:208:A:TRP:HE1	1:211:A:ALA:HB1	8	1.71	0.27	1.78
(1,1092)	1:199:B:GLN:HG2	1:173:A:GLN:HE21	8	1.37	0.62	1.34
(1,1091)	1:199:A:GLN:HG2	1:173:B:GLN:HE21	8	1.36	0.62	1.3
(1,590)	1:209:B:SER:HB3	1:208:B:TRP:H	8	0.79	0.65	0.8
(1,589)	1:209:A:SER:HB3	1:208:A:TRP:H	8	0.79	0.65	0.8
(1,1479)	1:179:A:TRP:HE1	1:201:A:MET:HE3	8	0.71	0.09	0.75
(1,1479)	1:179:A:TRP:HE1	1:201:A:MET:HE1	8	0.71	0.09	0.75
(1,1479)	1:179:A:TRP:HE1	1:201:A:MET:HE2	8	0.71	0.09	0.75
(1,1480)	1:179:B:TRP:HE1	1:201:B:MET:HE3	8	0.71	0.09	0.74
(1,1480)	1:179:B:TRP:HE1	1:201:B:MET:HE1	8	0.71	0.09	0.74
(1,1480)	1:179:B:TRP:HE1	1:201:B:MET:HE2	8	0.71	0.09	0.74
(1,1678)	1:199:B:GLN:HE22	1:198:B:ARG:HD3	8	0.56	0.49	0.36
(1,1103)	1:179:A:TRP:HE1	1:176:A:THR:HG21	8	0.45	0.16	0.44
(1,1103)	1:179:A:TRP:HE1	1:176:A:THR:HG23	8	0.45	0.16	0.44
(1,1103)	1:179:A:TRP:HE1	1:176:A:THR:HG22	8	0.45	0.16	0.44
(1,1104)	1:179:B:TRP:HE1	1:176:B:THR:HG21	8	0.45	0.16	0.43
(1,1104)	1:179:B:TRP:HE1	1:176:B:THR:HG23	8	0.45	0.16	0.43
(1,1104)	1:179:B:TRP:HE1	1:176:B:THR:HG22	8	0.45	0.16	0.43
(1,2873)	1:204:A:LEU:H	1:182:A:ILE:HD12	8	0.44	0.11	0.48

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2873)	1:204:A:LEU:H	1:182:B:ILE:HD13	8	0.44	0.11	0.48
(1,2873)	1:204:A:LEU:H	1:182:A:ILE:HD13	8	0.44	0.11	0.48
(1,2873)	1:204:A:LEU:H	1:182:B:ILE:HD12	8	0.44	0.11	0.48
(1,2874)	1:204:B:LEU:H	1:182:B:ILE:HD12	8	0.44	0.1	0.47
(1,2874)	1:204:B:LEU:H	1:182:A:ILE:HD13	8	0.44	0.1	0.47
(1,2874)	1:204:B:LEU:H	1:182:B:ILE:HD13	8	0.44	0.1	0.47
(1,2874)	1:204:B:LEU:H	1:182:A:ILE:HD12	8	0.44	0.1	0.47
(1,2081)	1:175:A:LEU:HD21	1:190:B:PHE:HZ	8	0.36	0.16	0.34
(1,2081)	1:175:A:LEU:HD23	1:190:B:PHE:HE1	8	0.36	0.16	0.34
(1,2081)	1:175:A:LEU:HD22	1:190:B:PHE:HZ	8	0.36	0.16	0.34
(1,2081)	1:175:A:LEU:HD23	1:190:B:PHE:HZ	8	0.36	0.16	0.34
(1,2711)	1:199:A:GLN:HE22	1:195:A:ALA:HA	8	0.32	0.11	0.32
(1,2711)	1:199:A:GLN:HE22	1:199:A:GLN:HA	8	0.32	0.11	0.32
(1,822)	1:208:B:TRP:HA	1:203:A:ARG:HG3	8	0.32	0.41	0.15
(1,2712)	1:199:B:GLN:HE22	1:195:B:ALA:HA	8	0.31	0.11	0.32
(1,2712)	1:199:B:GLN:HE22	1:199:B:GLN:HA	8	0.31	0.11	0.32
(1,2771)	1:175:A:LEU:H	1:190:B:PHE:HZ	8	0.29	0.13	0.28
(1,1262)	1:176:B:THR:HG22	1:177:B:VAL:HB	8	0.29	0.08	0.27
(1,1262)	1:176:B:THR:HG21	1:177:B:VAL:HB	8	0.29	0.08	0.27
(1,1262)	1:176:B:THR:HG23	1:177:B:VAL:HB	8	0.29	0.08	0.27
(1,1261)	1:176:A:THR:HG22	1:177:A:VAL:HB	8	0.29	0.08	0.27
(1,1261)	1:176:A:THR:HG21	1:177:A:VAL:HB	8	0.29	0.08	0.27
(1,1261)	1:176:A:THR:HG23	1:177:A:VAL:HB	8	0.29	0.08	0.27
(1,2565)	1:208:A:TRP:HE1	1:209:A:SER:HA	8	0.25	0.07	0.26
(1,2565)	1:208:A:TRP:HE1	1:208:A:TRP:HA	8	0.25	0.07	0.26
(1,2869)	1:209:A:SER:H	1:206:A:LYS:HE3	8	0.25	0.09	0.24
(1,2566)	1:208:B:TRP:HE1	1:209:B:SER:HA	8	0.25	0.07	0.26
(1,2566)	1:208:B:TRP:HE1	1:208:B:TRP:HA	8	0.25	0.07	0.26
(1,1694)	1:189:B:ASN:HD22	1:182:A:ILE:HD11	8	0.25	0.16	0.15
(1,1694)	1:189:B:ASN:HD22	1:182:A:ILE:HD12	8	0.25	0.16	0.15
(1,1694)	1:189:B:ASN:HD22	1:182:A:ILE:HD13	8	0.25	0.16	0.15
(1,2870)	1:209:B:SER:H	1:206:B:LYS:HE3	8	0.24	0.09	0.24
(1,2288)	1:182:B:ILE:HG21	1:183:B:GLU:HA	8	0.24	0.06	0.25
(1,2288)	1:182:B:ILE:HG22	1:183:B:GLU:HA	8	0.24	0.06	0.25
(1,2288)	1:182:B:ILE:HG23	1:183:B:GLU:HA	8	0.24	0.06	0.25
(1,2287)	1:182:A:ILE:HG21	1:183:A:GLU:HA	8	0.24	0.06	0.24
(1,2287)	1:182:A:ILE:HG22	1:183:A:GLU:HA	8	0.24	0.06	0.24
(1,2287)	1:182:A:ILE:HG23	1:183:A:GLU:HA	8	0.24	0.06	0.24
(1,275)	1:198:A:ARG:HG2	1:198:A:ARG:HD3	8	0.23	0.0	0.23
(1,276)	1:198:B:ARG:HG2	1:198:B:ARG:HD3	8	0.23	0.0	0.23
(1,1630)	1:203:B:ARG:H	1:179:B:TRP:HZ3	8	0.21	0.08	0.19
(1,1998)	1:191:B:GLU:H	1:186:B:LEU:HD12	8	0.21	0.08	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1998)	1:191:B:GLU:H	1:186:B:LEU:HD11	8	0.21	0.08	0.17
(1,1998)	1:191:B:GLU:H	1:186:B:LEU:HD13	8	0.21	0.08	0.17
(1,544)	1:199:B:GLN:HA	1:202:B:GLU:H	8	0.19	0.05	0.2
(1,543)	1:199:A:GLN:HA	1:202:A:GLU:H	8	0.19	0.04	0.19
(1,41)	1:196:A:ALA:H	1:195:A:ALA:HB3	8	0.19	0.06	0.18
(1,41)	1:196:A:ALA:H	1:195:A:ALA:HB2	8	0.19	0.06	0.18
(1,41)	1:196:A:ALA:H	1:195:A:ALA:HB1	8	0.19	0.06	0.18
(1,42)	1:196:B:ALA:H	1:195:B:ALA:HB3	8	0.18	0.06	0.16
(1,42)	1:196:B:ALA:H	1:195:B:ALA:HB2	8	0.18	0.06	0.16
(1,42)	1:196:B:ALA:H	1:195:B:ALA:HB1	8	0.18	0.06	0.16
(1,2484)	1:180:B:ASP:H	1:178:B:PRO:HD2	8	0.18	0.04	0.16
(1,2484)	1:180:B:ASP:H	1:182:B:ILE:HA	8	0.18	0.04	0.16
(1,1062)	1:189:B:ASN:HB2	1:191:B:GLU:H	8	0.14	0.04	0.12
(1,2515)	1:205:A:GLN:H	1:204:A:LEU:HB3	8	0.14	0.01	0.14
(1,1061)	1:189:A:ASN:HB2	1:191:A:GLU:H	8	0.13	0.04	0.12
(1,2818)	1:183:B:GLU:H	1:182:B:ILE:HG12	8	0.12	0.01	0.12
(1,2863)	1:173:B:GLN:H	1:203:A:ARG:HG3	7	1.01	0.64	0.79
(1,2864)	1:173:A:GLN:H	1:203:B:ARG:HG3	7	1.01	0.64	0.79
(1,1217)	1:201:A:MET:HE3	1:179:A:TRP:HB2	7	0.98	0.12	0.92
(1,1217)	1:201:A:MET:HE2	1:179:A:TRP:HB2	7	0.98	0.12	0.92
(1,1217)	1:201:A:MET:HE1	1:179:A:TRP:HB2	7	0.98	0.12	0.92
(1,1218)	1:201:B:MET:HE3	1:179:B:TRP:HB2	7	0.97	0.12	0.9
(1,1218)	1:201:B:MET:HE2	1:179:B:TRP:HB2	7	0.97	0.12	0.9
(1,1218)	1:201:B:MET:HE1	1:179:B:TRP:HB2	7	0.97	0.12	0.9
(1,2039)	1:203:A:ARG:H	1:205:A:GLN:HE22	7	0.64	0.35	0.61
(1,2040)	1:203:B:ARG:H	1:205:B:GLN:HE22	7	0.64	0.35	0.62
(1,1677)	1:199:A:GLN:HE22	1:198:A:ARG:HD3	7	0.62	0.49	0.42
(1,34)	1:205:B:GLN:HE22	1:201:B:MET:HE1	7	0.62	0.36	0.63
(1,34)	1:205:B:GLN:HE22	1:201:B:MET:HE3	7	0.62	0.36	0.63
(1,34)	1:205:B:GLN:HE22	1:201:B:MET:HE2	7	0.62	0.36	0.63
(1,33)	1:205:A:GLN:HE22	1:201:A:MET:HE1	7	0.62	0.36	0.63
(1,33)	1:205:A:GLN:HE22	1:201:A:MET:HE3	7	0.62	0.36	0.63
(1,33)	1:205:A:GLN:HE22	1:201:A:MET:HE2	7	0.62	0.36	0.63
(1,2436)	1:197:B:VAL:HG12	1:201:B:MET:HB2	7	0.6	0.24	0.72
(1,2436)	1:197:B:VAL:HG13	1:187:B:LYS:HD3	7	0.6	0.24	0.72
(1,2436)	1:201:B:MET:HB2	1:200:B:VAL:HG21	7	0.6	0.24	0.72
(1,2435)	1:197:A:VAL:HG12	1:201:A:MET:HB2	7	0.6	0.24	0.72
(1,2435)	1:197:A:VAL:HG13	1:187:A:LYS:HD3	7	0.6	0.24	0.72
(1,2435)	1:201:A:MET:HB2	1:200:A:VAL:HG21	7	0.6	0.24	0.72
(1,2768)	1:194:B:GLN:H	1:194:B:GLN:HB3	7	0.55	0.19	0.67
(1,2768)	1:175:B:LEU:H	1:173:B:GLN:HB3	7	0.55	0.19	0.67
(1,2767)	1:194:A:GLN:H	1:194:A:GLN:HB3	7	0.55	0.19	0.67

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2767)	1:175:A:LEU:H	1:173:A:GLN:HB3	7	0.55	0.19	0.67
(1,1986)	1:173:A:GLN:H	1:175:A:LEU:HD12	7	0.55	0.41	0.36
(1,1986)	1:173:A:GLN:H	1:175:A:LEU:HD11	7	0.55	0.41	0.36
(1,1985)	1:173:B:GLN:H	1:175:B:LEU:HD12	7	0.55	0.41	0.36
(1,1985)	1:173:B:GLN:H	1:175:B:LEU:HD11	7	0.55	0.41	0.36
(1,253)	1:175:A:LEU:HD13	1:196:B:ALA:HA	7	0.47	0.18	0.51
(1,253)	1:175:A:LEU:HD11	1:196:B:ALA:HA	7	0.47	0.18	0.51
(1,253)	1:175:A:LEU:HD12	1:196:B:ALA:HA	7	0.47	0.18	0.51
(1,2139)	1:206:A:LYS:HD3	1:203:A:ARG:HA	7	0.45	0.28	0.32
(1,2139)	1:206:A:LYS:HD3	1:206:A:LYS:HA	7	0.45	0.28	0.32
(1,2140)	1:206:B:LYS:HD3	1:203:B:ARG:HA	7	0.45	0.27	0.31
(1,2140)	1:206:B:LYS:HD3	1:206:B:LYS:HA	7	0.45	0.27	0.31
(1,2138)	1:201:B:MET:HB2	1:202:B:GLU:HA	7	0.41	0.28	0.24
(1,2138)	1:187:B:LYS:HD3	1:184:B:ALA:HA	7	0.41	0.28	0.24
(1,2137)	1:201:A:MET:HB2	1:202:A:GLU:HA	7	0.41	0.27	0.24
(1,2137)	1:187:A:LYS:HD3	1:184:A:ALA:HA	7	0.41	0.27	0.24
(1,2082)	1:175:B:LEU:HD21	1:190:A:PHE:HZ	7	0.41	0.14	0.36
(1,2082)	1:175:B:LEU:HD23	1:190:A:PHE:HE1	7	0.41	0.14	0.36
(1,2082)	1:175:B:LEU:HD22	1:190:A:PHE:HZ	7	0.41	0.14	0.36
(1,2082)	1:175:B:LEU:HD23	1:190:A:PHE:HZ	7	0.41	0.14	0.36
(1,916)	1:199:B:GLN:HG2	1:175:A:LEU:HD13	7	0.38	0.25	0.33
(1,916)	1:199:B:GLN:HG2	1:175:A:LEU:HD12	7	0.38	0.25	0.33
(1,915)	1:199:A:GLN:HG2	1:175:B:LEU:HD13	7	0.37	0.24	0.32
(1,915)	1:199:A:GLN:HG2	1:175:B:LEU:HD12	7	0.37	0.24	0.32
(1,2321)	1:197:A:VAL:HG13	1:187:A:LYS:HG3	7	0.37	0.09	0.35
(1,2321)	1:197:A:VAL:HG12	1:187:A:LYS:HG3	7	0.37	0.09	0.35
(1,2321)	1:197:A:VAL:HG11	1:187:A:LYS:HG3	7	0.37	0.09	0.35
(1,2322)	1:197:B:VAL:HG13	1:187:B:LYS:HG3	7	0.36	0.09	0.35
(1,2322)	1:197:B:VAL:HG12	1:187:B:LYS:HG3	7	0.36	0.09	0.35
(1,2322)	1:197:B:VAL:HG11	1:187:B:LYS:HG3	7	0.36	0.09	0.35
(1,821)	1:208:A:TRP:HA	1:203:B:ARG:HG3	7	0.35	0.44	0.16
(1,917)	1:173:A:GLN:HG2	1:175:A:LEU:HD13	7	0.34	0.14	0.37
(1,917)	1:173:A:GLN:HG2	1:175:A:LEU:HD11	7	0.34	0.14	0.37
(1,917)	1:173:A:GLN:HG3	1:175:A:LEU:HD11	7	0.34	0.14	0.37
(1,917)	1:173:A:GLN:HG2	1:175:A:LEU:HD12	7	0.34	0.14	0.37
(1,918)	1:173:B:GLN:HG2	1:175:B:LEU:HD13	7	0.34	0.14	0.36
(1,918)	1:173:B:GLN:HG2	1:175:B:LEU:HD11	7	0.34	0.14	0.36
(1,918)	1:173:B:GLN:HG3	1:175:B:LEU:HD11	7	0.34	0.14	0.36
(1,918)	1:173:B:GLN:HG2	1:175:B:LEU:HD12	7	0.34	0.14	0.36
(1,2710)	1:199:B:GLN:HE22	1:175:A:LEU:HA	7	0.3	0.16	0.28
(1,2709)	1:199:A:GLN:HE22	1:175:B:LEU:HA	7	0.3	0.14	0.27
(1,25)	1:201:A:MET:HE3	1:179:A:TRP:HB3	7	0.29	0.12	0.25

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,25)	1:201:A:MET:HE2	1:179:A:TRP:HB3	7	0.29	0.12	0.25
(1,25)	1:201:A:MET:HE1	1:179:A:TRP:HB3	7	0.29	0.12	0.25
(1,26)	1:201:B:MET:HE3	1:179:B:TRP:HB3	7	0.29	0.12	0.25
(1,26)	1:201:B:MET:HE2	1:179:B:TRP:HB3	7	0.29	0.12	0.25
(1,26)	1:201:B:MET:HE1	1:179:B:TRP:HB3	7	0.29	0.12	0.25
(1,1693)	1:189:A:ASN:HD22	1:182:B:ILE:HD11	7	0.27	0.15	0.17
(1,1693)	1:189:A:ASN:HD22	1:182:B:ILE:HD12	7	0.27	0.15	0.17
(1,1693)	1:189:A:ASN:HD22	1:182:B:ILE:HD13	7	0.27	0.15	0.17
(1,1196)	1:188:B:ASN:HA	1:191:B:GLU:HB2	7	0.25	0.09	0.24
(1,2721)	1:189:A:ASN:HD22	1:178:B:PRO:HG2	7	0.24	0.07	0.24
(1,2722)	1:189:B:ASN:HD22	1:178:A:PRO:HG2	7	0.24	0.07	0.24
(1,1629)	1:203:A:ARG:H	1:179:A:TRP:HZ3	7	0.22	0.07	0.18
(1,873)	1:185:A:LEU:HD13	1:188:A:ASN:HB2	7	0.21	0.09	0.17
(1,873)	1:185:A:LEU:HD12	1:188:A:ASN:HB2	7	0.21	0.09	0.17
(1,873)	1:185:A:LEU:HD11	1:188:A:ASN:HB2	7	0.21	0.09	0.17
(1,874)	1:185:B:LEU:HD13	1:188:B:ASN:HB2	7	0.21	0.09	0.17
(1,874)	1:185:B:LEU:HD12	1:188:B:ASN:HB2	7	0.21	0.09	0.17
(1,874)	1:185:B:LEU:HD11	1:188:B:ASN:HB2	7	0.21	0.09	0.17
(1,2470)	1:204:B:LEU:H	1:179:B:TRP:HZ3	7	0.18	0.08	0.15
(1,2469)	1:204:A:LEU:H	1:179:A:TRP:HZ3	7	0.18	0.08	0.14
(1,444)	1:192:B:ASN:H	1:192:B:ASN:HB2	7	0.17	0.02	0.17
(1,443)	1:192:A:ASN:H	1:192:A:ASN:HB2	7	0.17	0.02	0.16
(1,1541)	1:206:A:LYS:H	1:206:A:LYS:HE3	7	0.17	0.02	0.17
(1,1542)	1:206:B:LYS:H	1:206:B:LYS:HE3	7	0.17	0.03	0.16
(1,2501)	1:198:A:ARG:H	1:197:A:VAL:HG12	7	0.15	0.03	0.14
(1,2501)	1:198:A:ARG:H	1:197:A:VAL:HG11	7	0.15	0.03	0.14
(1,2501)	1:198:A:ARG:H	1:197:A:VAL:HG13	7	0.15	0.03	0.14
(1,2502)	1:198:B:ARG:H	1:197:B:VAL:HG12	7	0.15	0.02	0.14
(1,2502)	1:198:B:ARG:H	1:197:B:VAL:HG11	7	0.15	0.02	0.14
(1,2502)	1:198:B:ARG:H	1:197:B:VAL:HG13	7	0.15	0.02	0.14
(1,791)	1:202:A:GLU:HA	1:202:A:GLU:HG3	7	0.15	0.01	0.15
(1,782)	1:206:B:LYS:HG2	1:206:B:LYS:HA	7	0.15	0.02	0.14
(1,781)	1:206:A:LYS:HG2	1:206:A:LYS:HA	7	0.15	0.02	0.14
(1,792)	1:202:B:GLU:HA	1:202:B:GLU:HG3	7	0.15	0.01	0.14
(1,2526)	1:212:B:LYS:H	1:210:B:LEU:HB2	7	0.14	0.03	0.15
(1,2525)	1:212:A:LYS:H	1:210:A:LEU:HB2	7	0.13	0.03	0.14
(1,2532)	1:211:B:ALA:H	1:210:B:LEU:HB3	7	0.13	0.01	0.13
(1,2817)	1:183:A:GLU:H	1:182:A:ILE:HG12	7	0.12	0.01	0.12
(1,2272)	1:212:B:LYS:HG2	1:212:B:LYS:HA	6	0.69	0.02	0.69
(1,2272)	1:212:B:LYS:HG3	1:212:B:LYS:HA	6	0.69	0.02	0.69
(1,2271)	1:212:A:LYS:HG2	1:212:A:LYS:HA	6	0.69	0.02	0.68
(1,2861)	1:173:B:GLN:H	1:175:B:LEU:HB2	6	0.62	0.27	0.6

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2861)	1:173:B:GLN:H	1:212:B:LYS:HG2	6	0.62	0.27	0.6
(1,2862)	1:173:A:GLN:H	1:175:A:LEU:HB2	6	0.61	0.27	0.6
(1,2862)	1:173:A:GLN:H	1:212:A:LYS:HG2	6	0.61	0.27	0.6
(1,2403)	1:183:A:GLU:HA	1:201:A:MET:HB2	6	0.56	0.06	0.56
(1,2404)	1:183:B:GLU:HA	1:201:B:MET:HB2	6	0.56	0.06	0.56
(1,254)	1:175:B:LEU:HD13	1:196:A:ALA:HA	6	0.53	0.13	0.52
(1,254)	1:175:B:LEU:HD11	1:196:A:ALA:HA	6	0.53	0.13	0.52
(1,254)	1:175:B:LEU:HD12	1:196:A:ALA:HA	6	0.53	0.13	0.52
(1,2022)	1:179:B:TRP:HE1	1:205:B:GLN:HE22	6	0.53	0.15	0.56
(1,2021)	1:179:A:TRP:HE1	1:205:A:GLN:HE22	6	0.52	0.16	0.56
(1,2762)	1:175:B:LEU:H	1:175:B:LEU:HD12	6	0.48	0.22	0.52
(1,2762)	1:175:B:LEU:H	1:175:B:LEU:HD13	6	0.48	0.22	0.52
(1,2762)	1:175:B:LEU:H	1:175:B:LEU:HD11	6	0.48	0.22	0.52
(1,2761)	1:175:A:LEU:H	1:175:A:LEU:HD12	6	0.47	0.22	0.52
(1,2761)	1:175:A:LEU:H	1:175:A:LEU:HD13	6	0.47	0.22	0.52
(1,2761)	1:175:A:LEU:H	1:175:A:LEU:HD11	6	0.47	0.22	0.52
(1,2096)	1:175:B:LEU:HD13	1:199:A:GLN:HE22	6	0.42	0.14	0.39
(1,2096)	1:175:B:LEU:HD11	1:199:A:GLN:HE22	6	0.42	0.14	0.39
(1,2096)	1:175:B:LEU:HD12	1:199:A:GLN:HE22	6	0.42	0.14	0.39
(1,2095)	1:175:A:LEU:HD13	1:199:B:GLN:HE22	6	0.42	0.13	0.4
(1,2095)	1:175:A:LEU:HD11	1:199:B:GLN:HE22	6	0.42	0.13	0.4
(1,2095)	1:175:A:LEU:HD12	1:199:B:GLN:HE22	6	0.42	0.13	0.4
(1,1184)	1:199:B:GLN:HA	1:175:A:LEU:HD12	6	0.36	0.18	0.35
(1,1184)	1:199:B:GLN:HA	1:175:A:LEU:HD11	6	0.36	0.18	0.35
(1,1184)	1:199:B:GLN:HA	1:175:A:LEU:HD13	6	0.36	0.18	0.35
(1,2410)	1:197:B:VAL:HA	1:201:B:MET:HB2	6	0.35	0.05	0.34
(1,1183)	1:199:A:GLN:HA	1:175:B:LEU:HD12	6	0.35	0.18	0.32
(1,1183)	1:199:A:GLN:HA	1:175:B:LEU:HD11	6	0.35	0.18	0.32
(1,1183)	1:199:A:GLN:HA	1:175:B:LEU:HD13	6	0.35	0.18	0.32
(1,2409)	1:197:A:VAL:HA	1:201:A:MET:HB2	6	0.35	0.06	0.34
(1,1195)	1:188:A:ASN:HA	1:191:A:GLU:HB2	6	0.28	0.06	0.26
(1,2194)	1:173:B:GLN:HA	1:174:B:GLU:H	6	0.27	0.27	0.15
(1,2194)	1:173:B:GLN:HA	1:173:B:GLN:H	6	0.27	0.27	0.15
(1,2193)	1:173:A:GLN:HA	1:174:A:GLU:H	6	0.26	0.27	0.15
(1,2193)	1:173:A:GLN:HA	1:173:A:GLN:H	6	0.26	0.27	0.15
(1,1054)	1:199:B:GLN:HG3	1:175:A:LEU:HD13	6	0.25	0.04	0.24
(1,1054)	1:199:B:GLN:HG3	1:175:A:LEU:HD11	6	0.25	0.04	0.24
(1,1054)	1:199:B:GLN:HG3	1:175:A:LEU:HD12	6	0.25	0.04	0.24
(1,1053)	1:199:A:GLN:HG3	1:175:B:LEU:HD13	6	0.25	0.05	0.24
(1,1053)	1:199:A:GLN:HG3	1:175:B:LEU:HD11	6	0.25	0.05	0.24
(1,1053)	1:199:A:GLN:HG3	1:175:B:LEU:HD12	6	0.25	0.05	0.24
(1,1186)	1:175:B:LEU:HA	1:196:A:ALA:HB3	6	0.25	0.08	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1186)	1:175:B:LEU:HA	1:196:A:ALA:HB1	6	0.25	0.08	0.26
(1,1186)	1:175:B:LEU:HA	1:196:A:ALA:HB2	6	0.25	0.08	0.26
(1,1185)	1:175:A:LEU:HA	1:196:B:ALA:HB3	6	0.25	0.08	0.24
(1,1185)	1:175:A:LEU:HA	1:196:B:ALA:HB1	6	0.25	0.08	0.24
(1,1185)	1:175:A:LEU:HA	1:196:B:ALA:HB2	6	0.25	0.08	0.24
(1,223)	1:177:A:VAL:HG22	1:204:B:LEU:HD13	6	0.23	0.07	0.24
(1,223)	1:177:A:VAL:HG21	1:204:B:LEU:HD12	6	0.23	0.07	0.24
(1,223)	1:177:A:VAL:HG23	1:204:B:LEU:HD11	6	0.23	0.07	0.24
(1,223)	1:177:A:VAL:HG22	1:204:B:LEU:HD12	6	0.23	0.07	0.24
(1,223)	1:177:A:VAL:HG21	1:204:B:LEU:HD13	6	0.23	0.07	0.24
(1,229)	1:204:A:LEU:HD13	1:177:B:VAL:HG22	6	0.23	0.07	0.24
(1,229)	1:204:A:LEU:HD12	1:177:B:VAL:HG21	6	0.23	0.07	0.24
(1,229)	1:204:A:LEU:HD11	1:177:B:VAL:HG23	6	0.23	0.07	0.24
(1,229)	1:204:A:LEU:HD12	1:177:B:VAL:HG23	6	0.23	0.07	0.24
(1,229)	1:204:A:LEU:HD13	1:177:B:VAL:HG21	6	0.23	0.07	0.24
(1,230)	1:204:B:LEU:HD13	1:177:A:VAL:HG22	6	0.23	0.07	0.24
(1,230)	1:204:B:LEU:HD12	1:177:A:VAL:HG21	6	0.23	0.07	0.24
(1,230)	1:204:B:LEU:HD11	1:177:A:VAL:HG23	6	0.23	0.07	0.24
(1,230)	1:204:B:LEU:HD12	1:177:A:VAL:HG22	6	0.23	0.07	0.24
(1,230)	1:204:B:LEU:HD13	1:177:A:VAL:HG21	6	0.23	0.07	0.24
(1,224)	1:177:B:VAL:HG22	1:204:A:LEU:HD13	6	0.23	0.07	0.23
(1,224)	1:177:B:VAL:HG21	1:204:A:LEU:HD12	6	0.23	0.07	0.23
(1,224)	1:177:B:VAL:HG23	1:204:A:LEU:HD11	6	0.23	0.07	0.23
(1,224)	1:177:B:VAL:HG23	1:204:A:LEU:HD12	6	0.23	0.07	0.23
(1,224)	1:177:B:VAL:HG21	1:204:A:LEU:HD13	6	0.23	0.07	0.23
(1,2876)	1:205:B:GLN:H	1:177:A:VAL:HG22	6	0.21	0.06	0.19
(1,2876)	1:205:B:GLN:H	1:177:B:VAL:HG22	6	0.21	0.06	0.19
(1,2876)	1:205:B:GLN:H	1:177:A:VAL:HG23	6	0.21	0.06	0.19
(1,2876)	1:205:B:GLN:H	1:177:B:VAL:HG21	6	0.21	0.06	0.19
(1,2586)	1:179:B:TRP:HE1	1:205:B:GLN:HA	6	0.2	0.09	0.16
(1,2875)	1:205:A:GLN:H	1:177:B:VAL:HG22	6	0.2	0.06	0.18
(1,2875)	1:205:A:GLN:H	1:177:A:VAL:HG22	6	0.2	0.06	0.18
(1,2875)	1:205:A:GLN:H	1:177:B:VAL:HG23	6	0.2	0.06	0.18
(1,2875)	1:205:A:GLN:H	1:177:A:VAL:HG21	6	0.2	0.06	0.18
(1,2107)	1:177:A:VAL:HG21	1:190:B:PHE:HE2	6	0.18	0.06	0.15
(1,2107)	1:177:A:VAL:HG22	1:190:B:PHE:HE2	6	0.18	0.06	0.15
(1,2107)	1:177:A:VAL:HG23	1:190:B:PHE:HE2	6	0.18	0.06	0.15
(1,743)	1:184:A:ALA:HB2	1:181:A:ASP:HA	6	0.14	0.04	0.14
(1,743)	1:184:A:ALA:HB1	1:181:A:ASP:HA	6	0.14	0.04	0.14
(1,743)	1:184:A:ALA:HB3	1:181:A:ASP:HA	6	0.14	0.04	0.14
(1,744)	1:184:B:ALA:HB2	1:181:B:ASP:HA	6	0.14	0.04	0.14
(1,744)	1:184:B:ALA:HB1	1:181:B:ASP:HA	6	0.14	0.04	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,744)	1:184:B:ALA:HB3	1:181:B:ASP:HA	6	0.14	0.04	0.14
(1,1398)	1:202:B:GLU:H	1:200:B:VAL:HG11	6	0.14	0.02	0.14
(1,1398)	1:202:B:GLU:H	1:200:B:VAL:HG13	6	0.14	0.02	0.14
(1,1398)	1:202:B:GLU:H	1:200:B:VAL:HG12	6	0.14	0.02	0.14
(1,1397)	1:202:A:GLU:H	1:200:A:VAL:HG11	6	0.14	0.02	0.13
(1,1397)	1:202:A:GLU:H	1:200:A:VAL:HG13	6	0.14	0.02	0.13
(1,1397)	1:202:A:GLU:H	1:200:A:VAL:HG12	6	0.14	0.02	0.13
(1,2531)	1:211:A:ALA:H	1:210:A:LEU:HB3	6	0.13	0.01	0.14
(1,1115)	1:175:A:LEU:HD21	1:199:B:GLN:H	5	0.51	0.45	0.38
(1,1115)	1:175:A:LEU:HD23	1:199:B:GLN:H	5	0.51	0.45	0.38
(1,2370)	1:175:B:LEU:HG	1:199:A:GLN:HE22	5	0.28	0.12	0.33
(1,2369)	1:175:A:LEU:HG	1:199:B:GLN:HE22	5	0.27	0.11	0.32
(1,2585)	1:179:A:TRP:HE1	1:205:A:GLN:HA	5	0.22	0.08	0.18
(1,307)	1:199:A:GLN:HB3	1:200:A:VAL:HG12	5	0.19	0.06	0.18
(1,307)	1:199:A:GLN:HB3	1:200:A:VAL:HG11	5	0.19	0.06	0.18
(1,307)	1:199:A:GLN:HB3	1:200:A:VAL:HG13	5	0.19	0.06	0.18
(1,308)	1:199:B:GLN:HB3	1:200:B:VAL:HG12	5	0.19	0.06	0.18
(1,308)	1:199:B:GLN:HB3	1:200:B:VAL:HG11	5	0.19	0.06	0.18
(1,308)	1:199:B:GLN:HB3	1:200:B:VAL:HG13	5	0.19	0.06	0.18
(1,2108)	1:177:B:VAL:HG21	1:190:A:PHE:HE2	5	0.19	0.06	0.19
(1,2108)	1:177:B:VAL:HG22	1:190:A:PHE:HE2	5	0.19	0.06	0.19
(1,2108)	1:177:B:VAL:HG23	1:190:A:PHE:HE2	5	0.19	0.06	0.19
(1,1149)	1:178:A:PRO:HD3	1:177:A:VAL:HG21	5	0.16	0.03	0.16
(1,1149)	1:178:A:PRO:HD3	1:177:A:VAL:HG22	5	0.16	0.03	0.16
(1,1149)	1:178:A:PRO:HD3	1:177:A:VAL:HG23	5	0.16	0.03	0.16
(1,1150)	1:178:B:PRO:HD3	1:177:B:VAL:HG21	5	0.16	0.03	0.16
(1,1150)	1:178:B:PRO:HD3	1:177:B:VAL:HG22	5	0.16	0.03	0.16
(1,1150)	1:178:B:PRO:HD3	1:177:B:VAL:HG23	5	0.16	0.03	0.16
(1,246)	1:200:B:VAL:HG12	1:197:B:VAL:HA	5	0.15	0.05	0.13
(1,246)	1:200:B:VAL:HG13	1:197:B:VAL:HA	5	0.15	0.05	0.13
(1,2564)	1:209:B:SER:H	1:210:B:LEU:HD23	5	0.15	0.03	0.14
(1,2564)	1:209:B:SER:H	1:210:B:LEU:HD22	5	0.15	0.03	0.14
(1,2564)	1:209:B:SER:H	1:210:B:LEU:HD21	5	0.15	0.03	0.14
(1,2563)	1:209:A:SER:H	1:210:A:LEU:HD23	5	0.15	0.03	0.14
(1,2563)	1:209:A:SER:H	1:210:A:LEU:HD22	5	0.15	0.03	0.14
(1,2563)	1:209:A:SER:H	1:210:A:LEU:HD21	5	0.15	0.03	0.14
(1,2157)	1:181:A:ASP:H	1:182:A:ILE:HB	5	0.15	0.02	0.15
(1,2158)	1:181:B:ASP:H	1:182:B:ILE:HB	5	0.15	0.03	0.14
(1,2265)	1:210:A:LEU:HA	1:211:A:ALA:HB3	4	1.78	0.02	1.77
(1,2265)	1:210:A:LEU:HA	1:211:A:ALA:HB1	4	1.78	0.02	1.77
(1,2265)	1:210:A:LEU:HA	1:211:A:ALA:HB2	4	1.78	0.02	1.77
(1,2266)	1:210:B:LEU:HA	1:211:B:ALA:HB3	4	1.77	0.02	1.76

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2266)	1:210:B:LEU:HA	1:211:B:ALA:HB1	4	1.77	0.02	1.76
(1,2266)	1:210:B:LEU:HA	1:211:B:ALA:HB2	4	1.77	0.02	1.76
(1,2838)	1:179:B:TRP:H	1:180:B:ASP:HB3	4	1.2	0.03	1.2
(1,2837)	1:179:A:TRP:H	1:180:A:ASP:HB3	4	1.2	0.03	1.19
(1,1169)	1:206:A:LYS:HG3	1:209:A:SER:HB3	4	1.15	0.11	1.16
(1,1170)	1:206:B:LYS:HG3	1:209:B:SER:HB3	4	1.14	0.12	1.16
(1,587)	1:209:A:SER:H	1:209:A:SER:HB3	4	0.96	0.0	0.96
(1,588)	1:209:B:SER:H	1:209:B:SER:HB3	4	0.95	0.0	0.95
(1,585)	1:209:A:SER:HB3	1:210:A:LEU:H	4	0.9	0.02	0.9
(1,586)	1:209:B:SER:HB3	1:210:B:LEU:H	4	0.9	0.01	0.9
(1,171)	1:211:A:ALA:HB1	1:206:B:LYS:HE3	4	0.86	0.17	0.82
(1,171)	1:211:A:ALA:HB2	1:206:B:LYS:HE3	4	0.86	0.17	0.82
(1,171)	1:211:A:ALA:HB3	1:206:B:LYS:HE3	4	0.86	0.17	0.82
(1,172)	1:211:B:ALA:HB1	1:206:A:LYS:HE3	4	0.85	0.17	0.8
(1,172)	1:211:B:ALA:HB2	1:206:A:LYS:HE3	4	0.85	0.17	0.8
(1,172)	1:211:B:ALA:HB3	1:206:A:LYS:HE3	4	0.85	0.17	0.8
(1,1411)	1:212:A:LYS:H	1:212:A:LYS:HG2	4	0.72	0.48	0.74
(1,1412)	1:212:B:LYS:H	1:212:B:LYS:HG2	4	0.72	0.48	0.73
(1,113)	1:173:A:GLN:HE21	1:175:A:LEU:HD13	4	0.7	0.17	0.68
(1,113)	1:173:A:GLN:HE21	1:175:A:LEU:HD12	4	0.7	0.17	0.68
(1,113)	1:173:A:GLN:HE21	1:175:A:LEU:HD11	4	0.7	0.17	0.68
(1,114)	1:173:B:GLN:HE21	1:175:B:LEU:HD13	4	0.69	0.17	0.68
(1,114)	1:173:B:GLN:HE21	1:175:B:LEU:HD12	4	0.69	0.17	0.68
(1,114)	1:173:B:GLN:HE21	1:175:B:LEU:HD11	4	0.69	0.17	0.68
(1,1983)	1:173:B:GLN:H	1:173:B:GLN:HB2	4	0.67	0.05	0.66
(1,1984)	1:173:A:GLN:H	1:173:A:GLN:HB2	4	0.67	0.05	0.66
(1,1384)	1:180:B:ASP:H	1:180:B:ASP:HB3	4	0.61	0.01	0.61
(1,1383)	1:180:A:ASP:H	1:180:A:ASP:HB3	4	0.6	0.01	0.6
(1,1409)	1:212:A:LYS:H	1:212:A:LYS:HB3	4	0.6	0.44	0.62
(1,1410)	1:212:B:LYS:H	1:212:B:LYS:HB3	4	0.6	0.44	0.62
(1,1116)	1:175:B:LEU:HD21	1:199:A:GLN:H	4	0.6	0.46	0.48
(1,1116)	1:175:B:LEU:HD23	1:199:A:GLN:H	4	0.6	0.46	0.48
(1,2545)	1:181:A:ASP:H	1:180:A:ASP:HB3	4	0.6	0.04	0.6
(1,2545)	1:181:A:ASP:H	1:181:A:ASP:HB3	4	0.6	0.04	0.6
(1,2546)	1:181:B:ASP:H	1:180:B:ASP:HB3	4	0.6	0.04	0.6
(1,2546)	1:181:B:ASP:H	1:181:B:ASP:HB3	4	0.6	0.04	0.6
(1,1429)	1:211:A:ALA:H	1:206:B:LYS:HE3	4	0.57	0.17	0.56
(1,1430)	1:211:B:ALA:H	1:206:A:LYS:HE3	4	0.56	0.18	0.55
(1,311)	1:173:A:GLN:HB2	1:173:A:GLN:H	4	0.53	0.05	0.53
(1,312)	1:173:B:GLN:HB2	1:173:B:GLN:H	4	0.53	0.05	0.52
(1,1171)	1:209:A:SER:HB3	1:210:A:LEU:HD22	4	0.46	0.06	0.44
(1,1171)	1:209:A:SER:HB3	1:210:A:LEU:HD23	4	0.46	0.06	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1172)	1:209:B:SER:HB3	1:210:B:LEU:HD22	4	0.45	0.06	0.44
(1,1172)	1:209:B:SER:HB3	1:210:B:LEU:HD23	4	0.45	0.06	0.44
(1,1781)	1:175:A:LEU:H	1:177:A:VAL:HG21	4	0.39	0.13	0.42
(1,1781)	1:175:A:LEU:H	1:177:A:VAL:HG23	4	0.39	0.13	0.42
(1,1781)	1:175:A:LEU:H	1:177:A:VAL:HG22	4	0.39	0.13	0.42
(1,1782)	1:175:B:LEU:H	1:177:B:VAL:HG21	4	0.39	0.12	0.42
(1,1782)	1:175:B:LEU:H	1:177:B:VAL:HG23	4	0.39	0.12	0.42
(1,1782)	1:175:B:LEU:H	1:177:B:VAL:HG22	4	0.39	0.12	0.42
(1,319)	1:173:A:GLN:HG3	1:173:A:GLN:H	4	0.38	0.12	0.34
(1,320)	1:173:B:GLN:HG3	1:173:B:GLN:H	4	0.38	0.12	0.34
(1,217)	1:210:A:LEU:HD12	1:211:B:ALA:HA	4	0.36	0.13	0.39
(1,217)	1:210:A:LEU:HD11	1:211:B:ALA:HA	4	0.36	0.13	0.39
(1,218)	1:210:B:LEU:HD12	1:211:A:ALA:HA	4	0.36	0.13	0.39
(1,218)	1:210:B:LEU:HD11	1:211:A:ALA:HA	4	0.36	0.13	0.39
(1,2154)	1:205:B:GLN:HG2	1:205:B:GLN:H	4	0.34	0.39	0.12
(1,2153)	1:205:A:GLN:HG2	1:205:A:GLN:H	4	0.34	0.39	0.12
(1,309)	1:201:A:MET:HB2	1:202:A:GLU:H	4	0.32	0.05	0.34
(1,310)	1:201:B:MET:HB2	1:202:B:GLU:H	4	0.32	0.04	0.34
(1,1049)	1:212:A:LYS:HB3	1:212:A:LYS:HE3	4	0.32	0.18	0.32
(1,1050)	1:212:B:LYS:HB3	1:212:B:LYS:HE3	4	0.32	0.18	0.32
(1,1408)	1:212:B:LYS:H	1:203:A:ARG:HD3	4	0.24	0.17	0.16
(1,1407)	1:212:A:LYS:H	1:203:B:ARG:HD3	4	0.23	0.17	0.14
(1,2353)	1:211:A:ALA:H	1:212:A:LYS:HG2	4	0.23	0.04	0.22
(1,2353)	1:206:A:LYS:HG3	1:210:A:LEU:H	4	0.23	0.04	0.22
(1,2354)	1:211:B:ALA:H	1:212:B:LYS:HG2	4	0.23	0.04	0.22
(1,2354)	1:206:B:LYS:HG3	1:210:B:LEU:H	4	0.23	0.04	0.22
(1,2109)	1:177:A:VAL:HG22	1:179:A:TRP:HH2	4	0.19	0.07	0.17
(1,2109)	1:177:A:VAL:HG23	1:179:A:TRP:HH2	4	0.19	0.07	0.17
(1,2110)	1:177:B:VAL:HG22	1:179:B:TRP:HH2	4	0.19	0.08	0.16
(1,2110)	1:177:B:VAL:HG23	1:179:B:TRP:HH2	4	0.19	0.08	0.16
(1,2253)	1:211:A:ALA:HA	1:206:B:LYS:HG2	4	0.18	0.05	0.16
(1,2254)	1:211:B:ALA:HA	1:206:A:LYS:HG2	4	0.17	0.05	0.16
(1,2326)	1:197:B:VAL:HG11	1:198:B:ARG:HA	4	0.17	0.04	0.17
(1,2326)	1:197:B:VAL:HG12	1:198:B:ARG:HA	4	0.17	0.04	0.17
(1,2325)	1:197:A:VAL:HG11	1:198:A:ARG:HA	4	0.17	0.04	0.16
(1,2325)	1:197:A:VAL:HG12	1:198:A:ARG:HA	4	0.17	0.04	0.16
(1,245)	1:200:A:VAL:HG13	1:197:A:VAL:HA	4	0.16	0.05	0.16
(1,245)	1:200:A:VAL:HG12	1:197:A:VAL:HA	4	0.16	0.05	0.16
(1,2341)	1:204:A:LEU:HG	1:182:B:ILE:HD12	4	0.16	0.04	0.15
(1,2341)	1:204:A:LEU:HG	1:182:B:ILE:HD13	4	0.16	0.04	0.15
(1,2341)	1:204:A:LEU:HG	1:182:B:ILE:HD11	4	0.16	0.04	0.15
(1,2342)	1:204:B:LEU:HG	1:182:A:ILE:HD12	4	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2342)	1:204:B:LEU:HG	1:182:A:ILE:HD13	4	0.15	0.03	0.16
(1,1378)	1:180:B:ASP:H	1:183:B:GLU:HA	4	0.15	0.05	0.14
(1,1377)	1:180:A:ASP:H	1:183:A:GLU:HA	4	0.15	0.04	0.14
(1,1921)	1:179:A:TRP:H	1:179:A:TRP:HZ3	4	0.15	0.03	0.15
(1,1922)	1:179:B:TRP:H	1:179:B:TRP:HZ3	4	0.15	0.04	0.15
(1,1030)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	4	0.14	0.04	0.13
(1,1030)	1:182:B:ILE:HD12	1:178:B:PRO:HB2	4	0.14	0.04	0.13
(1,2106)	1:177:B:VAL:HG21	1:208:B:TRP:HE3	4	0.14	0.04	0.13
(1,2106)	1:177:B:VAL:HG22	1:208:B:TRP:HZ3	4	0.14	0.04	0.13
(1,2106)	1:177:B:VAL:HG22	1:208:B:TRP:HE3	4	0.14	0.04	0.13
(1,1029)	1:182:A:ILE:HD11	1:178:A:PRO:HB2	4	0.14	0.04	0.12
(1,1029)	1:182:A:ILE:HD12	1:178:A:PRO:HB2	4	0.14	0.04	0.12
(1,2105)	1:177:A:VAL:HG21	1:208:A:TRP:HE3	4	0.14	0.04	0.13
(1,2105)	1:177:A:VAL:HG22	1:208:A:TRP:HZ3	4	0.14	0.04	0.13
(1,2105)	1:177:A:VAL:HG22	1:208:A:TRP:HE3	4	0.14	0.04	0.13
(1,2097)	1:204:A:LEU:HD22	1:208:B:TRP:H	4	0.14	0.03	0.15
(1,2097)	1:204:A:LEU:HD21	1:208:B:TRP:H	4	0.14	0.03	0.15
(1,2097)	1:204:A:LEU:HD23	1:208:B:TRP:H	4	0.14	0.03	0.15
(1,2098)	1:204:B:LEU:HD22	1:208:A:TRP:H	4	0.14	0.01	0.14
(1,2098)	1:204:B:LEU:HD21	1:208:A:TRP:H	4	0.14	0.01	0.14
(1,2098)	1:204:B:LEU:HD23	1:208:A:TRP:H	4	0.14	0.01	0.14
(1,2704)	1:200:B:VAL:H	1:190:B:PHE:HE2	4	0.13	0.02	0.12
(1,1644)	1:201:B:MET:H	1:186:B:LEU:HA	4	0.13	0.03	0.12
(1,2703)	1:200:A:VAL:H	1:190:A:PHE:HE2	4	0.13	0.02	0.12
(1,1643)	1:201:A:MET:H	1:186:A:LEU:HA	4	0.12	0.02	0.12
(1,2256)	1:196:B:ALA:HA	1:175:A:LEU:HD21	4	0.12	0.01	0.12
(1,2256)	1:196:B:ALA:HA	1:175:A:LEU:HD22	4	0.12	0.01	0.12
(1,2588)	1:208:B:TRP:H	1:204:B:LEU:HB3	4	0.12	0.01	0.12
(1,764)	1:201:B:MET:HE1	1:201:B:MET:HA	3	1.7	0.26	1.58
(1,764)	1:201:B:MET:HE3	1:201:B:MET:HA	3	1.7	0.26	1.58
(1,763)	1:201:A:MET:HE1	1:201:A:MET:HA	3	1.7	0.25	1.58
(1,763)	1:201:A:MET:HE3	1:201:A:MET:HA	3	1.7	0.25	1.58
(1,191)	1:201:A:MET:HE1	1:182:A:ILE:HG21	3	1.25	0.41	1.45
(1,191)	1:201:A:MET:HE1	1:182:A:ILE:HG22	3	1.25	0.41	1.45
(1,191)	1:201:A:MET:HE2	1:182:A:ILE:HG22	3	1.25	0.41	1.45
(1,192)	1:201:B:MET:HE1	1:182:B:ILE:HG21	3	1.24	0.4	1.44
(1,192)	1:201:B:MET:HE1	1:182:B:ILE:HG22	3	1.24	0.4	1.44
(1,192)	1:201:B:MET:HE2	1:182:B:ILE:HG22	3	1.24	0.4	1.44
(1,1979)	1:173:B:GLN:H	1:212:B:LYS:HA	3	1.15	0.14	1.09
(1,1980)	1:173:A:GLN:H	1:212:A:LYS:HA	3	1.15	0.14	1.09
(1,94)	1:175:B:LEU:HD23	1:200:A:VAL:H	3	0.79	0.48	0.57
(1,94)	1:175:B:LEU:HD22	1:200:A:VAL:H	3	0.79	0.48	0.57

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,941)	1:175:A:LEU:HD23	1:200:B:VAL:HG11	3	0.79	0.44	0.55
(1,941)	1:175:A:LEU:HD22	1:200:B:VAL:HG12	3	0.79	0.44	0.55
(1,942)	1:175:B:LEU:HD23	1:200:A:VAL:HG11	3	0.79	0.44	0.56
(1,942)	1:175:B:LEU:HD22	1:200:A:VAL:HG12	3	0.79	0.44	0.56
(1,93)	1:175:A:LEU:HD23	1:200:B:VAL:H	3	0.78	0.48	0.54
(1,93)	1:175:A:LEU:HD22	1:200:B:VAL:H	3	0.78	0.48	0.54
(1,1558)	1:173:B:GLN:HE21	1:200:A:VAL:HG13	3	0.74	0.17	0.84
(1,1558)	1:173:B:GLN:HE21	1:200:A:VAL:HG12	3	0.74	0.17	0.84
(1,1557)	1:173:A:GLN:HE21	1:200:B:VAL:HG13	3	0.74	0.13	0.82
(1,1557)	1:173:A:GLN:HE21	1:200:B:VAL:HG12	3	0.74	0.13	0.82
(1,31)	1:201:A:MET:HE1	1:179:A:TRP:HZ3	3	0.69	0.52	0.44
(1,31)	1:201:A:MET:HE3	1:179:A:TRP:HZ3	3	0.69	0.52	0.44
(1,32)	1:201:B:MET:HE1	1:179:B:TRP:HZ3	3	0.69	0.52	0.44
(1,32)	1:201:B:MET:HE3	1:179:B:TRP:HZ3	3	0.69	0.52	0.44
(1,24)	1:201:B:MET:HE3	1:183:B:GLU:HA	3	0.62	0.28	0.57
(1,24)	1:201:B:MET:HE1	1:183:B:GLU:HA	3	0.62	0.28	0.57
(1,23)	1:201:A:MET:HE3	1:183:A:GLU:HA	3	0.62	0.28	0.57
(1,23)	1:201:A:MET:HE1	1:183:A:GLU:HA	3	0.62	0.28	0.57
(1,641)	1:198:A:ARG:H	1:198:A:ARG:HD3	3	0.55	0.21	0.69
(1,642)	1:198:B:ARG:H	1:198:B:ARG:HD3	3	0.55	0.21	0.69
(1,1584)	1:173:B:GLN:HE21	1:200:A:VAL:HA	3	0.53	0.17	0.43
(1,1583)	1:173:A:GLN:HE21	1:200:B:VAL:HA	3	0.52	0.15	0.43
(1,1145)	1:211:A:ALA:HA	1:206:B:LYS:HE3	3	0.5	0.13	0.46
(1,1146)	1:211:B:ALA:HA	1:206:A:LYS:HE3	3	0.49	0.12	0.44
(1,644)	1:199:B:GLN:H	1:198:B:ARG:HD3	3	0.46	0.24	0.6
(1,643)	1:199:A:GLN:H	1:198:A:ARG:HD3	3	0.45	0.24	0.6
(1,2668)	1:205:B:GLN:H	1:202:B:GLU:HB2	3	0.4	0.19	0.52
(1,2668)	1:205:B:GLN:H	1:201:B:MET:HE3	3	0.4	0.19	0.52
(1,2667)	1:205:A:GLN:H	1:202:A:GLU:HB2	3	0.4	0.19	0.52
(1,2667)	1:205:A:GLN:H	1:201:A:MET:HE3	3	0.4	0.19	0.52
(1,2394)	1:211:B:ALA:HA	1:207:A:GLY:HA2	3	0.3	0.13	0.34
(1,683)	1:211:A:ALA:HA	1:210:B:LEU:HD12	3	0.3	0.07	0.27
(1,684)	1:211:B:ALA:HA	1:210:A:LEU:HD12	3	0.3	0.07	0.27
(1,2393)	1:211:A:ALA:HA	1:207:B:GLY:HA2	3	0.3	0.11	0.32
(1,1191)	1:188:A:ASN:HA	1:191:A:GLU:HG2	3	0.29	0.18	0.18
(1,1192)	1:188:B:ASN:HA	1:191:B:GLU:HG2	3	0.29	0.18	0.18
(1,2091)	1:175:A:LEU:H	1:175:A:LEU:HD12	3	0.25	0.03	0.24
(1,2092)	1:175:B:LEU:H	1:175:B:LEU:HD12	3	0.25	0.02	0.25
(1,1735)	1:195:A:ALA:H	1:194:A:GLN:HG3	3	0.24	0.08	0.24
(1,2855)	1:174:A:GLU:H	1:196:B:ALA:HB1	3	0.24	0.14	0.18
(1,2855)	1:174:A:GLU:H	1:196:B:ALA:HB3	3	0.24	0.14	0.18
(1,2855)	1:174:A:GLU:H	1:196:B:ALA:HB2	3	0.24	0.14	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1736)	1:195:B:ALA:H	1:194:B:GLN:HG3	3	0.24	0.08	0.23
(1,1923)	1:179:A:TRP:H	1:205:A:GLN:HE22	3	0.14	0.03	0.13
(1,1924)	1:179:B:TRP:H	1:205:B:GLN:HE22	3	0.14	0.03	0.13
(1,2117)	1:182:A:ILE:HD13	1:178:A:PRO:HD2	3	0.13	0.03	0.12
(1,2117)	1:182:A:ILE:HD11	1:178:A:PRO:HD2	3	0.13	0.03	0.12
(1,2117)	1:182:A:ILE:HD12	1:178:A:PRO:HD2	3	0.13	0.03	0.12
(1,2118)	1:182:B:ILE:HD13	1:178:B:PRO:HD2	3	0.13	0.03	0.12
(1,2118)	1:182:B:ILE:HD11	1:178:B:PRO:HD2	3	0.13	0.03	0.12
(1,2118)	1:182:B:ILE:HD12	1:178:B:PRO:HD2	3	0.13	0.03	0.12
(1,2801)	1:186:A:LEU:H	1:185:A:LEU:HD22	3	0.13	0.01	0.14
(1,2802)	1:186:B:LEU:H	1:185:B:LEU:HD22	3	0.13	0.01	0.14
(1,2255)	1:196:A:ALA:HA	1:175:B:LEU:HD21	3	0.13	0.01	0.14
(1,2255)	1:196:A:ALA:HA	1:175:B:LEU:HD22	3	0.13	0.01	0.14
(1,259)	1:185:A:LEU:HD21	1:178:B:PRO:HB2	3	0.12	0.02	0.11
(1,260)	1:185:B:LEU:HD21	1:178:A:PRO:HB2	3	0.12	0.02	0.12
(1,2587)	1:208:A:TRP:H	1:204:A:LEU:HB3	3	0.12	0.01	0.12
(1,1647)	1:201:A:MET:H	1:200:A:VAL:HG11	3	0.1	0.0	0.1
(1,1647)	1:201:A:MET:H	1:200:A:VAL:HG13	3	0.1	0.0	0.1
(1,1648)	1:201:B:MET:H	1:200:B:VAL:HG11	3	0.1	0.0	0.1
(1,1648)	1:201:B:MET:H	1:200:B:VAL:HG13	3	0.1	0.0	0.1
(1,2832)	1:181:B:ASP:H	1:177:B:VAL:HA	3	0.1	0.0	0.1
(1,195)	1:201:A:MET:HE2	1:205:A:GLN:HG3	2	1.25	0.96	1.25
(1,196)	1:201:B:MET:HE2	1:205:B:GLN:HG3	2	1.25	0.96	1.25
(1,1975)	1:174:A:GLU:H	1:174:A:GLU:HB2	2	1.01	0.19	1.01
(1,1976)	1:174:B:GLU:H	1:174:B:GLU:HB2	2	1.01	0.19	1.01
(1,2184)	1:187:B:LYS:H	1:188:B:ASN:HB3	2	0.84	0.73	0.84
(1,909)	1:201:A:MET:HG2	1:201:A:MET:HA	2	0.74	0.04	0.74
(1,910)	1:201:B:MET:HG2	1:201:B:MET:HA	2	0.74	0.04	0.74
(1,186)	1:184:B:ALA:HB1	1:187:B:LYS:HE2	2	0.64	0.1	0.64
(1,185)	1:184:A:ALA:HB1	1:187:A:LYS:HE2	2	0.64	0.11	0.64
(1,765)	1:174:A:GLU:HA	1:174:A:GLU:HG2	2	0.64	0.0	0.64
(1,766)	1:174:B:GLU:HA	1:174:B:GLU:HG2	2	0.64	0.01	0.64
(1,346)	1:191:B:GLU:H	1:191:B:GLU:HG2	2	0.63	0.01	0.63
(1,345)	1:191:A:GLU:H	1:191:A:GLU:HG2	2	0.62	0.02	0.62
(1,869)	1:188:A:ASN:HB3	1:187:A:LYS:HB3	2	0.62	0.49	0.62
(1,870)	1:188:B:ASN:HB3	1:187:B:LYS:HB3	2	0.62	0.5	0.62
(1,2579)	1:208:A:TRP:HE1	1:175:A:LEU:HD11	2	0.56	0.09	0.56
(1,2580)	1:208:B:TRP:HE1	1:175:B:LEU:HD11	2	0.56	0.09	0.56
(1,27)	1:183:A:GLU:H	1:201:A:MET:HE1	2	0.54	0.21	0.54
(1,28)	1:183:B:GLU:H	1:201:B:MET:HE1	2	0.53	0.2	0.53
(1,2150)	1:175:B:LEU:H	1:173:B:GLN:HB3	2	0.53	0.25	0.53
(1,2150)	1:173:B:GLN:HB3	1:174:B:GLU:H	2	0.53	0.25	0.53

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2149)	1:175:A:LEU:H	1:173:A:GLN:HB3	2	0.52	0.26	0.52
(1,2149)	1:173:A:GLN:HB3	1:174:A:GLU:H	2	0.52	0.26	0.52
(1,1117)	1:175:A:LEU:HD23	1:208:A:TRP:HH2	2	0.47	0.31	0.47
(1,1117)	1:175:A:LEU:HD22	1:208:A:TRP:HH2	2	0.47	0.31	0.47
(1,1118)	1:175:B:LEU:HD23	1:208:B:TRP:HH2	2	0.47	0.31	0.47
(1,1118)	1:175:B:LEU:HD22	1:208:B:TRP:HH2	2	0.47	0.31	0.47
(1,279)	1:187:A:LYS:HG3	1:187:A:LYS:HE2	2	0.4	0.0	0.4
(1,280)	1:187:B:LYS:HG3	1:187:B:LYS:HE2	2	0.4	0.01	0.4
(1,975)	1:212:A:LYS:HB3	1:212:A:LYS:HA	2	0.36	0.0	0.36
(1,976)	1:212:B:LYS:HB3	1:212:B:LYS:HA	2	0.36	0.01	0.36
(1,2449)	1:184:A:ALA:H	1:187:A:LYS:HE2	2	0.36	0.07	0.36
(1,2450)	1:184:B:ALA:H	1:187:B:LYS:HE2	2	0.36	0.07	0.36
(1,1200)	1:203:B:ARG:HD3	1:212:A:LYS:HA	2	0.34	0.14	0.34
(1,1199)	1:203:A:ARG:HD3	1:212:B:LYS:HA	2	0.32	0.16	0.32
(1,181)	1:196:A:ALA:HB3	1:193:A:ASP:HB2	2	0.31	0.1	0.31
(1,181)	1:196:A:ALA:HB2	1:193:A:ASP:HB2	2	0.31	0.1	0.31
(1,182)	1:196:B:ALA:HB3	1:193:B:ASP:HB2	2	0.31	0.1	0.31
(1,182)	1:196:B:ALA:HB2	1:193:B:ASP:HB2	2	0.31	0.1	0.31
(1,2856)	1:174:B:GLU:H	1:196:A:ALA:HB3	2	0.31	0.15	0.31
(1,2856)	1:174:B:GLU:H	1:196:A:ALA:HB2	2	0.31	0.15	0.31
(1,724)	1:190:B:PHE:HA	1:191:B:GLU:HG2	2	0.3	0.2	0.3
(1,1297)	1:191:A:GLU:H	1:187:A:LYS:HG3	2	0.3	0.18	0.3
(1,1298)	1:191:B:GLU:H	1:187:B:LYS:HG3	2	0.3	0.18	0.3
(1,2051)	1:192:A:ASN:HD22	1:192:A:ASN:H	2	0.3	0.08	0.3
(1,2052)	1:192:B:ASN:HD22	1:192:B:ASN:H	2	0.3	0.08	0.3
(1,1988)	1:173:A:GLN:H	1:173:A:GLN:HE22	2	0.26	0.03	0.26
(1,1987)	1:173:B:GLN:H	1:173:B:GLN:HE22	2	0.25	0.04	0.25
(1,645)	1:198:A:ARG:HD3	1:198:A:ARG:HB2	2	0.24	0.03	0.24
(1,646)	1:198:B:ARG:HD3	1:198:B:ARG:HB2	2	0.24	0.03	0.24
(1,1577)	1:192:A:ASN:HD21	1:193:A:ASP:HA	2	0.2	0.09	0.2
(1,1578)	1:192:B:ASN:HD21	1:193:B:ASP:HA	2	0.19	0.09	0.19
(1,2572)	1:208:B:TRP:HE1	1:203:A:ARG:HB3	2	0.18	0.02	0.18
(1,2571)	1:208:A:TRP:HE1	1:203:B:ARG:HB3	2	0.17	0.03	0.17
(1,1981)	1:173:B:GLN:H	1:173:B:GLN:HG3	2	0.17	0.07	0.17
(1,1982)	1:173:A:GLN:H	1:173:A:GLN:HG3	2	0.17	0.07	0.17
(1,2553)	1:210:A:LEU:H	1:206:A:LYS:HE3	2	0.16	0.02	0.16
(1,2554)	1:210:B:LEU:H	1:206:B:LYS:HE3	2	0.16	0.03	0.16
(1,1109)	1:201:A:MET:H	1:197:A:VAL:HG13	2	0.16	0.01	0.16
(1,1109)	1:201:A:MET:H	1:197:A:VAL:HG12	2	0.16	0.01	0.16
(1,1110)	1:201:B:MET:H	1:197:B:VAL:HG13	2	0.15	0.01	0.15
(1,1110)	1:201:B:MET:H	1:197:B:VAL:HG12	2	0.15	0.01	0.15
(1,85)	1:197:A:VAL:HG23	1:190:A:PHE:HD2	2	0.15	0.0	0.15

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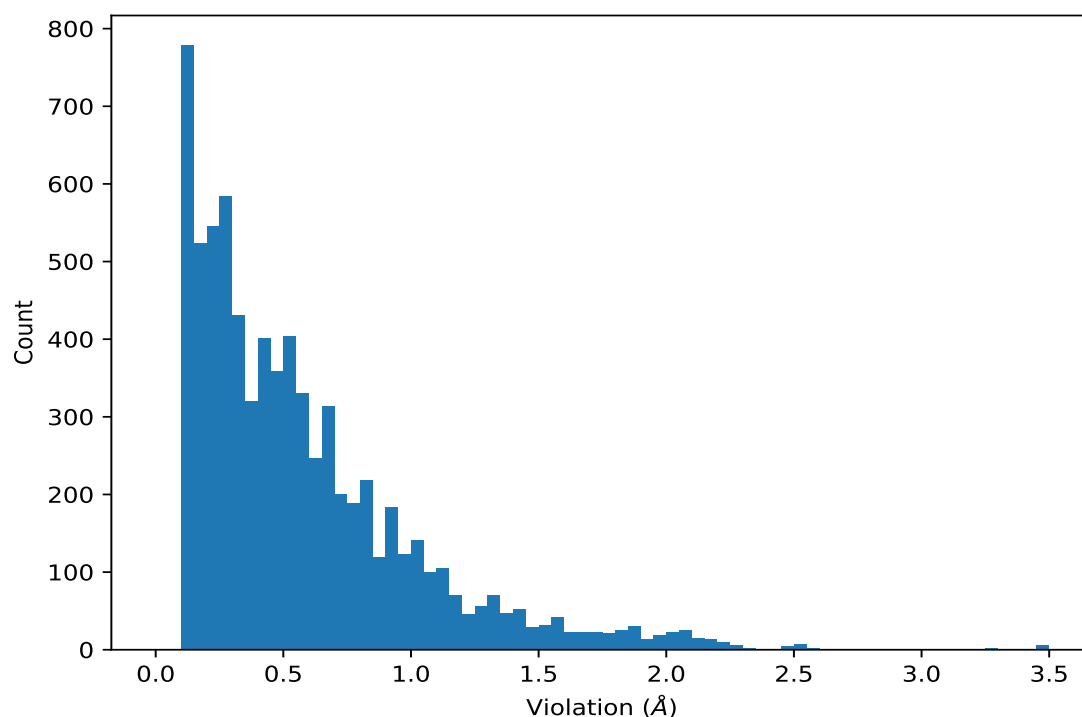
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,86)	1:197:B:VAL:HG23	1:190:B:PHE:HD2	2	0.15	0.0	0.15
(1,803)	1:203:A:ARG:HA	1:203:A:ARG:HG2	2	0.14	0.02	0.14
(1,804)	1:203:B:ARG:HA	1:203:B:ARG:HG2	2	0.13	0.03	0.13
(1,2559)	1:209:A:SER:H	1:206:A:LYS:HG2	2	0.11	0.0	0.11
(1,2831)	1:181:A:ASP:H	1:177:A:VAL:HA	2	0.11	0.0	0.11
(1,2560)	1:209:B:SER:H	1:206:B:LYS:HG2	2	0.11	0.0	0.11

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

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

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB3	1	3.49
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB3	1	3.48
(1,2630)	1:173:B:GLN:HE21	1:195:A:ALA:HB1	7	3.45
(1,2629)	1:173:A:GLN:HE21	1:195:B:ALA:HB1	7	3.45
(1,1466)	1:208:B:TRP:HE1	1:173:B:GLN:H	6	3.45
(1,1465)	1:208:A:TRP:HE1	1:173:A:GLN:H	6	3.45
(1,504)	1:189:B:ASN:HA	1:188:B:ASN:HD22	8	3.25
(1,503)	1:189:A:ASN:HA	1:188:A:ASN:HD22	8	3.25
(1,945)	1:175:A:LEU:HD23	1:199:B:GLN:HB3	7	2.6
(1,946)	1:175:B:LEU:HD23	1:199:A:GLN:HB3	7	2.59
(1,1466)	1:208:B:TRP:HE1	1:173:B:GLN:H	1	2.57
(1,1465)	1:208:A:TRP:HE1	1:173:A:GLN:H	1	2.55
(1,1466)	1:208:B:TRP:HE1	1:173:B:GLN:H	7	2.54
(1,887)	1:202:A:GLU:HG2	1:201:A:MET:HB2	10	2.54
(1,1465)	1:208:A:TRP:HE1	1:173:A:GLN:H	7	2.53
(1,888)	1:202:B:GLU:HG2	1:201:B:MET:HB2	10	2.53
(1,2302)	1:188:B:ASN:HB3	1:185:B:LEU:HB3	8	2.51
(1,2301)	1:188:A:ASN:HB3	1:185:A:LEU:HB3	8	2.51
(1,888)	1:202:B:GLU:HG2	1:201:B:MET:HB2	9	2.49
(1,887)	1:202:A:GLU:HG2	1:201:A:MET:HB2	9	2.49
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	4	2.48
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	4	2.46
(1,1466)	1:208:B:TRP:HE1	1:173:B:GLN:H	5	2.42
(1,1465)	1:208:A:TRP:HE1	1:173:A:GLN:H	5	2.4
(1,888)	1:202:B:GLU:HG2	1:201:B:MET:HB2	7	2.34
(1,887)	1:202:A:GLU:HG2	1:201:A:MET:HB2	7	2.34
(1,2350)	1:197:B:VAL:H	1:187:B:LYS:HG2	4	2.28
(1,2349)	1:197:A:VAL:H	1:187:A:LYS:HG2	4	2.28
(1,888)	1:202:B:GLU:HG2	1:201:B:MET:HB2	3	2.26
(1,887)	1:202:A:GLU:HG2	1:201:A:MET:HB2	3	2.26
(1,194)	1:201:B:MET:HE1	1:182:B:ILE:HD13	10	2.26
(1,193)	1:201:A:MET:HE1	1:182:A:ILE:HD13	10	2.25
(1,2646)	1:188:B:ASN:HD22	1:185:B:LEU:HB3	4	2.22
(1,2645)	1:188:A:ASN:HD22	1:185:A:LEU:HB3	4	2.21
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG23	5	2.21
(1,198)	1:201:B:MET:HE1	1:177:B:VAL:HG11	10	2.21
(1,197)	1:201:A:MET:HE1	1:177:A:VAL:HG11	10	2.21
(1,196)	1:201:B:MET:HE2	1:205:B:GLN:HG3	9	2.21
(1,195)	1:201:A:MET:HE2	1:205:A:GLN:HG3	9	2.21
(1,2350)	1:197:B:VAL:H	1:187:B:LYS:HG2	10	2.2
(1,2349)	1:197:A:VAL:H	1:187:A:LYS:HG2	10	2.2
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG23	5	2.2
(1,2646)	1:188:B:ASN:HD22	1:185:B:LEU:HB3	3	2.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2645)	1:188:A:ASN:HD22	1:185:A:LEU:HB3	3	2.19
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG21	6	2.19
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG21	6	2.19
(1,2646)	1:188:B:ASN:HD22	1:185:B:LEU:HB3	7	2.18
(1,2645)	1:188:A:ASN:HD22	1:185:A:LEU:HB3	7	2.18
(1,2350)	1:197:B:VAL:H	1:187:B:LYS:HG2	3	2.17
(1,2349)	1:197:A:VAL:H	1:187:A:LYS:HG2	3	2.17
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG23	7	2.17
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG23	7	2.16
(1,1091)	1:199:A:GLN:HG2	1:173:B:GLN:HE21	2	2.16
(1,2661)	1:192:A:ASN:HD22	1:194:A:GLN:HA	4	2.15
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	2	2.15
(1,2662)	1:192:B:ASN:HD22	1:194:B:GLN:HA	4	2.14
(1,2646)	1:188:B:ASN:HD22	1:185:B:LEU:HB3	2	2.14
(1,2645)	1:188:A:ASN:HD22	1:185:A:LEU:HB3	2	2.14
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	2	2.14
(1,2853)	1:176:A:THR:H	1:189:B:ASN:HB3	5	2.13
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG21	8	2.13
(1,1092)	1:199:B:GLN:HG2	1:173:A:GLN:HE21	2	2.13
(1,2854)	1:176:B:THR:H	1:189:A:ASN:HB3	5	2.12
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG21	8	2.11
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	10	2.11
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	10	2.11
(1,1091)	1:199:A:GLN:HG2	1:173:B:GLN:HE21	3	2.11
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD13	4	2.11
(1,2331)	1:212:A:LYS:HB3	1:211:A:ALA:H	5	2.1
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD13	4	2.1
(1,2332)	1:212:B:LYS:HB3	1:211:B:ALA:H	5	2.09
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD13	8	2.09
(1,2662)	1:192:B:ASN:HD22	1:194:B:GLN:HA	2	2.08
(1,2661)	1:192:A:ASN:HD22	1:194:A:GLN:HA	2	2.08
(1,2332)	1:212:B:LYS:HB3	1:211:B:ALA:H	8	2.08
(1,2331)	1:212:A:LYS:HB3	1:211:A:ALA:H	8	2.08
(1,2304)	1:188:B:ASN:HB2	1:187:B:LYS:HG3	1	2.08
(1,2303)	1:188:A:ASN:HB2	1:187:A:LYS:HG3	1	2.08
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	5	2.08
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD13	8	2.08
(1,2662)	1:192:B:ASN:HD22	1:194:B:GLN:HA	3	2.07
(1,2661)	1:192:A:ASN:HD22	1:194:A:GLN:HA	3	2.07
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	8	2.07
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	8	2.07
(1,1092)	1:199:B:GLN:HG2	1:173:A:GLN:HE21	3	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2646)	1:188:B:ASN:HD22	1:185:B:LEU:HB3	1	2.06
(1,2646)	1:188:B:ASN:HD22	1:185:B:LEU:HB3	5	2.06
(1,2646)	1:188:B:ASN:HD22	1:185:B:LEU:HB3	6	2.06
(1,2645)	1:188:A:ASN:HD22	1:185:A:LEU:HB3	1	2.06
(1,2645)	1:188:A:ASN:HD22	1:185:A:LEU:HB3	6	2.06
(1,2350)	1:197:B:VAL:H	1:187:B:LYS:HG2	2	2.06
(1,2349)	1:197:A:VAL:H	1:187:A:LYS:HG2	2	2.06
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	5	2.06
(1,1508)	1:208:B:TRP:H	1:203:A:ARG:HE	10	2.06
(1,764)	1:201:B:MET:HE1	1:201:B:MET:HA	10	2.06
(1,2645)	1:188:A:ASN:HD22	1:185:A:LEU:HB3	5	2.05
(1,1507)	1:208:A:TRP:H	1:203:B:ARG:HE	10	2.05
(1,763)	1:201:A:MET:HE1	1:201:A:MET:HA	10	2.05
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD11	8	2.05
(1,2065)	1:201:A:MET:HE3	1:184:A:ALA:H	9	2.04
(1,2576)	1:208:B:TRP:HE1	1:211:B:ALA:HB3	3	2.03
(1,2349)	1:197:A:VAL:H	1:187:A:LYS:HG2	5	2.03
(1,2066)	1:201:B:MET:HE3	1:184:B:ALA:H	9	2.03
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD11	8	2.03
(1,2575)	1:208:A:TRP:HE1	1:211:A:ALA:HB3	3	2.02
(1,2350)	1:197:B:VAL:H	1:187:B:LYS:HG2	5	2.02
(1,2349)	1:197:A:VAL:H	1:187:A:LYS:HG2	8	2.02
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD12	10	2.02
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD12	10	2.02
(1,2350)	1:193:B:ASP:H	1:187:B:LYS:HG2	6	2.01
(1,2350)	1:197:B:VAL:H	1:187:B:LYS:HG2	8	2.01
(1,2349)	1:193:A:ASP:H	1:187:A:LYS:HG2	6	2.01
(1,2304)	1:188:B:ASN:HB2	1:187:B:LYS:HG3	9	2.01
(1,2303)	1:188:A:ASN:HB2	1:187:A:LYS:HG3	9	2.0
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	9	2.0
(1,1466)	1:208:B:TRP:HE1	1:173:B:GLN:H	4	2.0
(1,1092)	1:199:B:GLN:HG2	1:173:A:GLN:HE21	4	2.0
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG22	1	1.99
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	9	1.99
(1,1465)	1:208:A:TRP:HE1	1:173:A:GLN:H	4	1.99
(1,2576)	1:208:B:TRP:HE1	1:211:B:ALA:HB3	2	1.98
(1,2575)	1:208:A:TRP:HE1	1:211:A:ALA:HB3	2	1.98
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG21	3	1.98
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG22	4	1.98
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG22	1	1.98
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG22	4	1.98
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG21	3	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:199:A:GLN:HG2	1:173:B:GLN:HE21	4	1.97
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD11	5	1.97
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD13	9	1.97
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD11	5	1.97
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG22	2	1.96
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG22	2	1.96
(1,946)	1:175:B:LEU:HD21	1:199:A:GLN:HB3	6	1.96
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD13	2	1.96
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD13	9	1.96
(1,2854)	1:176:B:THR:H	1:189:A:ASN:HB3	7	1.95
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD13	2	1.95
(1,2853)	1:176:A:THR:H	1:189:B:ASN:HB3	7	1.94
(1,2379)	1:182:A:ILE:HD13	1:185:B:LEU:H	9	1.94
(1,648)	1:195:B:ALA:HB2	1:198:B:ARG:HD3	10	1.94
(1,647)	1:195:A:ALA:HB2	1:198:A:ARG:HD3	10	1.94
(1,2146)	1:199:B:GLN:HB3	1:200:B:VAL:HG23	7	1.92
(1,2145)	1:199:A:GLN:HB3	1:200:A:VAL:HG23	7	1.92
(1,945)	1:175:A:LEU:HD21	1:199:B:GLN:HB3	6	1.92
(1,2576)	1:208:B:TRP:HE1	1:211:B:ALA:HB1	4	1.91
(1,2575)	1:208:A:TRP:HE1	1:211:A:ALA:HB1	4	1.91
(1,2380)	1:182:B:ILE:HD13	1:185:A:LEU:H	9	1.91
(1,2379)	1:182:A:ILE:HD11	1:185:B:LEU:H	10	1.91
(1,2349)	1:197:A:VAL:H	1:187:A:LYS:HG2	9	1.91
(1,2350)	1:197:B:VAL:H	1:187:B:LYS:HG2	9	1.9
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG12	6	1.9
(1,2706)	1:189:B:ASN:HD22	1:188:B:ASN:HA	2	1.89
(1,2705)	1:189:A:ASN:HD22	1:188:A:ASN:HA	2	1.89
(1,2705)	1:189:A:ASN:HD22	1:188:A:ASN:HA	4	1.89
(1,2705)	1:189:A:ASN:HD22	1:188:A:ASN:HA	8	1.89
(1,2661)	1:173:A:GLN:HE21	1:196:B:ALA:HA	5	1.89
(1,2380)	1:182:B:ILE:HD12	1:185:A:LEU:H	7	1.89
(1,2380)	1:182:B:ILE:HD11	1:185:A:LEU:H	10	1.89
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB3	3	1.89
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB3	3	1.89
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG12	6	1.89
(1,2706)	1:189:B:ASN:HD22	1:188:B:ASN:HA	4	1.88
(1,2706)	1:189:B:ASN:HD22	1:188:B:ASN:HA	8	1.88
(1,2662)	1:173:B:GLN:HE21	1:196:A:ALA:HA	5	1.88
(1,2379)	1:182:A:ILE:HD12	1:185:B:LEU:H	7	1.88
(1,2864)	1:173:A:GLN:H	1:203:B:ARG:HG3	4	1.87
(1,2863)	1:173:B:GLN:H	1:203:A:ARG:HG3	4	1.87
(1,2304)	1:188:B:ASN:HB2	1:187:B:LYS:HG3	10	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2303)	1:188:A:ASN:HB2	1:187:A:LYS:HG3	10	1.87
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD12	3	1.87
(1,2706)	1:189:B:ASN:HD22	1:181:A:ASP:HA	5	1.86
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	3	1.86
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	3	1.86
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD12	3	1.86
(1,2864)	1:173:A:GLN:H	1:203:B:ARG:HG3	7	1.85
(1,2863)	1:173:B:GLN:H	1:203:A:ARG:HG3	7	1.85
(1,2706)	1:189:B:ASN:HD22	1:188:B:ASN:HA	9	1.85
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB3	2	1.85
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB3	2	1.85
(1,2705)	1:189:A:ASN:HD22	1:181:B:ASP:HA	5	1.84
(1,2705)	1:189:A:ASN:HD22	1:181:B:ASP:HA	9	1.84
(1,2380)	1:182:B:ILE:HD11	1:185:A:LEU:H	1	1.84
(1,2379)	1:182:A:ILE:HD11	1:185:B:LEU:H	1	1.84
(1,2350)	1:193:B:ASP:H	1:187:B:LYS:HG2	7	1.84
(1,2349)	1:193:A:ASP:H	1:187:A:LYS:HG2	7	1.84
(1,2304)	1:188:B:ASN:HB2	1:187:B:LYS:HG3	7	1.84
(1,2303)	1:188:A:ASN:HB2	1:187:A:LYS:HG3	3	1.84
(1,2303)	1:188:A:ASN:HB2	1:187:A:LYS:HG3	7	1.84
(1,2304)	1:188:B:ASN:HB2	1:187:B:LYS:HG3	3	1.83
(1,2706)	1:189:B:ASN:HD22	1:181:A:ASP:HA	10	1.82
(1,2661)	1:173:A:GLN:HE21	1:196:B:ALA:HA	1	1.82
(1,2304)	1:188:B:ASN:HB2	1:187:B:LYS:HG3	6	1.82
(1,2303)	1:188:A:ASN:HB2	1:187:A:LYS:HG3	6	1.82
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG11	5	1.82
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG11	5	1.82
(1,2705)	1:189:A:ASN:HD22	1:181:B:ASP:HA	10	1.81
(1,2266)	1:210:B:LEU:HA	1:211:B:ALA:HB1	9	1.81
(1,2265)	1:210:A:LEU:HA	1:211:A:ALA:HB1	9	1.81
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG13	9	1.81
(1,2146)	1:199:B:GLN:HB3	1:196:B:ALA:HB3	10	1.81
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG13	9	1.81
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG12	3	1.8
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG12	3	1.8
(1,2145)	1:199:A:GLN:HB3	1:196:A:ALA:HB3	10	1.8
(1,2662)	1:173:B:GLN:HE21	1:196:A:ALA:HA	1	1.79
(1,2575)	1:208:A:TRP:HE1	1:211:A:ALA:HB3	7	1.79
(1,2030)	1:205:B:GLN:HE22	1:177:B:VAL:HG22	10	1.79
(1,2576)	1:208:B:TRP:HE1	1:211:B:ALA:HB3	7	1.78
(1,2304)	1:188:B:ASN:HB2	1:187:B:LYS:HG3	2	1.78
(1,2303)	1:188:A:ASN:HB2	1:187:A:LYS:HG3	2	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2265)	1:210:A:LEU:HA	1:211:A:ALA:HB2	6	1.78
(1,2029)	1:205:A:GLN:HE22	1:177:A:VAL:HG22	10	1.78
(1,2266)	1:210:B:LEU:HA	1:211:B:ALA:HB2	6	1.77
(1,2854)	1:176:B:THR:H	1:189:A:ASN:HB3	3	1.76
(1,2576)	1:208:B:TRP:HE1	1:211:B:ALA:HB2	1	1.76
(1,2575)	1:208:A:TRP:HE1	1:211:A:ALA:HB2	1	1.76
(1,2380)	1:182:B:ILE:HD11	1:185:A:LEU:H	8	1.76
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB2	8	1.76
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB2	8	1.76
(1,2266)	1:210:B:LEU:HA	1:211:B:ALA:HB2	5	1.76
(1,2265)	1:210:A:LEU:HA	1:211:A:ALA:HB2	5	1.76
(1,2266)	1:210:B:LEU:HA	1:211:B:ALA:HB3	8	1.75
(1,2265)	1:210:A:LEU:HA	1:211:A:ALA:HB3	8	1.75
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG11	4	1.75
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG11	4	1.75
(1,2661)	1:173:A:GLN:HE21	1:196:B:ALA:HA	10	1.74
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB3	7	1.74
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB3	7	1.74
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG12	2	1.74
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG12	2	1.74
(1,2066)	1:201:B:MET:HE1	1:184:B:ALA:H	10	1.74
(1,2065)	1:201:A:MET:HE1	1:184:A:ALA:H	10	1.74
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	7	1.74
(1,2661)	1:173:A:GLN:HE21	1:196:B:ALA:HA	9	1.73
(1,2379)	1:182:A:ILE:HD11	1:185:B:LEU:H	8	1.73
(1,2303)	1:188:A:ASN:HB2	1:187:A:LYS:HG3	5	1.73
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	7	1.73
(1,2853)	1:176:A:THR:H	1:189:B:ASN:HB3	3	1.72
(1,2380)	1:182:B:ILE:HD12	1:185:A:LEU:H	3	1.72
(1,2350)	1:197:B:VAL:H	1:187:B:LYS:HG2	1	1.72
(1,2349)	1:197:A:VAL:H	1:187:A:LYS:HG2	1	1.72
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB2	1	1.72
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB2	1	1.72
(1,2304)	1:188:B:ASN:HB2	1:187:B:LYS:HG3	5	1.72
(1,2662)	1:173:B:GLN:HE21	1:196:A:ALA:HA	10	1.71
(1,2379)	1:182:A:ILE:HD12	1:185:B:LEU:H	3	1.71
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG11	8	1.71
(1,2662)	1:173:B:GLN:HE21	1:196:A:ALA:HA	9	1.7
(1,2379)	1:182:A:ILE:HD11	1:185:B:LEU:H	6	1.7
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG11	8	1.7
(1,2854)	1:176:B:THR:H	1:189:A:ASN:HB3	1	1.69
(1,2853)	1:176:A:THR:H	1:189:B:ASN:HB3	1	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	1	1.68
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD13	6	1.68
(1,2854)	1:176:B:THR:H	1:189:A:ASN:HB3	2	1.67
(1,2380)	1:182:B:ILE:HD12	1:185:A:LEU:H	2	1.67
(1,2380)	1:182:B:ILE:HD11	1:185:A:LEU:H	6	1.67
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB1	4	1.67
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB1	5	1.67
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB1	4	1.67
(1,2146)	1:183:B:GLU:HB3	1:197:B:VAL:HG13	1	1.67
(1,2145)	1:183:A:GLU:HB3	1:197:A:VAL:HG13	1	1.67
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	1	1.67
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD13	6	1.67
(1,2706)	1:189:B:ASN:HD22	1:181:A:ASP:HA	3	1.66
(1,2705)	1:189:A:ASN:HD22	1:181:B:ASP:HA	3	1.66
(1,2380)	1:182:B:ILE:HD12	1:185:A:LEU:H	5	1.66
(1,2379)	1:182:A:ILE:HD12	1:185:B:LEU:H	5	1.66
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB1	5	1.66
(1,1687)	1:189:A:ASN:HD22	1:181:B:ASP:HB3	6	1.66
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB2	4	1.65
(1,2379)	1:182:A:ILE:HD12	1:185:B:LEU:H	2	1.65
(1,2853)	1:176:A:THR:H	1:189:B:ASN:HB3	4	1.64
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB2	4	1.64
(1,1688)	1:189:B:ASN:HD22	1:181:A:ASP:HB3	6	1.64
(1,2853)	1:176:A:THR:H	1:189:B:ASN:HB3	2	1.63
(1,2853)	1:176:A:THR:H	1:189:B:ASN:HB3	10	1.63
(1,2304)	1:188:B:ASN:HB2	1:187:B:LYS:HG3	4	1.63
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD13	7	1.63
(1,2576)	1:208:B:TRP:HE1	1:211:B:ALA:HB1	6	1.62
(1,2575)	1:208:A:TRP:HE1	1:211:A:ALA:HB1	6	1.62
(1,2303)	1:188:A:ASN:HB2	1:187:A:LYS:HG3	4	1.62
(1,1291)	1:191:A:GLU:H	1:193:A:ASP:HB3	5	1.62
(1,2854)	1:176:B:THR:H	1:189:A:ASN:HB3	4	1.61
(1,1292)	1:191:B:GLU:H	1:193:B:ASP:HB3	5	1.61
(1,192)	1:201:B:MET:HE1	1:182:B:ILE:HG22	10	1.61
(1,191)	1:201:A:MET:HE1	1:182:A:ILE:HG22	10	1.61
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD13	7	1.61
(1,2398)	1:195:B:ALA:HA	1:196:B:ALA:HB2	6	1.6
(1,2397)	1:195:A:ALA:HA	1:196:A:ALA:HB2	6	1.6
(1,952)	1:197:B:VAL:HG12	1:187:B:LYS:HG2	4	1.6
(1,951)	1:197:A:VAL:HG12	1:187:A:LYS:HG2	4	1.6
(1,2398)	1:195:B:ALA:HA	1:196:B:ALA:HB1	8	1.59
(1,2397)	1:195:A:ALA:HA	1:196:A:ALA:HB1	8	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:192:B:ASN:HB3	1:191:B:GLU:HB3	5	1.59
(1,891)	1:192:A:ASN:HB3	1:191:A:GLU:HB3	5	1.59
(1,197)	1:201:A:MET:HE1	1:177:A:VAL:HG11	9	1.59
(1,2854)	1:176:B:THR:H	1:189:A:ASN:HB3	10	1.58
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD23	10	1.58
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD22	4	1.58
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD21	9	1.58
(1,2398)	1:195:B:ALA:HA	1:196:B:ALA:HB2	1	1.58
(1,2398)	1:195:B:ALA:HA	1:196:B:ALA:HB3	9	1.58
(1,2397)	1:195:A:ALA:HA	1:196:A:ALA:HB3	9	1.58
(1,764)	1:201:B:MET:HE1	1:201:B:MET:HA	9	1.58
(1,763)	1:201:A:MET:HE1	1:201:A:MET:HA	9	1.58
(1,198)	1:201:B:MET:HE1	1:177:B:VAL:HG11	9	1.58
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD22	4	1.57
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD21	9	1.57
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD23	10	1.57
(1,2398)	1:195:B:ALA:HA	1:196:B:ALA:HB2	3	1.57
(1,2398)	1:195:B:ALA:HA	1:196:B:ALA:HB1	5	1.57
(1,2397)	1:195:A:ALA:HA	1:196:A:ALA:HB2	1	1.57
(1,2397)	1:195:A:ALA:HA	1:196:A:ALA:HB2	3	1.57
(1,2397)	1:195:A:ALA:HA	1:196:A:ALA:HB1	5	1.57
(1,2184)	1:187:B:LYS:H	1:188:B:ASN:HB3	8	1.57
(1,2183)	1:187:A:LYS:H	1:188:A:ASN:HB3	8	1.57
(1,193)	1:201:A:MET:HE1	1:182:A:ILE:HD12	9	1.57
(1,102)	1:189:B:ASN:HD22	1:185:B:LEU:HD11	1	1.57
(1,2854)	1:176:B:THR:H	1:173:B:GLN:HG3	6	1.56
(1,2853)	1:176:A:THR:H	1:173:A:GLN:HG3	6	1.56
(1,2646)	1:188:B:ASN:HD22	1:178:A:PRO:HG2	10	1.56
(1,2644)	1:188:B:ASN:HD22	1:185:B:LEU:HB2	4	1.56
(1,2643)	1:188:A:ASN:HD22	1:185:A:LEU:HB2	3	1.56
(1,933)	1:197:A:VAL:HG23	1:187:A:LYS:HG2	4	1.56
(1,648)	1:195:B:ALA:HB3	1:198:B:ARG:HD3	8	1.56
(1,647)	1:195:A:ALA:HB3	1:198:A:ARG:HD3	8	1.56
(1,194)	1:201:B:MET:HE1	1:182:B:ILE:HD12	9	1.56
(1,101)	1:189:A:ASN:HD22	1:185:A:LEU:HD11	1	1.56
(1,2644)	1:188:B:ASN:HD22	1:185:B:LEU:HB2	3	1.55
(1,2643)	1:188:A:ASN:HD22	1:185:A:LEU:HB2	4	1.55
(1,2398)	1:195:B:ALA:HA	1:197:B:VAL:HG23	2	1.55
(1,2379)	1:182:A:ILE:HD11	1:185:B:LEU:H	4	1.55
(1,934)	1:197:B:VAL:HG23	1:187:B:LYS:HG2	4	1.55
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD21	2	1.54
(1,2705)	1:189:A:ASN:HD22	1:181:B:ASP:HA	6	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2705)	1:189:A:ASN:HD22	1:181:B:ASP:HA	7	1.54
(1,2512)	1:176:B:THR:H	1:174:B:GLU:HB3	8	1.54
(1,2511)	1:176:A:THR:H	1:174:A:GLU:HB3	8	1.54
(1,2397)	1:195:A:ALA:HA	1:197:A:VAL:HG23	2	1.54
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD21	2	1.53
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD21	8	1.53
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD21	8	1.53
(1,2706)	1:189:B:ASN:HD22	1:181:A:ASP:HA	7	1.53
(1,2646)	1:188:B:ASN:HD22	1:178:A:PRO:HG2	9	1.53
(1,2398)	1:195:B:ALA:HA	1:197:B:VAL:HG22	10	1.53
(1,2397)	1:195:A:ALA:HA	1:197:A:VAL:HG22	10	1.53
(1,2645)	1:188:A:ASN:HD22	1:178:B:PRO:HG2	10	1.52
(1,2380)	1:182:B:ILE:HD11	1:185:A:LEU:H	4	1.52
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB1	6	1.52
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB1	6	1.52
(1,1554)	1:173:B:GLN:HE21	1:175:B:LEU:HB3	3	1.52
(1,1553)	1:173:A:GLN:HE21	1:175:A:LEU:HB3	3	1.52
(1,1084)	1:199:B:GLN:HB3	1:198:B:ARG:H	7	1.52
(1,1083)	1:199:A:GLN:HB3	1:198:A:ARG:H	7	1.52
(1,2706)	1:189:B:ASN:HD22	1:181:A:ASP:HA	6	1.51
(1,2398)	1:195:B:ALA:HA	1:197:B:VAL:HG22	7	1.51
(1,1466)	1:208:B:TRP:HE1	1:173:B:GLN:H	2	1.51
(1,1465)	1:208:A:TRP:HE1	1:173:A:GLN:H	2	1.51
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG21	7	1.5
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG21	7	1.5
(1,2645)	1:188:A:ASN:HD22	1:178:B:PRO:HG2	9	1.5
(1,2397)	1:195:A:ALA:HA	1:197:A:VAL:HG22	7	1.5
(1,2066)	1:201:B:MET:HE2	1:184:B:ALA:H	7	1.5
(1,2065)	1:201:A:MET:HE2	1:184:A:ALA:H	7	1.5
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD21	5	1.49
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG23	1	1.49
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG23	1	1.49
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB1	10	1.49
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB1	10	1.49
(1,2066)	1:201:B:MET:HE2	1:184:B:ALA:H	3	1.49
(1,2065)	1:201:A:MET:HE2	1:184:A:ALA:H	3	1.49
(1,952)	1:197:B:VAL:HG12	1:187:B:LYS:HG2	5	1.49
(1,951)	1:197:A:VAL:HG12	1:187:A:LYS:HG2	5	1.49
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD21	5	1.48
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB2	2	1.48
(1,1246)	1:175:B:LEU:HD13	1:177:B:VAL:HG22	7	1.48
(1,1245)	1:175:A:LEU:HD13	1:177:A:VAL:HG22	7	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:199:B:GLN:HB3	1:198:B:ARG:H	9	1.48
(1,1083)	1:199:A:GLN:HB3	1:198:A:ARG:H	9	1.48
(1,945)	1:175:A:LEU:HD21	1:199:B:GLN:HB3	8	1.48
(1,1180)	1:208:B:TRP:HA	1:203:A:ARG:HE	10	1.47
(1,952)	1:197:B:VAL:HG13	1:187:B:LYS:HG2	6	1.47
(1,952)	1:197:B:VAL:HG12	1:187:B:LYS:HG2	8	1.47
(1,951)	1:197:A:VAL:HG13	1:187:A:LYS:HG2	6	1.47
(1,951)	1:197:A:VAL:HG12	1:187:A:LYS:HG2	8	1.47
(1,764)	1:201:B:MET:HE3	1:201:B:MET:HA	7	1.47
(1,763)	1:201:A:MET:HE3	1:201:A:MET:HA	7	1.47
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB2	2	1.46
(1,1084)	1:199:B:GLN:HB3	1:198:B:ARG:H	1	1.46
(1,1083)	1:199:A:GLN:HB3	1:198:A:ARG:H	1	1.46
(1,946)	1:175:B:LEU:HD21	1:199:A:GLN:HB3	8	1.46
(1,752)	1:188:B:ASN:HB3	1:185:B:LEU:HA	8	1.46
(1,751)	1:188:A:ASN:HB3	1:185:A:LEU:HA	8	1.46
(1,2706)	1:189:B:ASN:HD22	1:181:A:ASP:HA	1	1.45
(1,1179)	1:208:A:TRP:HA	1:203:B:ARG:HE	10	1.45
(1,1084)	1:199:B:GLN:HB3	1:198:B:ARG:H	4	1.45
(1,1084)	1:199:B:GLN:HB3	1:198:B:ARG:H	6	1.45
(1,1083)	1:199:A:GLN:HB3	1:198:A:ARG:H	4	1.45
(1,1083)	1:199:A:GLN:HB3	1:198:A:ARG:H	6	1.45
(1,934)	1:197:B:VAL:HG21	1:187:B:LYS:HG2	10	1.45
(1,933)	1:197:A:VAL:HG21	1:187:A:LYS:HG2	10	1.45
(1,590)	1:209:B:SER:HB3	1:208:B:TRP:H	4	1.45
(1,191)	1:201:A:MET:HE1	1:182:A:ILE:HG21	9	1.45
(1,94)	1:175:B:LEU:HD22	1:200:A:VAL:H	7	1.45
(1,93)	1:175:A:LEU:HD22	1:200:B:VAL:H	7	1.45
(1,2705)	1:189:A:ASN:HD22	1:181:B:ASP:HA	1	1.44
(1,2643)	1:188:A:ASN:HD22	1:185:A:LEU:HB2	7	1.44
(1,1084)	1:199:B:GLN:HB3	1:198:B:ARG:H	3	1.44
(1,1084)	1:199:B:GLN:HB3	1:198:B:ARG:H	8	1.44
(1,1084)	1:199:B:GLN:HB3	1:198:B:ARG:H	10	1.44
(1,1083)	1:199:A:GLN:HB3	1:198:A:ARG:H	3	1.44
(1,1083)	1:199:A:GLN:HB3	1:198:A:ARG:H	8	1.44
(1,1083)	1:199:A:GLN:HB3	1:198:A:ARG:H	10	1.44
(1,590)	1:209:B:SER:HB3	1:208:B:TRP:H	8	1.44
(1,589)	1:209:A:SER:HB3	1:208:A:TRP:H	4	1.44
(1,589)	1:209:A:SER:HB3	1:208:A:TRP:H	8	1.44
(1,192)	1:201:B:MET:HE1	1:182:B:ILE:HG21	9	1.44
(1,2644)	1:188:B:ASN:HD22	1:185:B:LEU:HB2	7	1.43
(1,2336)	1:208:B:TRP:HB3	1:211:B:ALA:HB3	9	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2335)	1:208:A:TRP:HB3	1:211:A:ALA:HB3	9	1.43
(1,2079)	1:175:A:LEU:HD21	1:196:B:ALA:H	4	1.43
(1,1554)	1:173:B:GLN:HE21	1:175:B:LEU:HB3	2	1.43
(1,1553)	1:173:A:GLN:HE21	1:175:A:LEU:HB3	2	1.43
(1,952)	1:197:B:VAL:HG13	1:187:B:LYS:HG2	3	1.43
(1,952)	1:197:B:VAL:HG11	1:187:B:LYS:HG2	10	1.43
(1,951)	1:197:A:VAL:HG13	1:187:A:LYS:HG2	3	1.43
(1,934)	1:197:B:VAL:HG22	1:187:B:LYS:HG2	3	1.43
(1,590)	1:209:B:SER:HB3	1:208:B:TRP:H	5	1.43
(1,589)	1:209:A:SER:HB3	1:208:A:TRP:H	5	1.43
(1,589)	1:209:A:SER:HB3	1:208:A:TRP:H	6	1.43
(1,2863)	1:173:B:GLN:H	1:203:A:ARG:HG3	6	1.42
(1,2650)	1:188:B:ASN:HD22	1:178:A:PRO:HG3	5	1.42
(1,2644)	1:188:B:ASN:HD22	1:185:B:LEU:HB2	2	1.42
(1,2643)	1:188:A:ASN:HD22	1:185:A:LEU:HB2	2	1.42
(1,951)	1:197:A:VAL:HG11	1:187:A:LYS:HG2	10	1.42
(1,933)	1:197:A:VAL:HG22	1:187:A:LYS:HG2	3	1.42
(1,590)	1:209:B:SER:HB3	1:208:B:TRP:H	6	1.42
(1,32)	1:201:B:MET:HE1	1:179:B:TRP:HZ3	10	1.42
(1,31)	1:201:A:MET:HE1	1:179:A:TRP:HZ3	10	1.42
(1,2864)	1:173:A:GLN:H	1:203:B:ARG:HG3	6	1.41
(1,1084)	1:199:B:GLN:HB3	1:198:B:ARG:H	5	1.41
(1,1083)	1:199:A:GLN:HB3	1:198:A:ARG:H	5	1.41
(1,945)	1:175:A:LEU:HD22	1:199:B:GLN:HB3	9	1.41
(1,941)	1:175:A:LEU:HD22	1:200:B:VAL:HG12	7	1.41
(1,821)	1:208:A:TRP:HA	1:203:B:ARG:HG3	10	1.41
(1,2649)	1:188:A:ASN:HD22	1:178:B:PRO:HG3	5	1.4
(1,1678)	1:199:B:GLN:HE22	1:198:B:ARG:HD3	10	1.4
(1,942)	1:175:B:LEU:HD22	1:200:A:VAL:HG12	7	1.4
(1,822)	1:208:B:TRP:HA	1:203:A:ARG:HG3	10	1.4
(1,34)	1:205:B:GLN:HE22	1:201:B:MET:HE1	3	1.4
(1,33)	1:205:A:GLN:HE22	1:201:A:MET:HE1	3	1.4
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD21	5	1.39
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD21	9	1.39
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD21	5	1.39
(1,2040)	1:203:B:ARG:H	1:205:B:GLN:HE22	9	1.39
(1,2039)	1:203:A:ARG:H	1:205:A:GLN:HE22	9	1.39
(1,1677)	1:199:A:GLN:HE22	1:198:A:ARG:HD3	10	1.39
(1,1466)	1:208:B:TRP:HE1	1:173:B:GLN:H	3	1.39
(1,1092)	1:199:B:GLN:HG2	1:173:A:GLN:HE21	9	1.39
(1,2644)	1:188:B:ASN:HD22	1:185:B:LEU:HB2	1	1.38
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD21	9	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2080)	1:175:B:LEU:HD21	1:196:A:ALA:H	4	1.38
(1,1817)	1:192:A:ASN:H	1:187:A:LYS:HG2	7	1.38
(1,1291)	1:191:A:GLU:H	1:193:A:ASP:HB3	9	1.38
(1,1084)	1:199:B:GLN:HB3	1:198:B:ARG:H	2	1.38
(1,1083)	1:199:A:GLN:HB3	1:198:A:ARG:H	2	1.38
(1,2643)	1:188:A:ASN:HD22	1:185:A:LEU:HB2	1	1.37
(1,1818)	1:192:B:ASN:H	1:187:B:LYS:HG2	7	1.37
(1,1678)	1:199:B:GLN:HE22	1:198:B:ARG:HD3	8	1.37
(1,1677)	1:199:A:GLN:HE22	1:198:A:ARG:HD3	8	1.37
(1,1465)	1:208:A:TRP:HE1	1:173:A:GLN:H	3	1.37
(1,1292)	1:191:B:GLU:H	1:193:B:ASP:HB3	2	1.37
(1,1292)	1:191:B:GLU:H	1:193:B:ASP:HB3	9	1.37
(1,1291)	1:191:A:GLU:H	1:193:A:ASP:HB3	2	1.37
(1,946)	1:175:B:LEU:HD22	1:199:A:GLN:HB3	9	1.37
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD21	3	1.36
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD21	1	1.36
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD21	2	1.36
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD21	1	1.36
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD21	2	1.36
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD21	3	1.35
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD21	8	1.35
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD21	8	1.35
(1,1979)	1:173:B:GLN:H	1:212:B:LYS:HA	6	1.35
(1,1292)	1:191:B:GLU:H	1:193:B:ASP:HB3	8	1.35
(1,1291)	1:191:A:GLU:H	1:193:A:ASP:HB3	8	1.35
(1,1246)	1:175:B:LEU:HD13	1:177:B:VAL:HG23	6	1.35
(1,1245)	1:175:A:LEU:HD13	1:177:A:VAL:HG23	6	1.35
(1,892)	1:192:B:ASN:HB3	1:191:B:GLU:HB3	9	1.35
(1,891)	1:192:A:ASN:HB3	1:191:A:GLU:HB3	9	1.35
(1,158)	1:182:B:ILE:HD12	1:178:B:PRO:HD3	7	1.35
(1,157)	1:182:A:ILE:HD12	1:178:A:PRO:HD3	7	1.35
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD22	7	1.34
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD23	10	1.34
(1,1986)	1:173:A:GLN:H	1:175:A:LEU:HD11	7	1.34
(1,1980)	1:173:A:GLN:H	1:212:A:LYS:HA	6	1.34
(1,1482)	1:179:B:TRP:HE1	1:205:B:GLN:HB3	9	1.34
(1,1259)	1:176:A:THR:HG22	1:177:A:VAL:HG11	1	1.34
(1,1116)	1:175:B:LEU:HD23	1:199:A:GLN:H	7	1.34
(1,1115)	1:175:A:LEU:HD23	1:199:B:GLN:H	7	1.34
(1,892)	1:192:B:ASN:HB3	1:191:B:GLU:HB3	7	1.34
(1,891)	1:192:A:ASN:HB3	1:191:A:GLU:HB3	7	1.34
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD22	7	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD22	7	1.33
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG23	3	1.33
(1,2643)	1:188:A:ASN:HD22	1:185:A:LEU:HB2	6	1.33
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD21	6	1.33
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD23	10	1.33
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD21	6	1.33
(1,2397)	1:195:A:ALA:HA	1:197:A:VAL:HG21	4	1.33
(1,1985)	1:173:B:GLN:H	1:175:B:LEU:HD11	7	1.33
(1,1481)	1:179:A:TRP:HE1	1:205:A:GLN:HB3	9	1.33
(1,1260)	1:176:B:THR:HG22	1:177:B:VAL:HG11	1	1.33
(1,1091)	1:199:A:GLN:HG2	1:173:B:GLN:HE21	9	1.33
(1,934)	1:197:B:VAL:HG22	1:187:B:LYS:HG2	2	1.33
(1,934)	1:197:B:VAL:HG21	1:187:B:LYS:HG2	6	1.33
(1,933)	1:197:A:VAL:HG22	1:187:A:LYS:HG2	2	1.33
(1,933)	1:197:A:VAL:HG21	1:187:A:LYS:HG2	6	1.33
(1,892)	1:192:B:ASN:HB3	1:191:B:GLU:HB3	1	1.33
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG23	3	1.32
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG23	5	1.32
(1,2644)	1:188:B:ASN:HD22	1:185:B:LEU:HB2	6	1.32
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD21	3	1.32
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD22	7	1.32
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD22	7	1.32
(1,2398)	1:195:B:ALA:HA	1:197:B:VAL:HG21	4	1.32
(1,1484)	1:179:B:TRP:HE1	1:205:B:GLN:HG2	9	1.32
(1,1483)	1:179:A:TRP:HE1	1:205:A:GLN:HG2	9	1.32
(1,1292)	1:191:B:GLU:H	1:193:B:ASP:HB3	6	1.32
(1,1291)	1:191:A:GLU:H	1:193:A:ASP:HB3	6	1.32
(1,952)	1:197:B:VAL:HG13	1:187:B:LYS:HG2	2	1.32
(1,951)	1:197:A:VAL:HG13	1:187:A:LYS:HG2	2	1.32
(1,934)	1:197:B:VAL:HG21	1:187:B:LYS:HG2	5	1.32
(1,933)	1:197:A:VAL:HG21	1:187:A:LYS:HG2	5	1.32
(1,891)	1:192:A:ASN:HB3	1:191:A:GLU:HB3	1	1.32
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD22	7	1.31
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG23	5	1.31
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG21	2	1.31
(1,2649)	1:188:A:ASN:HD22	1:178:B:PRO:HG3	7	1.31
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD21	3	1.31
(1,1292)	1:191:B:GLU:H	1:193:B:ASP:HB3	1	1.31
(1,1291)	1:191:A:GLU:H	1:193:A:ASP:HB3	1	1.31
(1,1260)	1:176:B:THR:HG21	1:177:B:VAL:HG13	8	1.31
(1,1259)	1:176:A:THR:HG21	1:177:A:VAL:HG13	8	1.31
(1,1073)	1:192:A:ASN:H	1:187:A:LYS:HG3	7	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:197:B:VAL:HG21	1:187:B:LYS:HG2	8	1.31
(1,933)	1:197:A:VAL:HG21	1:187:A:LYS:HG2	8	1.31
(1,892)	1:192:B:ASN:HB3	1:191:B:GLU:HB3	2	1.31
(1,891)	1:192:A:ASN:HB3	1:191:A:GLU:HB3	2	1.31
(1,422)	1:196:B:ALA:H	1:193:B:ASP:HB2	7	1.31
(1,158)	1:182:B:ILE:HD13	1:178:B:PRO:HD3	9	1.31
(1,157)	1:182:A:ILE:HD13	1:178:A:PRO:HD3	9	1.31
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG21	2	1.3
(1,2650)	1:188:B:ASN:HD22	1:178:A:PRO:HG3	7	1.3
(1,2644)	1:188:B:ASN:HD22	1:185:B:LEU:HB2	5	1.3
(1,2643)	1:188:A:ASN:HD22	1:185:A:LEU:HB2	5	1.3
(1,2576)	1:208:B:TRP:HE1	1:211:B:ALA:HB1	10	1.3
(1,2103)	1:204:A:LEU:HD21	1:179:B:TRP:HE3	10	1.3
(1,2080)	1:175:B:LEU:HD21	1:196:A:ALA:H	2	1.3
(1,2079)	1:175:A:LEU:HD22	1:196:B:ALA:H	5	1.3
(1,1074)	1:192:B:ASN:H	1:187:B:LYS:HG3	7	1.3
(1,421)	1:196:A:ALA:H	1:193:A:ASP:HB2	7	1.3
(1,2575)	1:208:A:TRP:HE1	1:211:A:ALA:HB1	10	1.29
(1,2104)	1:204:B:LEU:HD21	1:179:A:TRP:HE3	10	1.29
(1,2080)	1:175:B:LEU:HD23	1:196:A:ALA:H	7	1.29
(1,2066)	1:201:B:MET:HE2	1:184:B:ALA:H	2	1.29
(1,2065)	1:201:A:MET:HE2	1:184:A:ALA:H	2	1.29
(1,1092)	1:199:B:GLN:HG2	1:173:A:GLN:HE21	10	1.29
(1,892)	1:192:B:ASN:HB3	1:191:B:GLU:HB3	4	1.29
(1,892)	1:192:B:ASN:HB3	1:191:B:GLU:HB3	8	1.29
(1,891)	1:192:A:ASN:HB3	1:191:A:GLU:HB3	4	1.29
(1,158)	1:182:B:ILE:HD11	1:178:B:PRO:HD3	10	1.29
(1,157)	1:182:A:ILE:HD11	1:178:A:PRO:HD3	10	1.29
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD21	6	1.28
(1,2576)	1:208:B:TRP:HE1	1:211:B:ALA:HB3	9	1.28
(1,2575)	1:208:A:TRP:HE1	1:211:A:ALA:HB3	9	1.28
(1,2464)	1:189:B:ASN:H	1:185:B:LEU:HD22	4	1.28
(1,2463)	1:189:A:ASN:H	1:185:A:LEU:HD22	4	1.28
(1,2079)	1:175:A:LEU:HD21	1:196:B:ALA:H	2	1.28
(1,2079)	1:175:A:LEU:HD23	1:196:B:ALA:H	7	1.28
(1,2079)	1:175:A:LEU:HD21	1:196:B:ALA:H	10	1.28
(1,1574)	1:188:B:ASN:HD22	1:189:B:ASN:HB2	8	1.28
(1,1573)	1:188:A:ASN:HD22	1:189:A:ASN:HB2	8	1.28
(1,1260)	1:176:B:THR:HG21	1:177:B:VAL:HG13	3	1.28
(1,1259)	1:176:A:THR:HG21	1:177:A:VAL:HG13	3	1.28
(1,1170)	1:206:B:LYS:HG3	1:209:B:SER:HB3	8	1.28
(1,1169)	1:206:A:LYS:HG3	1:209:A:SER:HB3	8	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:192:A:ASN:HB3	1:191:A:GLU:HB3	8	1.28
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD21	6	1.27
(1,2080)	1:175:B:LEU:HD22	1:196:A:ALA:H	5	1.27
(1,1292)	1:191:B:GLU:H	1:193:B:ASP:HB3	3	1.27
(1,1291)	1:191:A:GLU:H	1:193:A:ASP:HB3	3	1.27
(1,1260)	1:176:B:THR:HG21	1:177:B:VAL:HG11	9	1.27
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD21	2	1.26
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG23	8	1.26
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG23	8	1.26
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB3	5	1.26
(1,1554)	1:173:B:GLN:HE21	1:175:B:LEU:HB3	7	1.26
(1,1553)	1:173:A:GLN:HE21	1:175:A:LEU:HB3	7	1.26
(1,1260)	1:176:B:THR:HG22	1:177:B:VAL:HG13	2	1.26
(1,1260)	1:176:B:THR:HG23	1:177:B:VAL:HG13	4	1.26
(1,1259)	1:176:A:THR:HG22	1:177:A:VAL:HG13	2	1.26
(1,1259)	1:176:A:THR:HG23	1:177:A:VAL:HG13	4	1.26
(1,1259)	1:176:A:THR:HG21	1:177:A:VAL:HG11	9	1.26
(1,1091)	1:199:A:GLN:HG2	1:173:B:GLN:HE21	10	1.26
(1,892)	1:192:B:ASN:HB3	1:191:B:GLU:HB3	6	1.26
(1,891)	1:192:A:ASN:HB3	1:191:A:GLU:HB3	6	1.26
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD21	2	1.25
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD23	4	1.25
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD23	4	1.25
(1,2726)	1:189:B:ASN:HD22	1:185:B:LEU:HD21	1	1.25
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG23	8	1.25
(1,2650)	1:188:B:ASN:HD22	1:178:A:PRO:HG3	6	1.25
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB3	5	1.25
(1,2080)	1:175:B:LEU:HD21	1:196:A:ALA:H	1	1.25
(1,2080)	1:175:B:LEU:HD22	1:208:B:TRP:HZ2	3	1.25
(1,2079)	1:175:A:LEU:HD21	1:196:B:ALA:H	1	1.25
(1,2079)	1:175:A:LEU:HD22	1:208:A:TRP:HZ2	3	1.25
(1,2725)	1:189:A:ASN:HD22	1:185:A:LEU:HD21	1	1.24
(1,2080)	1:175:B:LEU:HD21	1:196:A:ALA:H	10	1.24
(1,2072)	1:211:B:ALA:HB1	1:208:A:TRP:H	3	1.24
(1,1291)	1:191:A:GLU:H	1:193:A:ASP:HB3	10	1.24
(1,951)	1:197:A:VAL:HG11	1:187:A:LYS:HG2	9	1.24
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD21	1	1.23
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD23	10	1.23
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD21	1	1.23
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG22	1	1.23
(1,2838)	1:179:B:TRP:H	1:180:B:ASP:HB3	4	1.23
(1,2837)	1:179:A:TRP:H	1:180:A:ASP:HB3	4	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG21	6	1.23
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB2	6	1.23
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB2	6	1.23
(1,1292)	1:191:B:GLU:H	1:193:B:ASP:HB3	10	1.23
(1,1259)	1:176:A:THR:HG22	1:177:A:VAL:HG11	10	1.23
(1,952)	1:197:B:VAL:HG11	1:187:B:LYS:HG2	9	1.23
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD22	3	1.22
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD23	10	1.22
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG22	1	1.22
(1,2838)	1:179:B:TRP:H	1:180:B:ASP:HB3	10	1.22
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG21	6	1.22
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG23	8	1.22
(1,2072)	1:211:B:ALA:HB1	1:208:A:TRP:H	2	1.22
(1,2071)	1:211:A:ALA:HB1	1:208:B:TRP:H	3	1.22
(1,1260)	1:176:B:THR:HG22	1:177:B:VAL:HG11	10	1.22
(1,1218)	1:201:B:MET:HE2	1:179:B:TRP:HB2	3	1.22
(1,1217)	1:201:A:MET:HE2	1:179:A:TRP:HB2	3	1.22
(1,1170)	1:206:B:LYS:HG3	1:209:B:SER:HB3	5	1.22
(1,1169)	1:206:A:LYS:HG3	1:209:A:SER:HB3	5	1.22
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD21	9	1.21
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD22	3	1.21
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD21	9	1.21
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG22	6	1.21
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG23	7	1.21
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG22	6	1.21
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG23	7	1.21
(1,2837)	1:179:A:TRP:H	1:180:A:ASP:HB3	10	1.21
(1,2071)	1:211:A:ALA:HB1	1:208:B:TRP:H	2	1.21
(1,2066)	1:201:B:MET:HE1	1:184:B:ALA:H	5	1.21
(1,2065)	1:201:A:MET:HE1	1:184:A:ALA:H	5	1.21
(1,1219)	1:185:A:LEU:HD22	1:177:B:VAL:HG12	8	1.21
(1,892)	1:192:B:ASN:HB3	1:191:B:GLU:HB3	3	1.21
(1,891)	1:192:A:ASN:HB3	1:191:A:GLU:HB3	10	1.21
(1,422)	1:196:B:ALA:H	1:193:B:ASP:HB2	4	1.21
(1,421)	1:196:A:ALA:H	1:193:A:ASP:HB2	4	1.21
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG21	3	1.2
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG23	4	1.2
(1,2649)	1:188:A:ASN:HD22	1:178:B:PRO:HG3	6	1.2
(1,2116)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	7	1.2
(1,2115)	1:182:A:ILE:HD11	1:178:A:PRO:HB2	7	1.2
(1,1976)	1:174:B:GLU:H	1:174:B:GLU:HB2	8	1.2
(1,1975)	1:174:A:GLU:H	1:174:A:GLU:HB2	8	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1412)	1:212:B:LYS:H	1:212:B:LYS:HG2	6	1.2
(1,1412)	1:212:B:LYS:H	1:212:B:LYS:HG2	9	1.2
(1,1411)	1:212:A:LYS:H	1:212:A:LYS:HG2	6	1.2
(1,1411)	1:212:A:LYS:H	1:212:A:LYS:HG2	9	1.2
(1,1259)	1:176:A:THR:HG22	1:177:A:VAL:HG11	5	1.2
(1,892)	1:192:B:ASN:HB3	1:191:B:GLU:HB3	10	1.2
(1,891)	1:192:A:ASN:HB3	1:191:A:GLU:HB3	3	1.2
(1,690)	1:199:B:GLN:HB3	1:196:B:ALA:HA	9	1.2
(1,689)	1:199:A:GLN:HB3	1:196:A:ALA:HA	9	1.2
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD23	6	1.19
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG23	4	1.19
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG21	3	1.19
(1,2116)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	3	1.19
(1,2115)	1:182:A:ILE:HD11	1:178:A:PRO:HB2	3	1.19
(1,2080)	1:175:B:LEU:HD21	1:196:A:ALA:H	8	1.19
(1,1260)	1:176:B:THR:HG22	1:177:B:VAL:HG11	5	1.19
(1,1258)	1:176:B:THR:HG21	1:177:B:VAL:HG22	3	1.19
(1,1257)	1:176:A:THR:HG21	1:177:A:VAL:HG22	3	1.19
(1,934)	1:197:B:VAL:HG21	1:187:B:LYS:HG2	7	1.19
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD23	6	1.18
(1,2838)	1:179:B:TRP:H	1:180:B:ASP:HB3	3	1.18
(1,2837)	1:179:A:TRP:H	1:180:A:ASP:HB3	3	1.18
(1,2662)	1:173:B:GLN:HE21	1:196:A:ALA:HA	7	1.18
(1,2649)	1:188:A:ASN:HD22	1:178:B:PRO:HG3	2	1.18
(1,2115)	1:182:A:ILE:HD11	1:178:A:PRO:HB2	1	1.18
(1,1722)	1:196:B:ALA:H	1:198:B:ARG:HG2	10	1.18
(1,933)	1:197:A:VAL:HG21	1:187:A:LYS:HG2	7	1.18
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG13	7	1.18
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG13	7	1.18
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD11	3	1.17
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD11	3	1.17
(1,2661)	1:173:A:GLN:HE21	1:196:B:ALA:HA	7	1.17
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB1	9	1.17
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB1	9	1.17
(1,2116)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	1	1.17
(1,1721)	1:196:A:ALA:H	1:198:A:ARG:HG2	10	1.17
(1,952)	1:197:B:VAL:HG13	1:187:B:LYS:HG2	7	1.17
(1,951)	1:197:A:VAL:HG13	1:187:A:LYS:HG2	7	1.17
(1,934)	1:197:B:VAL:HG23	1:187:B:LYS:HG2	9	1.17
(1,933)	1:197:A:VAL:HG23	1:187:A:LYS:HG2	9	1.17
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG22	9	1.16
(1,2838)	1:179:B:TRP:H	1:180:B:ASP:HB3	5	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2837)	1:179:A:TRP:H	1:180:A:ASP:HB3	5	1.16
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD11	1	1.16
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD13	4	1.16
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD11	8	1.16
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD11	1	1.16
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD13	4	1.16
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD11	8	1.16
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG23	4	1.16
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG23	4	1.16
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB1	3	1.16
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB1	3	1.16
(1,2116)	1:182:B:ILE:HD13	1:178:B:PRO:HB2	10	1.16
(1,2115)	1:182:A:ILE:HD13	1:178:A:PRO:HB2	10	1.16
(1,2066)	1:201:B:MET:HE2	1:184:B:ALA:H	1	1.16
(1,2065)	1:201:A:MET:HE2	1:184:A:ALA:H	1	1.16
(1,1722)	1:196:B:ALA:H	1:198:B:ARG:HG2	1	1.16
(1,1722)	1:196:B:ALA:H	1:198:B:ARG:HG2	7	1.16
(1,1721)	1:196:A:ALA:H	1:198:A:ARG:HG2	7	1.16
(1,1246)	1:175:B:LEU:HD11	1:177:B:VAL:HG21	10	1.16
(1,1245)	1:175:A:LEU:HD11	1:177:A:VAL:HG21	10	1.16
(1,1220)	1:185:B:LEU:HD22	1:177:A:VAL:HG12	8	1.16
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG22	9	1.15
(1,2629)	1:192:A:ASN:HD22	1:195:A:ALA:HB3	10	1.15
(1,2120)	1:177:B:VAL:HG11	1:182:B:ILE:HG23	8	1.15
(1,2119)	1:177:A:VAL:HG11	1:182:A:ILE:HG23	8	1.15
(1,2079)	1:175:A:LEU:HD21	1:196:B:ALA:H	8	1.15
(1,1721)	1:196:A:ALA:H	1:198:A:ARG:HG2	1	1.15
(1,940)	1:175:B:LEU:HD22	1:175:B:LEU:HB2	7	1.15
(1,939)	1:175:A:LEU:HD22	1:175:A:LEU:HB2	7	1.15
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB1	4	1.15
(1,282)	1:185:B:LEU:HD11	1:185:B:LEU:HB3	6	1.15
(1,282)	1:185:B:LEU:HD13	1:185:B:LEU:HB3	10	1.15
(1,281)	1:185:A:LEU:HD11	1:185:A:LEU:HB3	2	1.15
(1,281)	1:185:A:LEU:HD11	1:185:A:LEU:HB3	6	1.15
(1,281)	1:185:A:LEU:HD11	1:185:A:LEU:HB3	9	1.15
(1,281)	1:185:A:LEU:HD13	1:185:A:LEU:HB3	10	1.15
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG23	2	1.14
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG23	2	1.14
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD13	6	1.14
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD13	10	1.14
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD13	6	1.14
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD13	10	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2650)	1:188:B:ASN:HD22	1:178:A:PRO:HG3	2	1.14
(1,2630)	1:192:B:ASN:HD22	1:195:B:ALA:HB3	10	1.14
(1,2079)	1:175:A:LEU:HD22	1:196:B:ALA:H	9	1.14
(1,1258)	1:176:B:THR:HG21	1:177:B:VAL:HG22	8	1.14
(1,940)	1:175:B:LEU:HD21	1:175:B:LEU:HB2	9	1.14
(1,940)	1:175:B:LEU:HD23	1:175:B:LEU:HB2	10	1.14
(1,939)	1:175:A:LEU:HD23	1:175:A:LEU:HB2	10	1.14
(1,706)	1:195:B:ALA:HA	1:198:B:ARG:HG2	10	1.14
(1,705)	1:195:A:ALA:HA	1:198:A:ARG:HG2	10	1.14
(1,282)	1:185:B:LEU:HD12	1:185:B:LEU:HB3	1	1.14
(1,282)	1:185:B:LEU:HD11	1:185:B:LEU:HB3	2	1.14
(1,282)	1:185:B:LEU:HD11	1:185:B:LEU:HB3	4	1.14
(1,282)	1:185:B:LEU:HD12	1:185:B:LEU:HB3	5	1.14
(1,282)	1:185:B:LEU:HD11	1:185:B:LEU:HB3	7	1.14
(1,282)	1:185:B:LEU:HD12	1:185:B:LEU:HB3	8	1.14
(1,282)	1:185:B:LEU:HD11	1:185:B:LEU:HB3	9	1.14
(1,281)	1:185:A:LEU:HD12	1:185:A:LEU:HB3	1	1.14
(1,281)	1:185:A:LEU:HD11	1:185:A:LEU:HB3	4	1.14
(1,281)	1:185:A:LEU:HD12	1:185:A:LEU:HB3	5	1.14
(1,281)	1:185:A:LEU:HD11	1:185:A:LEU:HB3	7	1.14
(1,281)	1:185:A:LEU:HD12	1:185:A:LEU:HB3	8	1.14
(1,2116)	1:182:B:ILE:HD13	1:204:A:LEU:HG	9	1.13
(1,2115)	1:182:A:ILE:HD13	1:204:B:LEU:HG	9	1.13
(1,2066)	1:201:B:MET:HE3	1:184:B:ALA:H	6	1.13
(1,2066)	1:201:B:MET:HE2	1:184:B:ALA:H	8	1.13
(1,2065)	1:201:A:MET:HE3	1:184:A:ALA:H	6	1.13
(1,2065)	1:201:A:MET:HE2	1:184:A:ALA:H	8	1.13
(1,1260)	1:176:B:THR:HG22	1:177:B:VAL:HG13	7	1.13
(1,1258)	1:176:B:THR:HG22	1:177:B:VAL:HG23	1	1.13
(1,1257)	1:176:A:THR:HG22	1:177:A:VAL:HG23	1	1.13
(1,1257)	1:176:A:THR:HG21	1:177:A:VAL:HG22	8	1.13
(1,940)	1:175:B:LEU:HD23	1:175:B:LEU:HB2	4	1.13
(1,939)	1:175:A:LEU:HD23	1:175:A:LEU:HB2	4	1.13
(1,939)	1:175:A:LEU:HD21	1:175:A:LEU:HB2	9	1.13
(1,282)	1:185:B:LEU:HD13	1:185:B:LEU:HB3	3	1.13
(1,281)	1:185:A:LEU:HD13	1:185:A:LEU:HB3	3	1.13
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG22	5	1.12
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD13	5	1.12
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD13	5	1.12
(1,2120)	1:177:B:VAL:HG12	1:182:B:ILE:HG22	1	1.12
(1,2119)	1:177:A:VAL:HG12	1:182:A:ILE:HG22	1	1.12
(1,2071)	1:208:A:TRP:H	1:211:A:ALA:HB1	4	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2066)	1:201:B:MET:HE1	1:184:B:ALA:H	4	1.12
(1,2065)	1:201:A:MET:HE1	1:184:A:ALA:H	4	1.12
(1,1590)	1:202:B:GLU:H	1:205:B:GLN:HG3	9	1.12
(1,1589)	1:202:A:GLU:H	1:205:A:GLN:HG3	9	1.12
(1,1259)	1:176:A:THR:HG22	1:177:A:VAL:HG13	7	1.12
(1,940)	1:175:B:LEU:HD23	1:175:B:LEU:HB2	6	1.12
(1,939)	1:175:A:LEU:HD23	1:175:A:LEU:HB2	6	1.12
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB1	4	1.12
(1,173)	1:211:A:ALA:HB1	1:203:B:ARG:HD3	4	1.12
(1,171)	1:211:A:ALA:HB3	1:206:B:LYS:HE3	5	1.12
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG22	5	1.11
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB1	3	1.11
(1,1818)	1:192:B:ASN:H	1:187:B:LYS:HG2	2	1.11
(1,1817)	1:192:A:ASN:H	1:187:A:LYS:HG2	2	1.11
(1,1258)	1:176:B:THR:HG22	1:177:B:VAL:HG23	2	1.11
(1,1257)	1:176:A:THR:HG22	1:177:A:VAL:HG23	2	1.11
(1,1169)	1:206:A:LYS:HG3	1:209:A:SER:HB3	4	1.11
(1,940)	1:175:B:LEU:HD21	1:175:B:LEU:HB2	1	1.11
(1,940)	1:175:B:LEU:HD21	1:175:B:LEU:HB2	2	1.11
(1,940)	1:175:B:LEU:HD22	1:175:B:LEU:HB2	3	1.11
(1,939)	1:175:A:LEU:HD21	1:175:A:LEU:HB2	1	1.11
(1,939)	1:175:A:LEU:HD21	1:175:A:LEU:HB2	2	1.11
(1,939)	1:175:A:LEU:HD22	1:175:A:LEU:HB2	3	1.11
(1,870)	1:188:B:ASN:HB3	1:187:B:LYS:HB3	8	1.11
(1,869)	1:188:A:ASN:HB3	1:187:A:LYS:HB3	8	1.11
(1,690)	1:199:B:GLN:HB3	1:196:B:ALA:HA	6	1.11
(1,689)	1:199:A:GLN:HB3	1:196:A:ALA:HA	6	1.11
(1,172)	1:211:B:ALA:HB3	1:206:A:LYS:HE3	5	1.11
(1,158)	1:182:B:ILE:HD12	1:178:B:PRO:HD3	3	1.11
(1,157)	1:182:A:ILE:HD12	1:178:A:PRO:HD3	3	1.11
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG23	10	1.1
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG23	10	1.1
(1,2650)	1:188:B:ASN:HD22	1:178:A:PRO:HG3	4	1.1
(1,2570)	1:208:B:TRP:HE1	1:204:A:LEU:HG	7	1.1
(1,2569)	1:208:A:TRP:HE1	1:204:B:LEU:HG	7	1.1
(1,2072)	1:211:B:ALA:HB2	1:208:A:TRP:H	4	1.1
(1,1553)	1:173:A:GLN:HE21	1:175:A:LEU:HB3	4	1.1
(1,1260)	1:176:B:THR:HG21	1:177:B:VAL:HG13	6	1.1
(1,1259)	1:176:A:THR:HG21	1:177:A:VAL:HG13	6	1.1
(1,1170)	1:206:B:LYS:HG3	1:209:B:SER:HB3	4	1.1
(1,940)	1:175:B:LEU:HD23	1:175:B:LEU:HB2	8	1.1
(1,939)	1:175:A:LEU:HD23	1:175:A:LEU:HB2	8	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2724)	1:189:B:ASN:HD22	1:200:B:VAL:HG21	9	1.09
(1,2723)	1:189:A:ASN:HD22	1:200:A:VAL:HG21	9	1.09
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB1	3	1.09
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB1	2	1.09
(1,2373)	1:176:A:THR:HG23	1:190:B:PHE:HZ	4	1.09
(1,1980)	1:173:A:GLN:H	1:212:A:LYS:HA	7	1.09
(1,1979)	1:173:B:GLN:H	1:212:B:LYS:HA	7	1.09
(1,1554)	1:173:B:GLN:HE21	1:175:B:LEU:HB3	4	1.09
(1,1454)	1:209:B:SER:H	1:203:A:ARG:HE	10	1.09
(1,940)	1:175:B:LEU:HD21	1:175:B:LEU:HB2	5	1.09
(1,939)	1:175:A:LEU:HD21	1:175:A:LEU:HB2	5	1.09
(1,198)	1:201:B:MET:HE2	1:177:B:VAL:HG13	7	1.09
(1,197)	1:201:A:MET:HE2	1:177:A:VAL:HG13	7	1.09
(1,174)	1:211:B:ALA:HB1	1:203:A:ARG:HD3	4	1.09
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD23	5	1.09
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD23	5	1.09
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB3	7	1.08
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB3	7	1.08
(1,2374)	1:176:B:THR:HG23	1:190:A:PHE:HZ	4	1.08
(1,2373)	1:176:A:THR:HG21	1:190:B:PHE:HZ	9	1.08
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB1	3	1.08
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB1	3	1.08
(1,2148)	1:194:B:GLN:HB2	1:197:B:VAL:HG22	7	1.08
(1,2147)	1:194:A:GLN:HB2	1:197:A:VAL:HG22	7	1.08
(1,2071)	1:211:A:ALA:HB2	1:208:B:TRP:H	6	1.08
(1,2071)	1:211:A:ALA:HB1	1:208:B:TRP:H	9	1.08
(1,1453)	1:209:A:SER:H	1:203:B:ARG:HE	10	1.08
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG12	3	1.08
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG12	3	1.08
(1,1219)	1:185:A:LEU:HD22	1:177:B:VAL:HG13	5	1.08
(1,1218)	1:201:B:MET:HE3	1:179:B:TRP:HB2	6	1.08
(1,1217)	1:201:A:MET:HE3	1:179:A:TRP:HB2	6	1.08
(1,951)	1:197:A:VAL:HG13	1:187:A:LYS:HG2	1	1.08
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD11	2	1.07
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD11	2	1.07
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB1	2	1.07
(1,2116)	1:182:B:ILE:HD13	1:178:B:PRO:HB2	6	1.07
(1,2115)	1:182:A:ILE:HD11	1:178:A:PRO:HB2	2	1.07
(1,2115)	1:182:A:ILE:HD13	1:178:A:PRO:HB2	6	1.07
(1,2104)	1:204:B:LEU:HD23	1:179:A:TRP:HE3	7	1.07
(1,2103)	1:204:A:LEU:HD23	1:179:B:TRP:HE3	7	1.07
(1,2080)	1:175:B:LEU:HD22	1:196:A:ALA:H	9	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2071)	1:211:A:ALA:HB2	1:208:B:TRP:H	10	1.07
(1,1646)	1:201:B:MET:H	1:175:A:LEU:HB2	4	1.07
(1,1646)	1:201:B:MET:H	1:175:A:LEU:HB2	10	1.07
(1,1257)	1:176:A:THR:HG22	1:177:A:VAL:HG21	5	1.07
(1,1220)	1:185:B:LEU:HD22	1:177:A:VAL:HG13	5	1.07
(1,952)	1:197:B:VAL:HG13	1:187:B:LYS:HG2	1	1.07
(1,860)	1:200:B:VAL:HA	1:175:A:LEU:HB3	7	1.07
(1,249)	1:185:A:LEU:HD13	1:188:A:ASN:HB3	8	1.07
(1,198)	1:201:B:MET:HE2	1:177:B:VAL:HG13	3	1.07
(1,197)	1:201:A:MET:HE2	1:177:A:VAL:HG13	3	1.07
(1,170)	1:182:B:ILE:HD12	1:177:B:VAL:HG22	7	1.07
(1,169)	1:182:A:ILE:HD12	1:177:A:VAL:HG22	7	1.07
(1,57)	1:211:A:ALA:HB1	1:206:B:LYS:H	9	1.07
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB3	6	1.06
(1,2304)	1:188:B:ASN:HB2	1:185:B:LEU:HB3	8	1.06
(1,2303)	1:188:A:ASN:HB2	1:185:A:LEU:HB3	8	1.06
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB1	1	1.06
(1,2260)	1:190:B:PHE:HA	1:197:B:VAL:HG21	2	1.06
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB1	1	1.06
(1,2259)	1:190:A:PHE:HA	1:197:A:VAL:HG21	2	1.06
(1,2116)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	2	1.06
(1,2072)	1:211:B:ALA:HB3	1:208:A:TRP:H	1	1.06
(1,2072)	1:211:B:ALA:HB1	1:208:A:TRP:H	9	1.06
(1,2071)	1:211:A:ALA:HB3	1:208:B:TRP:H	1	1.06
(1,2020)	1:205:B:GLN:HE22	1:179:B:TRP:HD1	6	1.06
(1,2019)	1:205:A:GLN:HE22	1:179:A:TRP:HD1	6	1.06
(1,1722)	1:196:B:ALA:H	1:198:B:ARG:HG2	5	1.06
(1,1721)	1:196:A:ALA:H	1:198:A:ARG:HG2	5	1.06
(1,1258)	1:176:B:THR:HG22	1:177:B:VAL:HG21	5	1.06
(1,1258)	1:176:B:THR:HG21	1:177:B:VAL:HG21	9	1.06
(1,1257)	1:176:A:THR:HG21	1:177:A:VAL:HG21	9	1.06
(1,1246)	1:175:B:LEU:HD11	1:177:B:VAL:HG22	9	1.06
(1,1245)	1:175:A:LEU:HD11	1:177:A:VAL:HG22	9	1.06
(1,859)	1:200:A:VAL:HA	1:175:B:LEU:HB3	7	1.06
(1,414)	1:203:B:ARG:HD3	1:173:A:GLN:HE21	8	1.06
(1,413)	1:203:A:ARG:HD3	1:173:B:GLN:HE21	8	1.06
(1,250)	1:185:B:LEU:HD13	1:188:B:ASN:HB3	8	1.06
(1,57)	1:211:A:ALA:HB3	1:206:B:LYS:H	6	1.06
(1,2649)	1:188:A:ASN:HD22	1:178:B:PRO:HG3	4	1.05
(1,2644)	1:188:B:ASN:HD22	1:185:B:LEU:HB2	10	1.05
(1,2643)	1:188:A:ASN:HD22	1:185:A:LEU:HB2	9	1.05
(1,2643)	1:188:A:ASN:HD22	1:185:A:LEU:HB2	10	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2570)	1:208:B:TRP:HE1	1:204:A:LEU:HG	2	1.05
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB3	6	1.05
(1,2374)	1:176:B:THR:HG21	1:190:A:PHE:HZ	6	1.05
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD13	4	1.05
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB2	4	1.05
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB2	6	1.05
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB2	6	1.05
(1,2072)	1:211:B:ALA:HB2	1:208:A:TRP:H	6	1.05
(1,2071)	1:211:A:ALA:HB2	1:208:B:TRP:H	5	1.05
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG11	5	1.05
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG11	5	1.05
(1,1646)	1:201:B:MET:H	1:175:A:LEU:HB2	9	1.05
(1,1645)	1:201:A:MET:H	1:175:B:LEU:HB2	10	1.05
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB3	2	1.05
(1,58)	1:211:B:ALA:HB3	1:206:A:LYS:H	6	1.05
(1,58)	1:211:B:ALA:HB1	1:206:A:LYS:H	9	1.05
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD21	5	1.04
(1,2844)	1:177:B:VAL:H	1:175:B:LEU:HD23	8	1.04
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD21	5	1.04
(1,2843)	1:177:A:VAL:H	1:175:A:LEU:HD23	8	1.04
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD13	7	1.04
(1,2806)	1:185:B:LEU:H	1:186:B:LEU:HD12	9	1.04
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD13	7	1.04
(1,2805)	1:185:A:LEU:H	1:186:A:LEU:HD12	9	1.04
(1,2644)	1:188:B:ASN:HD22	1:185:B:LEU:HB2	9	1.04
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD13	4	1.04
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB2	4	1.04
(1,2104)	1:204:B:LEU:HD22	1:179:A:TRP:HE3	5	1.04
(1,2072)	1:211:B:ALA:HB2	1:208:A:TRP:H	5	1.04
(1,2072)	1:211:B:ALA:HB2	1:208:A:TRP:H	10	1.04
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE2	3	1.04
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE2	3	1.04
(1,1722)	1:196:B:ALA:H	1:198:B:ARG:HG2	9	1.04
(1,1721)	1:196:A:ALA:H	1:198:A:ARG:HG2	6	1.04
(1,1721)	1:196:A:ALA:H	1:198:A:ARG:HG2	9	1.04
(1,1645)	1:201:A:MET:H	1:175:B:LEU:HB2	4	1.04
(1,1645)	1:201:A:MET:H	1:175:B:LEU:HB2	8	1.04
(1,1580)	1:188:B:ASN:HD22	1:185:B:LEU:HA	4	1.04
(1,1410)	1:212:B:LYS:H	1:212:B:LYS:HB3	5	1.04
(1,1410)	1:212:B:LYS:H	1:212:B:LYS:HB3	8	1.04
(1,1409)	1:212:A:LYS:H	1:212:A:LYS:HB3	5	1.04
(1,1409)	1:212:A:LYS:H	1:212:A:LYS:HB3	8	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1220)	1:185:B:LEU:HD22	1:177:A:VAL:HG12	6	1.04
(1,706)	1:195:B:ALA:HA	1:198:B:ARG:HG2	7	1.04
(1,705)	1:195:A:ALA:HA	1:198:A:ARG:HG2	7	1.04
(1,170)	1:182:B:ILE:HD11	1:177:B:VAL:HG23	8	1.04
(1,170)	1:182:B:ILE:HD11	1:177:B:VAL:HG21	10	1.04
(1,169)	1:182:A:ILE:HD11	1:177:A:VAL:HG21	10	1.04
(1,2569)	1:208:A:TRP:HE1	1:204:B:LEU:HG	2	1.03
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG21	1	1.03
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG21	1	1.03
(1,2373)	1:176:A:THR:HG21	1:190:B:PHE:HZ	6	1.03
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB3	8	1.03
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB3	8	1.03
(1,2148)	1:183:B:GLU:HB2	1:197:B:VAL:HG11	5	1.03
(1,2147)	1:183:A:GLU:HB2	1:197:A:VAL:HG11	5	1.03
(1,2104)	1:204:B:LEU:HD23	1:179:A:TRP:HE3	9	1.03
(1,2103)	1:204:A:LEU:HD22	1:179:B:TRP:HE3	5	1.03
(1,2074)	1:211:B:ALA:HB1	1:208:B:TRP:HE3	4	1.03
(1,2073)	1:211:A:ALA:HB1	1:208:A:TRP:HE3	4	1.03
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG11	7	1.03
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG11	7	1.03
(1,1722)	1:196:B:ALA:H	1:198:B:ARG:HG2	3	1.03
(1,1722)	1:196:B:ALA:H	1:198:B:ARG:HG2	6	1.03
(1,1721)	1:196:A:ALA:H	1:198:A:ARG:HG2	3	1.03
(1,1646)	1:201:B:MET:H	1:175:A:LEU:HB2	5	1.03
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG12	2	1.03
(1,1258)	1:176:B:THR:HG23	1:177:B:VAL:HG23	4	1.03
(1,1257)	1:176:A:THR:HG23	1:177:A:VAL:HG23	4	1.03
(1,690)	1:199:B:GLN:HB3	1:196:B:ALA:HA	1	1.03
(1,689)	1:199:A:GLN:HB3	1:196:A:ALA:HA	1	1.03
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB3	2	1.03
(1,198)	1:201:B:MET:HE3	1:177:B:VAL:HG11	1	1.03
(1,197)	1:201:A:MET:HE3	1:177:A:VAL:HG11	1	1.03
(1,169)	1:182:A:ILE:HD11	1:177:A:VAL:HG23	8	1.03
(1,57)	1:211:A:ALA:HB1	1:206:B:LYS:H	1	1.03
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG11	3	1.02
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG11	3	1.02
(1,2840)	1:179:B:TRP:H	1:182:B:ILE:HG23	10	1.02
(1,2649)	1:188:A:ASN:HD22	1:178:B:PRO:HG3	1	1.02
(1,2649)	1:188:A:ASN:HD22	1:178:B:PRO:HG3	3	1.02
(1,2374)	1:176:B:THR:HG21	1:190:A:PHE:HZ	9	1.02
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB1	10	1.02
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB1	10	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2154)	1:205:B:GLN:HG2	1:205:B:GLN:H	9	1.02
(1,2153)	1:205:A:GLN:HG2	1:205:A:GLN:H	9	1.02
(1,2148)	1:194:B:GLN:HB2	1:197:B:VAL:HG22	10	1.02
(1,2147)	1:194:A:GLN:HB2	1:197:A:VAL:HG22	10	1.02
(1,2103)	1:204:A:LEU:HD23	1:179:B:TRP:HE3	9	1.02
(1,1979)	1:173:B:GLN:H	1:212:B:LYS:HA	4	1.02
(1,1646)	1:201:B:MET:H	1:175:A:LEU:HB2	8	1.02
(1,1579)	1:188:A:ASN:HD22	1:185:A:LEU:HA	4	1.02
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG13	5	1.02
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG12	2	1.02
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG13	5	1.02
(1,888)	1:202:B:GLU:HG2	1:201:B:MET:HB2	2	1.02
(1,888)	1:202:B:GLU:HG2	1:201:B:MET:HB2	8	1.02
(1,887)	1:202:A:GLU:HG2	1:201:A:MET:HB2	2	1.02
(1,887)	1:202:A:GLU:HG2	1:201:A:MET:HB2	8	1.02
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB3	3	1.02
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB3	3	1.02
(1,174)	1:211:B:ALA:HB3	1:203:A:ARG:HD3	2	1.02
(1,158)	1:182:B:ILE:HD11	1:178:B:PRO:HD3	1	1.02
(1,157)	1:182:A:ILE:HD11	1:178:A:PRO:HD3	1	1.02
(1,58)	1:211:B:ALA:HB1	1:206:A:LYS:H	1	1.02
(1,57)	1:211:A:ALA:HB2	1:206:B:LYS:H	10	1.02
(1,2872)	1:209:B:SER:H	1:204:A:LEU:HG	2	1.01
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD13	9	1.01
(1,2650)	1:188:B:ASN:HD22	1:178:A:PRO:HG3	1	1.01
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG22	8	1.01
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB2	7	1.01
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB2	9	1.01
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB2	7	1.01
(1,2148)	1:183:B:GLU:HB2	1:197:B:VAL:HG12	1	1.01
(1,2147)	1:183:A:GLU:HB2	1:197:A:VAL:HG12	1	1.01
(1,2120)	1:177:B:VAL:HG11	1:182:B:ILE:HG23	7	1.01
(1,2119)	1:177:A:VAL:HG11	1:182:A:ILE:HG23	7	1.01
(1,2116)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	4	1.01
(1,2115)	1:182:A:ILE:HD13	1:178:A:PRO:HB2	4	1.01
(1,2072)	1:211:B:ALA:HB1	1:208:A:TRP:H	7	1.01
(1,1980)	1:173:A:GLN:H	1:212:A:LYS:HA	4	1.01
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG23	2	1.01
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG21	9	1.01
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG23	2	1.01
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG21	9	1.01
(1,2839)	1:179:A:TRP:H	1:182:A:ILE:HG23	10	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2650)	1:188:B:ASN:HD22	1:178:A:PRO:HG3	3	1.0
(1,2569)	1:208:A:TRP:HE1	1:204:B:LEU:HG	9	1.0
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG22	8	1.0
(1,2374)	1:176:B:THR:HG22	1:190:A:PHE:HZ	2	1.0
(1,2373)	1:176:A:THR:HG22	1:190:B:PHE:HZ	2	1.0
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB2	9	1.0
(1,2148)	1:183:B:GLU:HB2	1:197:B:VAL:HG13	9	1.0
(1,2147)	1:183:A:GLU:HB2	1:197:A:VAL:HG13	9	1.0
(1,2116)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	8	1.0
(1,2115)	1:182:A:ILE:HD11	1:178:A:PRO:HB2	8	1.0
(1,2104)	1:204:B:LEU:HD21	1:179:A:TRP:HE3	8	1.0
(1,2103)	1:204:A:LEU:HD23	1:179:B:TRP:HE3	6	1.0
(1,2074)	1:211:B:ALA:HB3	1:208:B:TRP:HE3	2	1.0
(1,2073)	1:211:A:ALA:HB3	1:208:A:TRP:HE3	2	1.0
(1,2072)	1:211:B:ALA:HB3	1:208:A:TRP:H	8	1.0
(1,2071)	1:211:A:ALA:HB1	1:208:B:TRP:H	7	1.0
(1,1645)	1:201:A:MET:H	1:175:B:LEU:HB2	5	1.0
(1,1645)	1:201:A:MET:H	1:175:B:LEU:HB2	9	1.0
(1,1602)	1:202:B:GLU:H	1:205:B:GLN:HE22	9	1.0
(1,1601)	1:202:A:GLU:H	1:205:A:GLN:HE22	9	1.0
(1,1579)	1:188:A:ASN:HD22	1:185:A:LEU:HA	3	1.0
(1,1219)	1:185:A:LEU:HD22	1:177:B:VAL:HG12	6	1.0
(1,706)	1:195:B:ALA:HA	1:198:B:ARG:HG2	3	1.0
(1,173)	1:211:A:ALA:HB3	1:203:B:ARG:HD3	2	1.0
(1,158)	1:182:B:ILE:HD12	1:178:B:PRO:HD3	5	1.0
(1,157)	1:182:A:ILE:HD12	1:178:A:PRO:HD3	5	1.0
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD21	3	1.0
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD21	3	1.0
(1,58)	1:211:B:ALA:HB2	1:206:A:LYS:H	2	1.0
(1,58)	1:211:B:ALA:HB2	1:206:A:LYS:H	3	1.0
(1,57)	1:211:A:ALA:HB3	1:206:B:LYS:H	4	1.0
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG12	5	0.99
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG12	5	0.99
(1,2871)	1:209:A:SER:H	1:204:B:LEU:HG	2	0.99
(1,2862)	1:173:A:GLN:H	1:175:A:LEU:HB2	7	0.99
(1,2861)	1:173:B:GLN:H	1:175:B:LEU:HB2	7	0.99
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD11	10	0.99
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD13	9	0.99
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB3	9	0.99
(1,2373)	1:176:A:THR:HG22	1:190:B:PHE:HZ	7	0.99
(1,2120)	1:177:B:VAL:HG11	1:182:B:ILE:HG23	2	0.99
(1,2119)	1:177:A:VAL:HG11	1:182:A:ILE:HG23	2	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2104)	1:204:B:LEU:HD22	1:179:A:TRP:HE3	2	0.99
(1,1645)	1:201:A:MET:H	1:175:B:LEU:HB2	2	0.99
(1,1580)	1:188:B:ASN:HD22	1:185:B:LEU:HA	3	0.99
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG12	6	0.99
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG13	9	0.99
(1,1258)	1:176:B:THR:HG22	1:177:B:VAL:HG23	10	0.99
(1,1257)	1:176:A:THR:HG22	1:177:A:VAL:HG23	10	0.99
(1,1246)	1:175:B:LEU:HD13	1:177:B:VAL:HG23	4	0.99
(1,1245)	1:175:A:LEU:HD13	1:177:A:VAL:HG23	4	0.99
(1,1219)	1:185:A:LEU:HD22	1:177:B:VAL:HG12	2	0.99
(1,933)	1:197:A:VAL:HG23	1:187:A:LYS:HG2	1	0.99
(1,706)	1:195:B:ALA:HA	1:198:B:ARG:HG2	9	0.99
(1,705)	1:195:A:ALA:HA	1:198:A:ARG:HG2	3	0.99
(1,690)	1:199:B:GLN:HB3	1:196:B:ALA:HA	8	0.99
(1,689)	1:199:A:GLN:HB3	1:196:A:ALA:HA	8	0.99
(1,174)	1:211:B:ALA:HB3	1:203:A:ARG:HD3	3	0.99
(1,158)	1:182:B:ILE:HD12	1:178:B:PRO:HD3	2	0.99
(1,157)	1:182:A:ILE:HD12	1:178:A:PRO:HD3	2	0.99
(1,58)	1:211:B:ALA:HB2	1:206:A:LYS:H	10	0.99
(1,57)	1:211:A:ALA:HB3	1:206:B:LYS:H	5	0.99
(1,2872)	1:209:B:SER:H	1:204:A:LEU:HG	1	0.98
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB2	2	0.98
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB2	2	0.98
(1,2592)	1:208:B:TRP:H	1:211:B:ALA:HB1	4	0.98
(1,2570)	1:208:B:TRP:HE1	1:204:A:LEU:HG	8	0.98
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB3	9	0.98
(1,2374)	1:176:B:THR:HG22	1:190:A:PHE:HZ	7	0.98
(1,2259)	1:190:A:PHE:HA	1:196:A:ALA:HB3	5	0.98
(1,2148)	1:183:B:GLU:HB2	1:197:B:VAL:HG12	6	0.98
(1,2147)	1:183:A:GLU:HB2	1:197:A:VAL:HG12	6	0.98
(1,2120)	1:177:B:VAL:HG12	1:182:B:ILE:HG22	9	0.98
(1,2104)	1:204:B:LEU:HD23	1:179:A:TRP:HE3	1	0.98
(1,2103)	1:204:A:LEU:HD23	1:179:B:TRP:HE3	1	0.98
(1,2103)	1:204:A:LEU:HD22	1:179:B:TRP:HE3	2	0.98
(1,2103)	1:204:A:LEU:HD21	1:179:B:TRP:HE3	8	0.98
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG12	3	0.98
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG23	3	0.98
(1,1646)	1:201:B:MET:H	1:175:A:LEU:HB2	2	0.98
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG12	6	0.98
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG13	9	0.98
(1,1170)	1:206:B:LYS:HG3	1:209:B:SER:HB3	6	0.98
(1,1169)	1:206:A:LYS:HG3	1:209:A:SER:HB3	6	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:197:B:VAL:HG23	1:187:B:LYS:HG2	1	0.98
(1,705)	1:195:A:ALA:HA	1:198:A:ARG:HG2	9	0.98
(1,690)	1:199:B:GLN:HB3	1:196:B:ALA:HA	7	0.98
(1,689)	1:199:A:GLN:HB3	1:196:A:ALA:HA	7	0.98
(1,173)	1:211:A:ALA:HB3	1:203:B:ARG:HD3	3	0.98
(1,58)	1:211:B:ALA:HB3	1:206:A:LYS:H	5	0.98
(1,57)	1:211:A:ALA:HB2	1:206:B:LYS:H	2	0.98
(1,57)	1:211:A:ALA:HB2	1:206:B:LYS:H	3	0.98
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB1	6	0.98
(1,24)	1:201:B:MET:HE3	1:183:B:GLU:HA	9	0.98
(1,23)	1:201:A:MET:HE3	1:183:A:GLU:HA	9	0.98
(1,2871)	1:209:A:SER:H	1:204:B:LEU:HG	1	0.97
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD11	10	0.97
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB2	4	0.97
(1,2570)	1:208:B:TRP:HE1	1:204:A:LEU:HG	9	0.97
(1,2260)	1:190:B:PHE:HA	1:196:B:ALA:HB3	5	0.97
(1,2148)	1:183:B:GLU:HB2	1:197:B:VAL:HG12	2	0.97
(1,2119)	1:177:A:VAL:HG12	1:182:A:ILE:HG22	9	0.97
(1,2104)	1:204:B:LEU:HD23	1:179:A:TRP:HE3	6	0.97
(1,2071)	1:211:A:ALA:HB3	1:208:B:TRP:H	8	0.97
(1,2062)	1:177:B:VAL:HG12	1:182:B:ILE:HG12	8	0.97
(1,2061)	1:177:A:VAL:HG12	1:182:A:ILE:HG12	8	0.97
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG12	3	0.97
(1,1818)	1:192:B:ASN:H	1:187:B:LYS:HG2	5	0.97
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG23	3	0.97
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG21	5	0.97
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG21	5	0.97
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG13	1	0.97
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG13	1	0.97
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG12	7	0.97
(1,1218)	1:201:B:MET:HE2	1:179:B:TRP:HB2	8	0.97
(1,706)	1:195:B:ALA:HA	1:198:B:ARG:HG2	1	0.97
(1,690)	1:199:B:GLN:HB3	1:196:B:ALA:HA	5	0.97
(1,689)	1:199:A:GLN:HB3	1:196:A:ALA:HA	5	0.97
(1,170)	1:182:B:ILE:HD11	1:177:B:VAL:HG21	4	0.97
(1,169)	1:182:A:ILE:HD11	1:177:A:VAL:HG21	4	0.97
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB1	6	0.97
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB1	9	0.97
(1,2871)	1:209:A:SER:H	1:204:B:LEU:HG	10	0.96
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD12	7	0.96
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD12	7	0.96
(1,2569)	1:208:A:TRP:HE1	1:204:B:LEU:HG	8	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2147)	1:183:A:GLU:HB2	1:197:A:VAL:HG12	2	0.96
(1,2079)	1:175:A:LEU:HD21	1:196:B:ALA:H	6	0.96
(1,1818)	1:192:B:ASN:H	1:187:B:LYS:HG2	4	0.96
(1,1817)	1:192:A:ASN:H	1:187:A:LYS:HG2	4	0.96
(1,1817)	1:192:A:ASN:H	1:187:A:LYS:HG2	5	0.96
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG22	6	0.96
(1,1722)	1:196:B:ALA:H	1:198:B:ARG:HG2	4	0.96
(1,1721)	1:196:A:ALA:H	1:198:A:ARG:HG2	4	0.96
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG12	7	0.96
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG12	8	0.96
(1,1220)	1:185:B:LEU:HD22	1:177:A:VAL:HG12	2	0.96
(1,1217)	1:201:A:MET:HE2	1:179:A:TRP:HB2	8	0.96
(1,705)	1:195:A:ALA:HA	1:198:A:ARG:HG2	1	0.96
(1,690)	1:199:B:GLN:HB3	1:196:B:ALA:HA	3	0.96
(1,689)	1:199:A:GLN:HB3	1:196:A:ALA:HA	3	0.96
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB2	8	0.96
(1,588)	1:209:B:SER:H	1:209:B:SER:HB3	8	0.96
(1,587)	1:209:A:SER:H	1:209:A:SER:HB3	4	0.96
(1,587)	1:209:A:SER:H	1:209:A:SER:HB3	5	0.96
(1,587)	1:209:A:SER:H	1:209:A:SER:HB3	6	0.96
(1,587)	1:209:A:SER:H	1:209:A:SER:HB3	8	0.96
(1,198)	1:201:B:MET:HE3	1:177:B:VAL:HG13	2	0.96
(1,197)	1:201:A:MET:HE3	1:177:A:VAL:HG13	2	0.96
(1,158)	1:182:B:ILE:HD11	1:178:B:PRO:HD3	6	0.96
(1,157)	1:182:A:ILE:HD11	1:178:A:PRO:HD3	4	0.96
(1,157)	1:182:A:ILE:HD11	1:178:A:PRO:HD3	6	0.96
(1,58)	1:211:B:ALA:HB3	1:206:A:LYS:H	4	0.96
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB1	9	0.96
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG11	4	0.95
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB1	9	0.95
(1,2569)	1:208:A:TRP:HE1	1:204:B:LEU:HG	10	0.95
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB2	1	0.95
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB2	1	0.95
(1,2120)	1:177:B:VAL:HG11	1:182:B:ILE:HG21	3	0.95
(1,2120)	1:177:B:VAL:HG11	1:182:B:ILE:HG23	4	0.95
(1,2119)	1:177:A:VAL:HG11	1:182:A:ILE:HG21	3	0.95
(1,2119)	1:177:A:VAL:HG11	1:182:A:ILE:HG23	4	0.95
(1,2104)	1:204:B:LEU:HD21	1:179:A:TRP:HE3	3	0.95
(1,2103)	1:204:A:LEU:HD21	1:179:B:TRP:HE3	3	0.95
(1,2080)	1:175:B:LEU:HD21	1:196:A:ALA:H	6	0.95
(1,2074)	1:211:B:ALA:HB3	1:208:B:TRP:HE3	3	0.95
(1,2073)	1:211:A:ALA:HB3	1:208:A:TRP:HE3	3	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2062)	1:177:B:VAL:HG13	1:182:B:ILE:HG12	7	0.95
(1,2062)	1:177:B:VAL:HG13	1:182:B:ILE:HG12	10	0.95
(1,2061)	1:177:A:VAL:HG13	1:182:A:ILE:HG12	7	0.95
(1,2061)	1:177:A:VAL:HG13	1:182:A:ILE:HG12	10	0.95
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG23	1	0.95
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG23	1	0.95
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG22	6	0.95
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG12	8	0.95
(1,706)	1:195:B:ALA:HA	1:198:B:ARG:HG2	6	0.95
(1,705)	1:195:A:ALA:HA	1:198:A:ARG:HG2	5	0.95
(1,588)	1:209:B:SER:H	1:209:B:SER:HB3	4	0.95
(1,588)	1:209:B:SER:H	1:209:B:SER:HB3	5	0.95
(1,588)	1:209:B:SER:H	1:209:B:SER:HB3	6	0.95
(1,198)	1:201:B:MET:HE2	1:177:B:VAL:HG11	5	0.95
(1,197)	1:201:A:MET:HE2	1:177:A:VAL:HG11	5	0.95
(1,158)	1:182:B:ILE:HD11	1:178:B:PRO:HD3	4	0.95
(1,114)	1:173:B:GLN:HE21	1:175:B:LEU:HD11	7	0.95
(1,113)	1:173:A:GLN:HE21	1:175:A:LEU:HD11	7	0.95
(1,2872)	1:209:B:SER:H	1:204:A:LEU:HG	7	0.94
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB2	6	0.94
(1,2569)	1:208:A:TRP:HE1	1:204:B:LEU:HG	1	0.94
(1,2374)	1:176:B:THR:HG22	1:190:A:PHE:HZ	10	0.94
(1,2373)	1:176:A:THR:HG22	1:190:B:PHE:HZ	10	0.94
(1,2324)	1:204:B:LEU:HD12	1:200:B:VAL:HA	7	0.94
(1,2323)	1:204:A:LEU:HD12	1:200:A:VAL:HA	7	0.94
(1,2116)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	5	0.94
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG13	1	0.94
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG13	1	0.94
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG21	7	0.94
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG21	7	0.94
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG13	10	0.94
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG13	10	0.94
(1,1220)	1:185:B:LEU:HD23	1:177:A:VAL:HG12	4	0.94
(1,946)	1:175:B:LEU:HD21	1:199:A:GLN:HB3	10	0.94
(1,945)	1:175:A:LEU:HD21	1:199:B:GLN:HB3	10	0.94
(1,887)	1:202:A:GLU:HG2	1:201:A:MET:HB2	5	0.94
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG12	8	0.94
(1,706)	1:195:B:ALA:HA	1:198:B:ARG:HG2	5	0.94
(1,705)	1:195:A:ALA:HA	1:198:A:ARG:HG2	6	0.94
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB2	8	0.94
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG11	4	0.93
(1,2872)	1:209:B:SER:H	1:204:A:LEU:HG	3	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2872)	1:209:B:SER:H	1:204:A:LEU:HG	10	0.93
(1,2871)	1:209:A:SER:H	1:204:B:LEU:HG	7	0.93
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB2	4	0.93
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB2	10	0.93
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB3	1	0.93
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB1	9	0.93
(1,2570)	1:208:B:TRP:HE1	1:204:A:LEU:HG	1	0.93
(1,2570)	1:208:B:TRP:HE1	1:204:A:LEU:HG	10	0.93
(1,2569)	1:208:A:TRP:HE1	1:204:B:LEU:HG	4	0.93
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG23	3	0.93
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG23	3	0.93
(1,2120)	1:177:B:VAL:HG11	1:182:B:ILE:HG22	6	0.93
(1,2119)	1:177:A:VAL:HG12	1:182:A:ILE:HG22	5	0.93
(1,2119)	1:177:A:VAL:HG11	1:182:A:ILE:HG22	6	0.93
(1,2115)	1:182:A:ILE:HD11	1:178:A:PRO:HB2	5	0.93
(1,2062)	1:177:B:VAL:HG12	1:182:B:ILE:HG12	4	0.93
(1,2061)	1:177:A:VAL:HG12	1:182:A:ILE:HG12	4	0.93
(1,1646)	1:201:B:MET:H	1:175:A:LEU:HB2	1	0.93
(1,1645)	1:201:A:MET:H	1:175:B:LEU:HB2	1	0.93
(1,1258)	1:176:B:THR:HG21	1:177:B:VAL:HG22	6	0.93
(1,1257)	1:176:A:THR:HG21	1:177:A:VAL:HG22	6	0.93
(1,946)	1:175:B:LEU:HD21	1:199:A:GLN:HB3	4	0.93
(1,888)	1:202:B:GLU:HG2	1:201:B:MET:HB2	5	0.93
(1,887)	1:202:A:GLU:HG2	1:201:A:MET:HB2	1	0.93
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG12	8	0.93
(1,690)	1:199:B:GLN:HB3	1:196:B:ALA:HA	4	0.93
(1,689)	1:199:A:GLN:HB3	1:196:A:ALA:HA	4	0.93
(1,585)	1:209:A:SER:HB3	1:210:A:LEU:H	4	0.93
(1,174)	1:211:B:ALA:HB2	1:203:A:ARG:HD3	8	0.93
(1,170)	1:182:B:ILE:HD11	1:177:B:VAL:HG21	1	0.93
(1,169)	1:182:A:ILE:HD11	1:177:A:VAL:HG21	1	0.93
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB2	5	0.93
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB2	5	0.93
(1,2871)	1:209:A:SER:H	1:204:B:LEU:HG	3	0.92
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD21	8	0.92
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD11	1	0.92
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD11	1	0.92
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB2	4	0.92
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG23	2	0.92
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG23	2	0.92
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB3	1	0.92
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB2	6	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG22	4	0.92
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG22	4	0.92
(1,2373)	1:176:A:THR:HG22	1:190:B:PHE:HZ	1	0.92
(1,2120)	1:177:B:VAL:HG12	1:182:B:ILE:HG22	5	0.92
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG12	4	0.92
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG23	10	0.92
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG23	10	0.92
(1,1372)	1:176:B:THR:H	1:177:B:VAL:HG12	4	0.92
(1,1371)	1:176:A:THR:H	1:177:A:VAL:HG12	4	0.92
(1,1217)	1:201:A:MET:HE2	1:179:A:TRP:HB2	5	0.92
(1,1092)	1:199:B:GLN:HG2	1:173:A:GLN:HE21	5	0.92
(1,916)	1:199:B:GLN:HG2	1:175:A:LEU:HD12	7	0.92
(1,888)	1:202:B:GLU:HG2	1:201:B:MET:HB2	1	0.92
(1,888)	1:202:B:GLU:HG2	1:201:B:MET:HB2	4	0.92
(1,888)	1:202:B:GLU:HG2	1:201:B:MET:HB2	6	0.92
(1,586)	1:209:B:SER:HB3	1:210:B:LEU:H	4	0.92
(1,171)	1:211:A:ALA:HB1	1:206:B:LYS:HE3	8	0.92
(1,2872)	1:209:B:SER:H	1:204:A:LEU:HG	5	0.91
(1,2871)	1:209:A:SER:H	1:204:B:LEU:HG	5	0.91
(1,2871)	1:209:A:SER:H	1:204:B:LEU:HG	9	0.91
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD21	8	0.91
(1,2777)	1:193:A:ASP:H	1:197:A:VAL:HG22	7	0.91
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB2	5	0.91
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB2	5	0.91
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB2	10	0.91
(1,2569)	1:208:A:TRP:HE1	1:204:B:LEU:HG	5	0.91
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG22	7	0.91
(1,2374)	1:176:B:THR:HG22	1:190:A:PHE:HZ	1	0.91
(1,2374)	1:176:B:THR:HG21	1:190:A:PHE:HZ	8	0.91
(1,2373)	1:176:A:THR:HG21	1:190:B:PHE:HZ	8	0.91
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD11	5	0.91
(1,2103)	1:204:A:LEU:HD22	1:179:B:TRP:HE3	4	0.91
(1,2074)	1:211:B:ALA:HB2	1:208:B:TRP:HE3	8	0.91
(1,2073)	1:211:A:ALA:HB2	1:208:A:TRP:HE3	8	0.91
(1,2062)	1:177:B:VAL:HG13	1:182:B:ILE:HG12	5	0.91
(1,2061)	1:177:A:VAL:HG13	1:182:A:ILE:HG12	5	0.91
(1,2020)	1:205:B:GLN:HE22	1:179:B:TRP:HD1	7	0.91
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG11	9	0.91
(1,1645)	1:201:A:MET:H	1:175:B:LEU:HB2	3	0.91
(1,1258)	1:176:B:THR:HG22	1:177:B:VAL:HG21	7	0.91
(1,1257)	1:176:A:THR:HG22	1:177:A:VAL:HG21	7	0.91
(1,1217)	1:201:A:MET:HE1	1:179:A:TRP:HB2	4	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	1:175:A:LEU:HD21	1:199:B:GLN:HB3	4	0.91
(1,915)	1:199:A:GLN:HG2	1:175:B:LEU:HD12	7	0.91
(1,887)	1:202:A:GLU:HG2	1:201:A:MET:HB2	4	0.91
(1,887)	1:202:A:GLU:HG2	1:201:A:MET:HB2	6	0.91
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB1	6	0.91
(1,170)	1:182:B:ILE:HD12	1:177:B:VAL:HG22	5	0.91
(1,169)	1:182:A:ILE:HD12	1:177:A:VAL:HG22	5	0.91
(1,160)	1:182:B:ILE:HD12	1:177:B:VAL:HA	7	0.91
(1,159)	1:182:A:ILE:HD12	1:177:A:VAL:HA	7	0.91
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD23	1	0.91
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD23	1	0.91
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB3	1	0.91
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB2	8	0.91
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB3	1	0.91
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB1	4	0.91
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB2	8	0.91
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG11	2	0.9
(1,2872)	1:209:B:SER:H	1:204:A:LEU:HG	8	0.9
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD23	9	0.9
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD23	9	0.9
(1,2778)	1:193:B:ASP:H	1:197:B:VAL:HG22	7	0.9
(1,2570)	1:208:B:TRP:HE1	1:204:A:LEU:HG	4	0.9
(1,2570)	1:208:B:TRP:HE1	1:204:A:LEU:HG	5	0.9
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG22	7	0.9
(1,2486)	1:180:B:ASP:H	1:183:B:GLU:HB3	1	0.9
(1,2485)	1:180:A:ASP:H	1:183:A:GLU:HB3	1	0.9
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB1	8	0.9
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB1	8	0.9
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD11	5	0.9
(1,2120)	1:177:B:VAL:HG12	1:182:B:ILE:HG23	10	0.9
(1,2019)	1:205:A:GLN:HE22	1:179:A:TRP:HD1	7	0.9
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG13	2	0.9
(1,1219)	1:185:A:LEU:HD23	1:177:B:VAL:HG12	4	0.9
(1,1218)	1:201:B:MET:HE1	1:179:B:TRP:HB2	4	0.9
(1,1218)	1:201:B:MET:HE2	1:179:B:TRP:HB2	5	0.9
(1,1123)	1:211:A:ALA:HB1	1:204:B:LEU:H	10	0.9
(1,1091)	1:199:A:GLN:HG2	1:173:B:GLN:HE21	5	0.9
(1,586)	1:209:B:SER:HB3	1:210:B:LEU:H	6	0.9
(1,585)	1:209:A:SER:HB3	1:210:A:LEU:H	5	0.9
(1,173)	1:211:A:ALA:HB2	1:203:B:ARG:HD3	8	0.9
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB1	4	0.9
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB1	7	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB1	7	0.9
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG11	6	0.89
(1,2861)	1:173:B:GLN:H	1:175:B:LEU:HB2	1	0.89
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB2	10	0.89
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB2	10	0.89
(1,2228)	1:208:B:TRP:HA	1:212:B:LYS:H	10	0.89
(1,2227)	1:208:A:TRP:HA	1:212:A:LYS:H	10	0.89
(1,2119)	1:177:A:VAL:HG12	1:182:A:ILE:HG23	10	0.89
(1,2104)	1:204:B:LEU:HD22	1:179:A:TRP:HE3	4	0.89
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB2	7	0.89
(1,2020)	1:205:B:GLN:HE22	1:179:B:TRP:HD1	5	0.89
(1,2019)	1:205:A:GLN:HE22	1:179:A:TRP:HD1	5	0.89
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG12	4	0.89
(1,1818)	1:192:B:ASN:H	1:187:B:LYS:HG2	10	0.89
(1,1817)	1:192:A:ASN:H	1:187:A:LYS:HG2	10	0.89
(1,1770)	1:175:B:LEU:H	1:175:B:LEU:HB3	5	0.89
(1,1769)	1:175:A:LEU:H	1:175:A:LEU:HB3	5	0.89
(1,1220)	1:185:B:LEU:HD22	1:177:A:VAL:HG13	1	0.89
(1,1220)	1:185:B:LEU:HD23	1:177:A:VAL:HG12	7	0.89
(1,1220)	1:185:B:LEU:HD21	1:177:A:VAL:HG13	10	0.89
(1,1219)	1:185:A:LEU:HD22	1:177:B:VAL:HG13	1	0.89
(1,1219)	1:185:A:LEU:HD23	1:177:B:VAL:HG12	7	0.89
(1,1218)	1:201:B:MET:HE3	1:179:B:TRP:HB2	1	0.89
(1,1217)	1:201:A:MET:HE3	1:179:A:TRP:HB2	1	0.89
(1,1123)	1:211:A:ALA:HB3	1:204:B:LEU:H	9	0.89
(1,586)	1:209:B:SER:HB3	1:210:B:LEU:H	5	0.89
(1,586)	1:209:B:SER:HB3	1:210:B:LEU:H	8	0.89
(1,585)	1:209:A:SER:HB3	1:210:A:LEU:H	6	0.89
(1,172)	1:211:B:ALA:HB1	1:206:A:LYS:HE3	8	0.89
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG11	8	0.88
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG11	2	0.88
(1,2872)	1:209:B:SER:H	1:204:A:LEU:HG	9	0.88
(1,2862)	1:173:A:GLN:H	1:175:A:LEU:HB2	1	0.88
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB1	7	0.88
(1,2332)	1:212:B:LYS:HB3	1:211:B:ALA:H	6	0.88
(1,2331)	1:212:A:LYS:HB3	1:211:A:ALA:H	6	0.88
(1,2074)	1:211:B:ALA:HB2	1:208:B:TRP:HE3	1	0.88
(1,2074)	1:211:B:ALA:HB3	1:208:B:TRP:HE3	7	0.88
(1,2073)	1:211:A:ALA:HB2	1:208:A:TRP:HE3	1	0.88
(1,2073)	1:211:A:ALA:HB3	1:208:A:TRP:HE3	7	0.88
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB2	7	0.88
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG11	9	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG13	2	0.88
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG22	8	0.88
(1,1646)	1:201:B:MET:H	1:175:A:LEU:HB2	3	0.88
(1,1558)	1:173:B:GLN:HE21	1:200:A:VAL:HG13	2	0.88
(1,690)	1:199:B:GLN:HB3	1:196:B:ALA:HA	2	0.88
(1,689)	1:199:A:GLN:HB3	1:196:A:ALA:HA	2	0.88
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB1	6	0.88
(1,585)	1:209:A:SER:HB3	1:210:A:LEU:H	8	0.88
(1,173)	1:211:A:ALA:HB1	1:203:B:ARG:HD3	6	0.88
(1,159)	1:182:A:ILE:HD13	1:177:A:VAL:HA	9	0.88
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB3	3	0.88
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG13	10	0.87
(1,2871)	1:209:A:SER:H	1:204:B:LEU:HG	6	0.87
(1,2836)	1:179:B:TRP:H	1:183:B:GLU:HA	7	0.87
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG22	8	0.87
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB1	7	0.87
(1,2591)	1:208:A:TRP:H	1:211:B:ALA:HB3	8	0.87
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB2	3	0.87
(1,2194)	1:173:B:GLN:HA	1:173:B:GLN:H	8	0.87
(1,2193)	1:173:A:GLN:HA	1:173:A:GLN:H	8	0.87
(1,1818)	1:192:B:ASN:H	1:187:B:LYS:HG2	3	0.87
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG22	8	0.87
(1,1770)	1:175:B:LEU:H	1:175:B:LEU:HB3	1	0.87
(1,1770)	1:175:B:LEU:H	1:175:B:LEU:HB3	3	0.87
(1,1769)	1:175:A:LEU:H	1:175:A:LEU:HB3	1	0.87
(1,1769)	1:175:A:LEU:H	1:175:A:LEU:HB3	3	0.87
(1,1646)	1:201:B:MET:H	1:175:A:LEU:HB2	6	0.87
(1,1645)	1:201:A:MET:H	1:175:B:LEU:HB2	6	0.87
(1,1580)	1:188:B:ASN:HD22	1:185:B:LEU:HA	2	0.87
(1,1579)	1:188:A:ASN:HD22	1:185:A:LEU:HA	2	0.87
(1,1124)	1:211:B:ALA:HB1	1:204:A:LEU:H	10	0.87
(1,198)	1:201:B:MET:HE1	1:177:B:VAL:HG13	6	0.87
(1,197)	1:201:A:MET:HE1	1:177:A:VAL:HG13	6	0.87
(1,170)	1:182:B:ILE:HD12	1:177:B:VAL:HG21	2	0.87
(1,170)	1:182:B:ILE:HD13	1:177:B:VAL:HG22	9	0.87
(1,169)	1:182:A:ILE:HD12	1:177:A:VAL:HG21	2	0.87
(1,169)	1:182:A:ILE:HD13	1:177:A:VAL:HG22	9	0.87
(1,160)	1:182:B:ILE:HD13	1:177:B:VAL:HA	9	0.87
(1,160)	1:182:B:ILE:HD11	1:177:B:VAL:HA	10	0.87
(1,159)	1:182:A:ILE:HD11	1:177:A:VAL:HA	10	0.87
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB3	3	0.87
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG11	6	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG11	8	0.86
(1,2871)	1:209:A:SER:H	1:204:B:LEU:HG	8	0.86
(1,2835)	1:179:A:TRP:H	1:183:A:GLU:HA	7	0.86
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG23	3	0.86
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG22	6	0.86
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG22	8	0.86
(1,2630)	1:173:B:GLN:HE21	1:195:A:ALA:HB3	8	0.86
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG21	5	0.86
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG21	5	0.86
(1,2474)	1:197:B:VAL:H	1:190:B:PHE:H	7	0.86
(1,2473)	1:197:A:VAL:H	1:190:A:PHE:H	7	0.86
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB2	3	0.86
(1,2148)	1:183:B:GLU:HB2	1:197:B:VAL:HG12	3	0.86
(1,2147)	1:183:A:GLU:HB2	1:197:A:VAL:HG12	3	0.86
(1,2062)	1:177:B:VAL:HG13	1:182:B:ILE:HG12	1	0.86
(1,2062)	1:177:B:VAL:HG12	1:182:B:ILE:HG12	2	0.86
(1,2062)	1:177:B:VAL:HG12	1:182:B:ILE:HG12	6	0.86
(1,2061)	1:177:A:VAL:HG13	1:182:A:ILE:HG12	1	0.86
(1,2061)	1:177:A:VAL:HG12	1:182:A:ILE:HG12	2	0.86
(1,2061)	1:177:A:VAL:HG12	1:182:A:ILE:HG12	6	0.86
(1,1986)	1:173:A:GLN:H	1:175:A:LEU:HD11	4	0.86
(1,1985)	1:173:B:GLN:H	1:175:B:LEU:HD11	4	0.86
(1,1817)	1:192:A:ASN:H	1:187:A:LYS:HG2	3	0.86
(1,1219)	1:185:A:LEU:HD21	1:177:B:VAL:HG13	10	0.86
(1,1124)	1:211:B:ALA:HB3	1:204:A:LEU:H	9	0.86
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB2	1	0.86
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB2	1	0.86
(1,170)	1:182:B:ILE:HD11	1:177:B:VAL:HG23	6	0.86
(1,169)	1:182:A:ILE:HD11	1:177:A:VAL:HG23	6	0.86
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB2	7	0.86
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB1	10	0.86
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB2	7	0.86
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB1	10	0.86
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB3	2	0.86
(1,46)	1:199:B:GLN:H	1:196:B:ALA:HB3	10	0.86
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB3	10	0.86
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG13	10	0.85
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG12	1	0.85
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG23	3	0.85
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG22	6	0.85
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG22	2	0.85
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG22	2	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG21	6	0.85
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG23	7	0.85
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG23	7	0.85
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD13	10	0.85
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD13	10	0.85
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE1	6	0.85
(1,1788)	1:179:B:TRP:H	1:177:B:VAL:HG23	4	0.85
(1,1787)	1:179:A:TRP:H	1:177:A:VAL:HG23	4	0.85
(1,1658)	1:200:B:VAL:H	1:199:B:GLN:HB3	9	0.85
(1,1657)	1:200:A:VAL:H	1:199:A:GLN:HB3	9	0.85
(1,1646)	1:201:B:MET:H	1:175:A:LEU:HB2	7	0.85
(1,1645)	1:201:A:MET:H	1:175:B:LEU:HB2	7	0.85
(1,1580)	1:188:B:ASN:HD22	1:185:B:LEU:HA	7	0.85
(1,1579)	1:188:A:ASN:HD22	1:185:A:LEU:HA	7	0.85
(1,1218)	1:201:B:MET:HE3	1:179:B:TRP:HB2	2	0.85
(1,1217)	1:201:A:MET:HE3	1:179:A:TRP:HB2	2	0.85
(1,1072)	1:175:B:LEU:HD13	1:201:A:MET:H	7	0.85
(1,750)	1:185:B:LEU:HD21	1:185:B:LEU:HA	7	0.85
(1,749)	1:185:A:LEU:HD21	1:185:A:LEU:HA	7	0.85
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB3	7	0.85
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB3	7	0.85
(1,158)	1:182:B:ILE:HD11	1:178:B:PRO:HD3	8	0.85
(1,157)	1:182:A:ILE:HD11	1:178:A:PRO:HD3	8	0.85
(1,45)	1:199:A:GLN:H	1:196:A:ALA:HB3	2	0.85
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG12	1	0.84
(1,2872)	1:209:B:SER:H	1:204:A:LEU:HG	6	0.84
(1,2871)	1:209:A:SER:H	1:204:B:LEU:HG	4	0.84
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD22	2	0.84
(1,2836)	1:179:B:TRP:H	1:183:B:GLU:HA	9	0.84
(1,2835)	1:179:A:TRP:H	1:183:A:GLU:HA	9	0.84
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD11	8	0.84
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG21	9	0.84
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG21	9	0.84
(1,2592)	1:208:B:TRP:H	1:211:A:ALA:HB3	8	0.84
(1,2570)	1:208:B:TRP:HE1	1:204:A:LEU:HG	3	0.84
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG21	6	0.84
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG22	3	0.84
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD13	2	0.84
(1,2234)	1:200:B:VAL:HA	1:190:B:PHE:HE2	7	0.84
(1,2233)	1:200:A:VAL:HA	1:190:A:PHE:HE2	7	0.84
(1,2148)	1:183:B:GLU:HB2	1:197:B:VAL:HG11	4	0.84
(1,2147)	1:183:A:GLU:HB2	1:197:A:VAL:HG11	4	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2138)	1:201:B:MET:HB2	1:202:B:GLU:HA	1	0.84
(1,2137)	1:201:A:MET:HB2	1:202:A:GLU:HA	1	0.84
(1,2074)	1:211:B:ALA:HB1	1:208:B:TRP:HE3	5	0.84
(1,2073)	1:211:A:ALA:HB1	1:208:A:TRP:HE3	5	0.84
(1,2019)	1:205:A:GLN:HE22	1:179:A:TRP:HD1	8	0.84
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE1	6	0.84
(1,1721)	1:196:A:ALA:H	1:198:A:ARG:HG2	8	0.84
(1,1558)	1:173:B:GLN:HE21	1:200:A:VAL:HG12	3	0.84
(1,1557)	1:173:A:GLN:HE21	1:200:B:VAL:HG13	2	0.84
(1,1246)	1:175:B:LEU:HD11	1:177:B:VAL:HG23	1	0.84
(1,1245)	1:175:A:LEU:HD11	1:177:A:VAL:HG23	1	0.84
(1,1245)	1:175:A:LEU:HD13	1:177:A:VAL:HG23	8	0.84
(1,1071)	1:175:A:LEU:HD13	1:201:B:MET:H	7	0.84
(1,750)	1:185:B:LEU:HD23	1:185:B:LEU:HA	3	0.84
(1,749)	1:185:A:LEU:HD23	1:185:A:LEU:HA	3	0.84
(1,174)	1:211:B:ALA:HB1	1:203:A:ARG:HD3	6	0.84
(1,58)	1:211:B:ALA:HB2	1:206:A:LYS:H	7	0.84
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD23	1	0.83
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD23	1	0.83
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG22	5	0.83
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG22	5	0.83
(1,2569)	1:208:A:TRP:HE1	1:204:B:LEU:HG	3	0.83
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG22	3	0.83
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD11	3	0.83
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD13	6	0.83
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD11	3	0.83
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD13	6	0.83
(1,2373)	1:176:A:THR:HG22	1:190:B:PHE:HZ	5	0.83
(1,2362)	1:196:B:ALA:H	1:194:B:GLN:HB3	4	0.83
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD11	8	0.83
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD13	2	0.83
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD11	8	0.83
(1,2062)	1:177:B:VAL:HG13	1:182:B:ILE:HG12	9	0.83
(1,2061)	1:177:A:VAL:HG13	1:182:A:ILE:HG12	9	0.83
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG11	6	0.83
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG12	10	0.83
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG11	6	0.83
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG12	10	0.83
(1,1722)	1:196:B:ALA:H	1:198:B:ARG:HG2	8	0.83
(1,1246)	1:175:B:LEU:HD13	1:177:B:VAL:HG23	8	0.83
(1,1245)	1:175:A:LEU:HD11	1:177:A:VAL:HG21	5	0.83
(1,1220)	1:185:B:LEU:HD22	1:177:A:VAL:HG13	9	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1219)	1:185:A:LEU:HD22	1:177:B:VAL:HG12	3	0.83
(1,1092)	1:199:B:GLN:HG2	1:173:A:GLN:HE21	1	0.83
(1,749)	1:185:A:LEU:HD23	1:185:A:LEU:HA	1	0.83
(1,749)	1:185:A:LEU:HD23	1:185:A:LEU:HA	5	0.83
(1,749)	1:185:A:LEU:HD22	1:185:A:LEU:HA	10	0.83
(1,690)	1:199:B:GLN:HB3	1:196:B:ALA:HA	10	0.83
(1,689)	1:199:A:GLN:HB3	1:196:A:ALA:HA	10	0.83
(1,173)	1:211:A:ALA:HB2	1:203:B:ARG:HD3	1	0.83
(1,57)	1:211:A:ALA:HB2	1:206:B:LYS:H	7	0.83
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB1	3	0.83
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB1	3	0.83
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG12	9	0.82
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD22	2	0.82
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG21	1	0.82
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG21	1	0.82
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG23	2	0.82
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG22	4	0.82
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG22	5	0.82
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG22	10	0.82
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG23	2	0.82
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG22	4	0.82
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG22	10	0.82
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD12	9	0.82
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD12	9	0.82
(1,2361)	1:196:A:ALA:H	1:194:A:GLN:HB3	4	0.82
(1,2074)	1:211:B:ALA:HB3	1:208:B:TRP:HE3	9	0.82
(1,2073)	1:211:A:ALA:HB1	1:208:A:TRP:HE3	6	0.82
(1,2073)	1:211:A:ALA:HB3	1:208:A:TRP:HE3	9	0.82
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB2	4	0.82
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB2	4	0.82
(1,2020)	1:205:B:GLN:HE22	1:179:B:TRP:HD1	8	0.82
(1,1976)	1:174:B:GLU:H	1:174:B:GLU:HB2	9	0.82
(1,1975)	1:174:A:GLU:H	1:174:A:GLU:HB2	9	0.82
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE3	8	0.82
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE3	8	0.82
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG11	1	0.82
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG11	2	0.82
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG11	2	0.82
(1,1658)	1:200:B:VAL:H	1:199:B:GLN:HB3	1	0.82
(1,1657)	1:200:A:VAL:H	1:199:A:GLN:HB3	1	0.82
(1,1579)	1:188:A:ASN:HD22	1:185:A:LEU:HA	6	0.82
(1,1557)	1:173:A:GLN:HE21	1:200:B:VAL:HG12	3	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1246)	1:175:B:LEU:HD12	1:177:B:VAL:HG23	2	0.82
(1,1246)	1:175:B:LEU:HD11	1:177:B:VAL:HG21	5	0.82
(1,1245)	1:175:A:LEU:HD12	1:177:A:VAL:HG23	2	0.82
(1,1219)	1:185:A:LEU:HD22	1:177:B:VAL:HG13	9	0.82
(1,1124)	1:211:B:ALA:HB1	1:204:A:LEU:H	5	0.82
(1,1123)	1:211:A:ALA:HB1	1:204:B:LEU:H	4	0.82
(1,1123)	1:211:A:ALA:HB1	1:204:B:LEU:H	5	0.82
(1,750)	1:185:B:LEU:HD23	1:185:B:LEU:HA	1	0.82
(1,750)	1:185:B:LEU:HD23	1:185:B:LEU:HA	2	0.82
(1,750)	1:185:B:LEU:HD21	1:185:B:LEU:HA	4	0.82
(1,750)	1:185:B:LEU:HD23	1:185:B:LEU:HA	5	0.82
(1,750)	1:185:B:LEU:HD23	1:185:B:LEU:HA	8	0.82
(1,750)	1:185:B:LEU:HD23	1:185:B:LEU:HA	9	0.82
(1,750)	1:185:B:LEU:HD22	1:185:B:LEU:HA	10	0.82
(1,749)	1:185:A:LEU:HD23	1:185:A:LEU:HA	2	0.82
(1,749)	1:185:A:LEU:HD21	1:185:A:LEU:HA	4	0.82
(1,749)	1:185:A:LEU:HD23	1:185:A:LEU:HA	6	0.82
(1,749)	1:185:A:LEU:HD23	1:185:A:LEU:HA	8	0.82
(1,749)	1:185:A:LEU:HD23	1:185:A:LEU:HA	9	0.82
(1,174)	1:211:B:ALA:HB2	1:203:A:ARG:HD3	1	0.82
(1,174)	1:211:B:ALA:HB3	1:203:A:ARG:HD3	7	0.82
(1,173)	1:211:A:ALA:HB3	1:203:B:ARG:HD3	7	0.82
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD13	10	0.82
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD13	10	0.82
(1,106)	1:185:B:LEU:HD22	1:183:A:GLU:H	7	0.82
(1,105)	1:185:A:LEU:HD22	1:183:B:GLU:H	7	0.82
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD21	3	0.81
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD21	3	0.81
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD11	8	0.81
(1,2629)	1:173:A:GLN:HE21	1:195:B:ALA:HB3	8	0.81
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG22	1	0.81
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG23	6	0.81
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG22	1	0.81
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG22	5	0.81
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG23	6	0.81
(1,2324)	1:204:B:LEU:HD12	1:200:B:VAL:HA	10	0.81
(1,2323)	1:204:A:LEU:HD12	1:200:A:VAL:HA	10	0.81
(1,2148)	1:183:B:GLU:HB2	1:197:B:VAL:HG11	8	0.81
(1,2147)	1:183:A:GLU:HB2	1:197:A:VAL:HG11	8	0.81
(1,2139)	1:206:A:LYS:HD3	1:206:A:LYS:HA	9	0.81
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG21	1	0.81
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG21	1	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2074)	1:211:B:ALA:HB1	1:208:B:TRP:HE3	6	0.81
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG11	10	0.81
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG11	1	0.81
(1,1658)	1:200:B:VAL:H	1:199:B:GLN:HB3	3	0.81
(1,1658)	1:200:B:VAL:H	1:199:B:GLN:HB3	6	0.81
(1,1657)	1:200:A:VAL:H	1:199:A:GLN:HB3	3	0.81
(1,1657)	1:200:A:VAL:H	1:199:A:GLN:HB3	6	0.81
(1,1580)	1:188:B:ASN:HD22	1:185:B:LEU:HA	6	0.81
(1,1553)	1:173:A:GLN:HE21	1:175:A:LEU:HB3	1	0.81
(1,1430)	1:211:B:ALA:H	1:206:A:LYS:HE3	5	0.81
(1,1429)	1:211:A:ALA:H	1:206:B:LYS:HE3	5	0.81
(1,1220)	1:185:B:LEU:HD22	1:177:A:VAL:HG12	3	0.81
(1,1091)	1:199:A:GLN:HG2	1:173:B:GLN:HE21	1	0.81
(1,1074)	1:192:B:ASN:H	1:187:B:LYS:HG3	1	0.81
(1,1073)	1:192:A:ASN:H	1:187:A:LYS:HG3	1	0.81
(1,750)	1:185:B:LEU:HD23	1:185:B:LEU:HA	6	0.81
(1,198)	1:201:B:MET:HE3	1:177:B:VAL:HG13	8	0.81
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD11	3	0.81
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD13	1	0.81
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD11	3	0.81
(1,2878)	1:203:B:ARG:H	1:177:A:VAL:HG11	7	0.8
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG12	9	0.8
(1,2872)	1:209:B:SER:H	1:204:A:LEU:HG	4	0.8
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD12	3	0.8
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG22	8	0.8
(1,2412)	1:199:B:GLN:HA	1:200:B:VAL:HG23	9	0.8
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG22	8	0.8
(1,2411)	1:199:A:GLN:HA	1:200:A:VAL:HG23	9	0.8
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD11	7	0.8
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD11	7	0.8
(1,2324)	1:204:B:LEU:HD11	1:200:B:VAL:HA	9	0.8
(1,2323)	1:204:A:LEU:HD11	1:200:A:VAL:HA	9	0.8
(1,2140)	1:206:B:LYS:HD3	1:206:B:LYS:HA	9	0.8
(1,2073)	1:211:A:ALA:HB1	1:208:A:TRP:HE3	10	0.8
(1,1480)	1:179:B:TRP:HE1	1:201:B:MET:HE1	6	0.8
(1,1479)	1:179:A:TRP:HE1	1:201:A:MET:HE1	6	0.8
(1,1124)	1:211:B:ALA:HB2	1:204:A:LEU:H	1	0.8
(1,1123)	1:211:A:ALA:HB2	1:204:B:LEU:H	1	0.8
(1,972)	1:204:B:LEU:HD23	1:182:A:ILE:HD12	8	0.8
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB1	5	0.8
(1,197)	1:201:A:MET:HE3	1:177:A:VAL:HG13	8	0.8
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD13	1	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB2	6	0.8
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB2	6	0.8
(1,2877)	1:203:A:ARG:H	1:177:B:VAL:HG11	7	0.79
(1,2864)	1:173:A:GLN:H	1:203:B:ARG:HG3	2	0.79
(1,2863)	1:173:B:GLN:H	1:203:A:ARG:HG3	2	0.79
(1,2436)	1:201:B:MET:HB2	1:200:B:VAL:HG21	4	0.79
(1,2436)	1:201:B:MET:HB2	1:200:B:VAL:HG21	5	0.79
(1,2435)	1:201:A:MET:HB2	1:200:A:VAL:HG21	4	0.79
(1,2435)	1:201:A:MET:HB2	1:200:A:VAL:HG21	5	0.79
(1,2374)	1:176:B:THR:HG22	1:190:A:PHE:HZ	5	0.79
(1,2332)	1:212:B:LYS:HB3	1:211:B:ALA:H	9	0.79
(1,2331)	1:212:A:LYS:HB3	1:211:A:ALA:H	9	0.79
(1,2234)	1:200:B:VAL:HA	1:190:B:PHE:HE2	2	0.79
(1,2233)	1:200:A:VAL:HA	1:190:A:PHE:HE2	2	0.79
(1,2188)	1:193:B:ASP:H	1:192:B:ASN:HB2	3	0.79
(1,2187)	1:193:A:ASP:H	1:192:A:ASN:HB2	3	0.79
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG22	8	0.79
(1,2074)	1:211:B:ALA:HB1	1:208:B:TRP:HE3	10	0.79
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG13	5	0.79
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG13	5	0.79
(1,1612)	1:204:B:LEU:H	1:205:B:GLN:HG3	9	0.79
(1,1611)	1:204:A:LEU:H	1:205:A:GLN:HG3	9	0.79
(1,1580)	1:188:B:ASN:HD22	1:185:B:LEU:HA	1	0.79
(1,1580)	1:188:B:ASN:HD22	1:185:B:LEU:HA	5	0.79
(1,1579)	1:188:A:ASN:HD22	1:185:A:LEU:HA	5	0.79
(1,1554)	1:173:B:GLN:HE21	1:175:B:LEU:HB3	1	0.79
(1,1479)	1:179:A:TRP:HE1	1:201:A:MET:HE3	8	0.79
(1,1123)	1:211:A:ALA:HB1	1:204:B:LEU:H	6	0.79
(1,1105)	1:176:A:THR:HG21	1:179:A:TRP:HD1	1	0.79
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB1	5	0.79
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB1	2	0.79
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB2	4	0.79
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB3	5	0.79
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB2	4	0.79
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB3	5	0.79
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB3	8	0.79
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD12	3	0.78
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD11	6	0.78
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB3	1	0.78
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB3	1	0.78
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB3	4	0.78
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB3	4	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2234)	1:200:B:VAL:HA	1:190:B:PHE:HE2	8	0.78
(1,2233)	1:200:A:VAL:HA	1:190:A:PHE:HE2	8	0.78
(1,2188)	1:193:B:ASP:H	1:192:B:ASN:HB2	4	0.78
(1,2187)	1:193:A:ASP:H	1:192:A:ASN:HB2	4	0.78
(1,2150)	1:173:B:GLN:HB3	1:174:B:GLU:H	6	0.78
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG22	8	0.78
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB3	5	0.78
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB3	5	0.78
(1,2022)	1:179:B:TRP:HE1	1:205:B:GLN:HE22	6	0.78
(1,2021)	1:179:A:TRP:HE1	1:205:A:GLN:HE22	6	0.78
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG11	10	0.78
(1,1657)	1:200:A:VAL:H	1:199:A:GLN:HB3	7	0.78
(1,1579)	1:188:A:ASN:HD22	1:185:A:LEU:HA	1	0.78
(1,1554)	1:173:B:GLN:HE21	1:175:B:LEU:HB3	5	0.78
(1,1553)	1:173:A:GLN:HE21	1:175:A:LEU:HB3	5	0.78
(1,1480)	1:179:B:TRP:HE1	1:201:B:MET:HE2	4	0.78
(1,1480)	1:179:B:TRP:HE1	1:201:B:MET:HE3	8	0.78
(1,1479)	1:179:A:TRP:HE1	1:201:A:MET:HE2	4	0.78
(1,1124)	1:211:B:ALA:HB3	1:204:A:LEU:H	2	0.78
(1,1118)	1:175:B:LEU:HD22	1:208:B:TRP:HH2	7	0.78
(1,1117)	1:175:A:LEU:HD22	1:208:A:TRP:HH2	7	0.78
(1,1106)	1:176:B:THR:HG21	1:179:B:TRP:HD1	1	0.78
(1,971)	1:204:A:LEU:HD21	1:182:B:ILE:HD12	4	0.78
(1,910)	1:201:B:MET:HG2	1:201:B:MET:HA	3	0.78
(1,909)	1:201:A:MET:HG2	1:201:A:MET:HA	3	0.78
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG12	6	0.78
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD13	10	0.78
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD13	10	0.78
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD11	2	0.78
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD13	6	0.78
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD11	2	0.78
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD13	4	0.78
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD13	6	0.78
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB1	1	0.78
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB3	8	0.78
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB1	1	0.78
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB1	2	0.78
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB2	6	0.77
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB2	6	0.77
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB1	8	0.77
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG21	9	0.77
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD11	2	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD11	2	0.77
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD13	6	0.77
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD13	7	0.77
(1,2234)	1:200:B:VAL:HA	1:190:B:PHE:HE2	5	0.77
(1,2188)	1:193:B:ASP:H	1:192:B:ASN:HB2	2	0.77
(1,2187)	1:193:A:ASP:H	1:192:A:ASN:HB2	2	0.77
(1,2149)	1:173:A:GLN:HB3	1:174:A:GLU:H	6	0.77
(1,2062)	1:177:B:VAL:HG12	1:182:B:ILE:HG12	3	0.77
(1,2061)	1:177:A:VAL:HG12	1:182:A:ILE:HG12	3	0.77
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE2	4	0.77
(1,1722)	1:196:B:ALA:H	1:198:B:ARG:HG2	2	0.77
(1,1721)	1:196:A:ALA:H	1:198:A:ARG:HG2	2	0.77
(1,1658)	1:200:B:VAL:H	1:199:B:GLN:HB3	7	0.77
(1,1584)	1:173:B:GLN:HE21	1:200:A:VAL:HA	2	0.77
(1,1124)	1:211:B:ALA:HB1	1:204:A:LEU:H	4	0.77
(1,174)	1:211:B:ALA:HB1	1:203:A:ARG:HD3	5	0.77
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD12	9	0.77
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD12	9	0.77
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD13	4	0.77
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD11	5	0.77
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD11	5	0.77
(1,106)	1:185:B:LEU:HD22	1:183:A:GLU:H	4	0.77
(1,48)	1:198:B:ARG:H	1:196:B:ALA:HB2	9	0.77
(1,47)	1:198:A:ARG:H	1:196:A:ALA:HB2	9	0.77
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB1	8	0.76
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG21	9	0.76
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB1	5	0.76
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG13	7	0.76
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG13	7	0.76
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG12	7	0.76
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD12	3	0.76
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD13	7	0.76
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD12	3	0.76
(1,2234)	1:200:B:VAL:HA	1:190:B:PHE:HE2	3	0.76
(1,2233)	1:200:A:VAL:HA	1:190:A:PHE:HE2	3	0.76
(1,2233)	1:200:A:VAL:HA	1:190:A:PHE:HE2	5	0.76
(1,2188)	1:193:B:ASP:H	1:192:B:ASN:HB2	10	0.76
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG22	4	0.76
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG21	6	0.76
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG22	4	0.76
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG21	6	0.76
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB1	10	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE3	1	0.76
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE2	4	0.76
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE3	1	0.76
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE2	5	0.76
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG11	3	0.76
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG11	3	0.76
(1,1658)	1:200:B:VAL:H	1:199:B:GLN:HB3	4	0.76
(1,1658)	1:200:B:VAL:H	1:199:B:GLN:HB3	5	0.76
(1,1658)	1:200:B:VAL:H	1:199:B:GLN:HB3	8	0.76
(1,1657)	1:200:A:VAL:H	1:199:A:GLN:HB3	4	0.76
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG12	6	0.76
(1,173)	1:211:A:ALA:HB1	1:203:B:ARG:HD3	5	0.76
(1,2836)	1:179:B:TRP:H	1:183:B:GLU:HA	1	0.75
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD12	2	0.75
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD11	6	0.75
(1,2656)	1:188:B:ASN:HD21	1:185:B:LEU:HD23	8	0.75
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB1	5	0.75
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD13	1	0.75
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD13	4	0.75
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD11	5	0.75
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD13	1	0.75
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD13	4	0.75
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD11	5	0.75
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG12	7	0.75
(1,2324)	1:204:B:LEU:HD11	1:200:B:VAL:HA	2	0.75
(1,2323)	1:204:A:LEU:HD11	1:200:A:VAL:HA	2	0.75
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD13	6	0.75
(1,2234)	1:200:B:VAL:HA	1:190:B:PHE:HE2	6	0.75
(1,2233)	1:200:A:VAL:HA	1:190:A:PHE:HE2	6	0.75
(1,2187)	1:193:A:ASP:H	1:192:A:ASN:HB2	10	0.75
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG23	3	0.75
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG23	3	0.75
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB1	10	0.75
(1,1984)	1:173:A:GLN:H	1:173:A:GLN:HB2	6	0.75
(1,1983)	1:173:B:GLN:H	1:173:B:GLN:HB2	6	0.75
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG12	6	0.75
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE3	2	0.75
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE2	5	0.75
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE3	2	0.75
(1,1657)	1:200:A:VAL:H	1:199:A:GLN:HB3	5	0.75
(1,1657)	1:200:A:VAL:H	1:199:A:GLN:HB3	8	0.75
(1,1480)	1:179:B:TRP:HE1	1:201:B:MET:HE3	1	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1479)	1:179:A:TRP:HE1	1:201:A:MET:HE3	1	0.75
(1,1479)	1:179:A:TRP:HE1	1:201:A:MET:HE2	5	0.75
(1,1124)	1:211:B:ALA:HB1	1:204:A:LEU:H	6	0.75
(1,1123)	1:211:A:ALA:HB3	1:204:B:LEU:H	2	0.75
(1,1010)	1:208:B:TRP:HB3	1:208:B:TRP:HE3	1	0.75
(1,1010)	1:208:B:TRP:HB3	1:208:B:TRP:HE3	3	0.75
(1,1009)	1:208:A:TRP:HB3	1:208:A:TRP:HE3	3	0.75
(1,971)	1:204:A:LEU:HD23	1:182:B:ILE:HD12	8	0.75
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG11	7	0.75
(1,434)	1:188:B:ASN:H	1:188:B:ASN:HB3	8	0.75
(1,433)	1:188:A:ASN:H	1:188:A:ASN:HB3	8	0.75
(1,198)	1:201:B:MET:HE2	1:177:B:VAL:HG13	4	0.75
(1,197)	1:201:A:MET:HE2	1:177:A:VAL:HG13	4	0.75
(1,194)	1:201:B:MET:HE2	1:182:B:ILE:HD11	7	0.75
(1,193)	1:201:A:MET:HE2	1:182:A:ILE:HD11	7	0.75
(1,186)	1:184:B:ALA:HB1	1:187:B:LYS:HE2	7	0.75
(1,185)	1:184:A:ALA:HB1	1:187:A:LYS:HE2	7	0.75
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD12	9	0.75
(1,105)	1:185:A:LEU:HD21	1:183:B:GLU:H	3	0.75
(1,105)	1:185:A:LEU:HD22	1:183:B:GLU:H	4	0.75
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB1	5	0.75
(1,58)	1:211:B:ALA:HB1	1:206:A:LYS:H	8	0.75
(1,27)	1:183:A:GLU:H	1:201:A:MET:HE1	9	0.75
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD23	7	0.74
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD23	7	0.74
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD21	5	0.74
(1,2836)	1:179:B:TRP:H	1:183:B:GLU:HA	2	0.74
(1,2835)	1:179:A:TRP:H	1:183:A:GLU:HA	1	0.74
(1,2835)	1:179:A:TRP:H	1:183:A:GLU:HA	2	0.74
(1,2835)	1:179:A:TRP:H	1:183:A:GLU:HA	3	0.74
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD12	5	0.74
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD12	5	0.74
(1,2655)	1:188:A:ASN:HD21	1:185:A:LEU:HD23	8	0.74
(1,2436)	1:197:B:VAL:HG12	1:201:B:MET:HB2	6	0.74
(1,2362)	1:196:B:ALA:H	1:194:B:GLN:HB3	7	0.74
(1,2361)	1:196:A:ALA:H	1:194:A:GLN:HB3	5	0.74
(1,2361)	1:196:A:ALA:H	1:194:A:GLN:HB3	7	0.74
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD13	9	0.74
(1,2140)	1:206:B:LYS:HD3	1:206:B:LYS:HA	6	0.74
(1,2139)	1:206:A:LYS:HD3	1:206:A:LYS:HA	6	0.74
(1,2122)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	10	0.74
(1,2121)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	10	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1658)	1:200:B:VAL:H	1:199:B:GLN:HB3	10	0.74
(1,1657)	1:200:A:VAL:H	1:199:A:GLN:HB3	10	0.74
(1,1583)	1:173:A:GLN:HE21	1:200:B:VAL:HA	2	0.74
(1,1480)	1:179:B:TRP:HE1	1:201:B:MET:HE2	5	0.74
(1,1246)	1:175:B:LEU:HD11	1:177:B:VAL:HG22	3	0.74
(1,1245)	1:175:A:LEU:HD11	1:177:A:VAL:HG22	3	0.74
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG11	6	0.74
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG11	6	0.74
(1,1010)	1:208:B:TRP:HB3	1:208:B:TRP:HE3	2	0.74
(1,1010)	1:208:B:TRP:HB3	1:208:B:TRP:HE3	5	0.74
(1,1010)	1:208:B:TRP:HB3	1:208:B:TRP:HE3	7	0.74
(1,1010)	1:208:B:TRP:HB3	1:208:B:TRP:HE3	8	0.74
(1,1009)	1:208:A:TRP:HB3	1:208:A:TRP:HE3	1	0.74
(1,1009)	1:208:A:TRP:HB3	1:208:A:TRP:HE3	2	0.74
(1,1009)	1:208:A:TRP:HB3	1:208:A:TRP:HE3	5	0.74
(1,1009)	1:208:A:TRP:HB3	1:208:A:TRP:HE3	7	0.74
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG11	7	0.74
(1,160)	1:182:B:ILE:HD12	1:177:B:VAL:HA	3	0.74
(1,159)	1:182:A:ILE:HD12	1:177:A:VAL:HA	3	0.74
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD11	3	0.74
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD11	3	0.74
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD11	7	0.74
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD12	9	0.74
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD11	7	0.74
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD23	10	0.74
(1,106)	1:185:B:LEU:HD21	1:183:A:GLU:H	3	0.74
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB1	5	0.74
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB3	3	0.74
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD22	4	0.73
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD21	5	0.73
(1,2836)	1:179:B:TRP:H	1:183:B:GLU:HA	3	0.73
(1,2486)	1:180:B:ASP:H	1:183:B:GLU:HB3	2	0.73
(1,2485)	1:180:A:ASP:H	1:183:A:GLU:HB3	2	0.73
(1,2435)	1:197:A:VAL:HG12	1:201:A:MET:HB2	6	0.73
(1,2414)	1:192:B:ASN:HB2	1:191:B:GLU:HA	5	0.73
(1,2413)	1:192:A:ASN:HB2	1:191:A:GLU:HA	5	0.73
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG11	3	0.73
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG11	3	0.73
(1,2362)	1:196:B:ALA:H	1:194:B:GLN:HB3	5	0.73
(1,2362)	1:196:B:ALA:H	1:194:B:GLN:HB3	10	0.73
(1,2361)	1:196:A:ALA:H	1:194:A:GLN:HB3	10	0.73
(1,2234)	1:200:B:VAL:HA	1:190:B:PHE:HE2	1	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2233)	1:200:A:VAL:HA	1:190:A:PHE:HE2	1	0.73
(1,2188)	1:193:B:ASP:H	1:192:B:ASN:HB2	6	0.73
(1,2188)	1:193:B:ASP:H	1:192:B:ASN:HB2	9	0.73
(1,2187)	1:193:A:ASP:H	1:192:A:ASN:HB2	9	0.73
(1,2140)	1:206:B:LYS:HD3	1:206:B:LYS:HA	4	0.73
(1,2139)	1:206:A:LYS:HD3	1:206:A:LYS:HA	4	0.73
(1,2122)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	2	0.73
(1,2122)	1:182:B:ILE:HG21	1:182:B:ILE:HG13	3	0.73
(1,2122)	1:182:B:ILE:HG22	1:182:B:ILE:HG13	5	0.73
(1,2122)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	7	0.73
(1,2122)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	8	0.73
(1,2122)	1:182:B:ILE:HG22	1:182:B:ILE:HG13	9	0.73
(1,2121)	1:182:A:ILE:HG21	1:182:A:ILE:HG13	3	0.73
(1,2121)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	4	0.73
(1,2121)	1:182:A:ILE:HG22	1:182:A:ILE:HG13	5	0.73
(1,2121)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	7	0.73
(1,2121)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	8	0.73
(1,2121)	1:182:A:ILE:HG22	1:182:A:ILE:HG13	9	0.73
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG21	5	0.73
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG21	5	0.73
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB2	9	0.73
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB2	9	0.73
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG12	6	0.73
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG13	8	0.73
(1,1770)	1:175:B:LEU:H	1:175:B:LEU:HB3	4	0.73
(1,1769)	1:175:A:LEU:H	1:175:A:LEU:HB3	4	0.73
(1,1010)	1:208:B:TRP:HB3	1:208:B:TRP:HE3	6	0.73
(1,1010)	1:208:B:TRP:HB3	1:208:B:TRP:HE3	10	0.73
(1,1009)	1:208:A:TRP:HB3	1:208:A:TRP:HE3	4	0.73
(1,1009)	1:208:A:TRP:HB3	1:208:A:TRP:HE3	6	0.73
(1,1009)	1:208:A:TRP:HB3	1:208:A:TRP:HE3	8	0.73
(1,1009)	1:208:A:TRP:HB3	1:208:A:TRP:HE3	10	0.73
(1,972)	1:204:B:LEU:HD21	1:182:A:ILE:HD12	4	0.73
(1,945)	1:175:A:LEU:HD22	1:199:B:GLN:HB3	1	0.73
(1,171)	1:211:A:ALA:HB2	1:206:B:LYS:HE3	2	0.73
(1,170)	1:182:B:ILE:HD12	1:177:B:VAL:HG23	3	0.73
(1,160)	1:182:B:ILE:HD12	1:177:B:VAL:HA	5	0.73
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD11	2	0.73
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD11	2	0.73
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD23	10	0.73
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB3	2	0.73
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB3	3	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB2	8	0.73
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB2	8	0.73
(1,28)	1:183:B:GLU:H	1:201:B:MET:HE1	9	0.73
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD12	2	0.72
(1,2485)	1:180:A:ASP:H	1:183:A:GLU:HB3	5	0.72
(1,2436)	1:197:B:VAL:HG12	1:201:B:MET:HB2	1	0.72
(1,2435)	1:197:A:VAL:HG12	1:201:A:MET:HB2	1	0.72
(1,2414)	1:192:B:ASN:HB2	1:191:B:GLU:HA	2	0.72
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG11	4	0.72
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG13	5	0.72
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG11	4	0.72
(1,2362)	1:196:B:ALA:H	1:194:B:GLN:HB3	9	0.72
(1,2361)	1:196:A:ALA:H	1:194:A:GLN:HB3	9	0.72
(1,2272)	1:212:B:LYS:HG3	1:212:B:LYS:HA	10	0.72
(1,2271)	1:212:A:LYS:HG2	1:212:A:LYS:HA	10	0.72
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD13	9	0.72
(1,2188)	1:193:B:ASP:H	1:192:B:ASN:HB2	8	0.72
(1,2187)	1:193:A:ASP:H	1:192:A:ASN:HB2	6	0.72
(1,2187)	1:193:A:ASP:H	1:192:A:ASN:HB2	8	0.72
(1,2122)	1:182:B:ILE:HG22	1:182:B:ILE:HG13	1	0.72
(1,2122)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	4	0.72
(1,2122)	1:182:B:ILE:HG22	1:182:B:ILE:HG13	6	0.72
(1,2121)	1:182:A:ILE:HG22	1:182:A:ILE:HG13	1	0.72
(1,2121)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	2	0.72
(1,2121)	1:182:A:ILE:HG22	1:182:A:ILE:HG13	6	0.72
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB1	3	0.72
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB1	3	0.72
(1,1986)	1:173:A:GLN:H	1:175:A:LEU:HD12	3	0.72
(1,1985)	1:173:B:GLN:H	1:175:B:LEU:HD12	3	0.72
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG13	8	0.72
(1,1770)	1:175:B:LEU:H	1:175:B:LEU:HB3	2	0.72
(1,1769)	1:175:A:LEU:H	1:175:A:LEU:HB3	2	0.72
(1,1658)	1:200:B:VAL:H	1:199:B:GLN:HB3	2	0.72
(1,1657)	1:200:A:VAL:H	1:199:A:GLN:HB3	2	0.72
(1,1010)	1:208:B:TRP:HB3	1:208:B:TRP:HE3	4	0.72
(1,1010)	1:208:B:TRP:HB3	1:208:B:TRP:HE3	9	0.72
(1,1009)	1:208:A:TRP:HB3	1:208:A:TRP:HE3	9	0.72
(1,972)	1:204:B:LEU:HD21	1:182:A:ILE:HD13	5	0.72
(1,971)	1:204:A:LEU:HD21	1:182:B:ILE:HD13	5	0.72
(1,946)	1:175:B:LEU:HD22	1:199:A:GLN:HB3	1	0.72
(1,420)	1:193:B:ASP:H	1:193:B:ASP:HB3	7	0.72
(1,419)	1:193:A:ASP:H	1:193:A:ASP:HB3	7	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:182:A:ILE:HD12	1:177:A:VAL:HG23	3	0.72
(1,159)	1:182:A:ILE:HD12	1:177:A:VAL:HA	5	0.72
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD11	5	0.72
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD13	6	0.72
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD11	7	0.72
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD11	5	0.72
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD13	6	0.72
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD11	7	0.72
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG22	3	0.72
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG22	3	0.72
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD21	9	0.72
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB3	2	0.72
(1,2862)	1:173:A:GLN:H	1:175:A:LEU:HB2	4	0.71
(1,2861)	1:173:B:GLN:H	1:175:B:LEU:HB2	4	0.71
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD22	4	0.71
(1,2836)	1:179:B:TRP:H	1:183:B:GLU:HA	8	0.71
(1,2835)	1:179:A:TRP:H	1:183:A:GLU:HA	8	0.71
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB1	3	0.71
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB3	10	0.71
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB1	3	0.71
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB3	10	0.71
(1,2762)	1:175:B:LEU:H	1:175:B:LEU:HD12	5	0.71
(1,2761)	1:175:A:LEU:H	1:175:A:LEU:HD12	5	0.71
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD23	4	0.71
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD23	4	0.71
(1,2486)	1:180:B:ASP:H	1:183:B:GLU:HB3	5	0.71
(1,2413)	1:192:A:ASN:HB2	1:191:A:GLU:HA	2	0.71
(1,2378)	1:181:B:ASP:H	1:182:B:ILE:HD13	8	0.71
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG11	6	0.71
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG11	8	0.71
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG13	5	0.71
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG11	8	0.71
(1,2302)	1:188:B:ASN:HB3	1:185:B:LEU:HB3	1	0.71
(1,2301)	1:188:A:ASN:HB3	1:185:A:LEU:HB3	1	0.71
(1,2272)	1:212:B:LYS:HG2	1:212:B:LYS:HA	2	0.71
(1,2271)	1:212:A:LYS:HG2	1:212:A:LYS:HA	2	0.71
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG22	1	0.71
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG22	1	0.71
(1,2081)	1:175:A:LEU:HD22	1:190:B:PHE:HZ	3	0.71
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB1	1	0.71
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB1	1	0.71
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG13	4	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1738)	1:195:B:ALA:H	1:194:B:GLN:HB3	4	0.71
(1,1124)	1:211:B:ALA:HB3	1:204:A:LEU:H	3	0.71
(1,1122)	1:184:B:ALA:HB1	1:182:B:ILE:H	10	0.71
(1,1121)	1:184:A:ALA:HB1	1:182:A:ILE:H	10	0.71
(1,1105)	1:176:A:THR:HG23	1:179:A:TRP:HD1	3	0.71
(1,910)	1:201:B:MET:HG2	1:201:B:MET:HA	7	0.71
(1,909)	1:201:A:MET:HG2	1:201:A:MET:HA	7	0.71
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD21	8	0.71
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD21	9	0.71
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD21	8	0.71
(1,106)	1:185:B:LEU:HD21	1:183:A:GLU:H	5	0.71
(1,57)	1:211:A:ALA:HB1	1:206:B:LYS:H	8	0.71
(1,34)	1:205:B:GLN:HE22	1:201:B:MET:HE3	4	0.71
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD21	10	0.7
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD21	8	0.7
(1,2836)	1:179:B:TRP:H	1:183:B:GLU:HA	10	0.7
(1,2835)	1:179:A:TRP:H	1:183:A:GLU:HA	5	0.7
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD23	5	0.7
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD22	8	0.7
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD22	10	0.7
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD22	2	0.7
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD22	2	0.7
(1,2436)	1:201:B:MET:HB2	1:200:B:VAL:HG21	8	0.7
(1,2435)	1:201:A:MET:HB2	1:200:A:VAL:HG21	8	0.7
(1,2414)	1:192:B:ASN:HB2	1:191:B:GLU:HA	3	0.7
(1,2413)	1:192:A:ASN:HB2	1:191:A:GLU:HA	3	0.7
(1,2377)	1:181:A:ASP:H	1:182:A:ILE:HD13	8	0.7
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG11	6	0.7
(1,2362)	1:196:B:ALA:H	1:194:B:GLN:HB3	1	0.7
(1,2361)	1:196:A:ALA:H	1:194:A:GLN:HB3	1	0.7
(1,2301)	1:188:A:ASN:HB3	1:185:A:LEU:HB3	7	0.7
(1,2234)	1:200:B:VAL:HA	1:190:B:PHE:HE2	9	0.7
(1,2233)	1:200:A:VAL:HA	1:190:A:PHE:HE2	9	0.7
(1,2082)	1:175:B:LEU:HD22	1:190:A:PHE:HZ	3	0.7
(1,1872)	1:184:B:ALA:H	1:197:B:VAL:HG12	9	0.7
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG13	4	0.7
(1,1871)	1:184:A:ALA:H	1:197:A:VAL:HG12	9	0.7
(1,1737)	1:195:A:ALA:H	1:194:A:GLN:HB3	4	0.7
(1,1480)	1:179:B:TRP:HE1	1:201:B:MET:HE3	2	0.7
(1,1479)	1:179:A:TRP:HE1	1:201:A:MET:HE3	2	0.7
(1,1122)	1:184:B:ALA:HB1	1:182:B:ILE:H	3	0.7
(1,1121)	1:184:A:ALA:HB1	1:182:A:ILE:H	3	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:176:B:THR:HG23	1:179:B:TRP:HD1	3	0.7
(1,945)	1:175:A:LEU:HD22	1:199:B:GLN:HB3	5	0.7
(1,642)	1:198:B:ARG:H	1:198:B:ARG:HD3	8	0.7
(1,641)	1:198:A:ARG:H	1:198:A:ARG:HD3	8	0.7
(1,438)	1:188:B:ASN:HD22	1:188:B:ASN:HB3	8	0.7
(1,437)	1:188:A:ASN:HD22	1:188:A:ASN:HB3	8	0.7
(1,254)	1:175:B:LEU:HD11	1:196:A:ALA:HA	3	0.7
(1,172)	1:211:B:ALA:HB2	1:206:A:LYS:HE3	2	0.7
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD13	4	0.7
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD13	4	0.7
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD22	4	0.7
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD22	4	0.7
(1,114)	1:173:B:GLN:HE21	1:175:B:LEU:HD12	3	0.7
(1,113)	1:173:A:GLN:HE21	1:175:A:LEU:HD12	3	0.7
(1,105)	1:185:A:LEU:HD21	1:183:B:GLU:H	5	0.7
(1,33)	1:205:A:GLN:HE22	1:201:A:MET:HE3	4	0.7
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD22	5	0.69
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD22	5	0.69
(1,2836)	1:179:B:TRP:H	1:183:B:GLU:HA	4	0.69
(1,2836)	1:179:B:TRP:H	1:183:B:GLU:HA	5	0.69
(1,2835)	1:179:A:TRP:H	1:183:A:GLU:HA	4	0.69
(1,2835)	1:179:A:TRP:H	1:183:A:GLU:HA	10	0.69
(1,2670)	1:202:B:GLU:H	1:179:B:TRP:HZ3	7	0.69
(1,2669)	1:202:A:GLU:H	1:179:A:TRP:HZ3	7	0.69
(1,2664)	1:173:B:GLN:HE21	1:212:B:LYS:HA	8	0.69
(1,2663)	1:173:A:GLN:HE21	1:212:A:LYS:HA	8	0.69
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD22	3	0.69
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD21	6	0.69
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD22	10	0.69
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD21	1	0.69
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD22	3	0.69
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD23	5	0.69
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD21	6	0.69
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD22	8	0.69
(1,2508)	1:176:B:THR:H	1:176:B:THR:HG21	8	0.69
(1,2507)	1:176:A:THR:H	1:176:A:THR:HG21	8	0.69
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD22	5	0.69
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD22	6	0.69
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD22	5	0.69
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD22	6	0.69
(1,2414)	1:192:B:ASN:HB2	1:191:B:GLU:HA	4	0.69
(1,2414)	1:192:B:ASN:HB2	1:191:B:GLU:HA	10	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2413)	1:192:A:ASN:HB2	1:191:A:GLU:HA	4	0.69
(1,2413)	1:192:A:ASN:HB2	1:191:A:GLU:HA	10	0.69
(1,2361)	1:196:A:ALA:H	1:194:A:GLN:HB3	6	0.69
(1,2302)	1:188:B:ASN:HB3	1:185:B:LEU:HB3	4	0.69
(1,2302)	1:188:B:ASN:HB3	1:185:B:LEU:HB3	7	0.69
(1,2272)	1:212:B:LYS:HG2	1:212:B:LYS:HA	1	0.69
(1,2272)	1:212:B:LYS:HG2	1:212:B:LYS:HA	3	0.69
(1,2271)	1:212:A:LYS:HG2	1:212:A:LYS:HA	1	0.69
(1,2234)	1:200:B:VAL:HA	1:190:B:PHE:HE2	10	0.69
(1,2233)	1:200:A:VAL:HA	1:190:A:PHE:HE2	10	0.69
(1,2187)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	7	0.69
(1,2138)	1:187:B:LYS:HD3	1:184:B:ALA:HA	2	0.69
(1,2137)	1:187:A:LYS:HD3	1:184:A:ALA:HA	2	0.69
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG22	2	0.69
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG22	2	0.69
(1,1124)	1:211:B:ALA:HB3	1:204:A:LEU:H	7	0.69
(1,1123)	1:211:A:ALA:HB3	1:204:B:LEU:H	3	0.69
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB2	4	0.69
(1,642)	1:198:B:ARG:H	1:198:B:ARG:HD3	10	0.69
(1,641)	1:198:A:ARG:H	1:198:A:ARG:HD3	10	0.69
(1,398)	1:175:B:LEU:HB2	1:190:A:PHE:HZ	5	0.69
(1,171)	1:211:A:ALA:HB2	1:206:B:LYS:HE3	7	0.69
(1,160)	1:182:B:ILE:HD11	1:177:B:VAL:HA	6	0.69
(1,159)	1:182:A:ILE:HD11	1:177:A:VAL:HA	6	0.69
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD13	1	0.69
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD13	1	0.69
(1,106)	1:185:B:LEU:HD23	1:183:A:GLU:H	10	0.69
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB1	4	0.69
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB1	4	0.69
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD21	10	0.68
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD21	6	0.68
(1,2836)	1:179:B:TRP:H	1:183:B:GLU:HA	6	0.68
(1,2835)	1:179:A:TRP:H	1:183:A:GLU:HA	6	0.68
(1,2762)	1:175:B:LEU:H	1:175:B:LEU:HD12	3	0.68
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD21	4	0.68
(1,2573)	1:208:A:TRP:HE1	1:203:B:ARG:HD2	8	0.68
(1,2544)	1:185:B:LEU:H	1:185:B:LEU:HD23	4	0.68
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD21	1	0.68
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD23	2	0.68
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD23	2	0.68
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD21	9	0.68
(1,2438)	1:199:B:GLN:HG3	1:196:B:ALA:HB2	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2437)	1:199:A:GLN:HG3	1:196:A:ALA:HB2	2	0.68
(1,2414)	1:192:B:ASN:HB2	1:191:B:GLU:HA	8	0.68
(1,2413)	1:192:A:ASN:HB2	1:191:A:GLU:HA	8	0.68
(1,2362)	1:196:B:ALA:H	1:194:B:GLN:HB3	6	0.68
(1,2361)	1:196:A:ALA:H	1:194:A:GLN:HB3	8	0.68
(1,2324)	1:204:B:LEU:HD13	1:200:B:VAL:HA	3	0.68
(1,2324)	1:204:B:LEU:HD11	1:200:B:VAL:HA	4	0.68
(1,2323)	1:204:A:LEU:HD13	1:200:A:VAL:HA	3	0.68
(1,2323)	1:204:A:LEU:HD11	1:200:A:VAL:HA	4	0.68
(1,2301)	1:188:A:ASN:HB3	1:185:A:LEU:HB3	4	0.68
(1,2272)	1:212:B:LYS:HG2	1:212:B:LYS:HA	7	0.68
(1,2271)	1:212:A:LYS:HG2	1:212:A:LYS:HA	3	0.68
(1,2234)	1:200:B:VAL:HA	1:190:B:PHE:HE2	4	0.68
(1,2188)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	7	0.68
(1,2040)	1:203:B:ARG:H	1:205:B:GLN:HE22	7	0.68
(1,2039)	1:203:A:ARG:H	1:205:A:GLN:HE22	10	0.68
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE1	10	0.68
(1,1818)	1:192:B:ASN:H	1:187:B:LYS:HG2	9	0.68
(1,1817)	1:192:A:ASN:H	1:187:A:LYS:HG2	9	0.68
(1,1184)	1:199:B:GLN:HA	1:175:A:LEU:HD11	7	0.68
(1,1183)	1:199:A:GLN:HA	1:175:B:LEU:HD11	7	0.68
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG11	8	0.68
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG13	9	0.68
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG11	8	0.68
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG13	9	0.68
(1,1145)	1:211:A:ALA:HA	1:206:B:LYS:HE3	5	0.68
(1,1124)	1:211:B:ALA:HB2	1:204:A:LEU:H	8	0.68
(1,1123)	1:211:A:ALA:HB3	1:204:B:LEU:H	7	0.68
(1,1122)	1:184:B:ALA:HB3	1:182:B:ILE:H	6	0.68
(1,1106)	1:176:B:THR:HG23	1:179:B:TRP:HD1	8	0.68
(1,1105)	1:176:A:THR:HG21	1:179:A:TRP:HD1	2	0.68
(1,397)	1:175:A:LEU:HB2	1:190:B:PHE:HZ	5	0.68
(1,354)	1:174:B:GLU:H	1:174:B:GLU:HG3	2	0.68
(1,353)	1:174:A:GLU:H	1:174:A:GLU:HG3	2	0.68
(1,192)	1:201:B:MET:HE2	1:182:B:ILE:HG22	7	0.68
(1,191)	1:201:A:MET:HE2	1:182:A:ILE:HG22	7	0.68
(1,172)	1:211:B:ALA:HB2	1:206:A:LYS:HE3	7	0.68
(1,152)	1:183:B:GLU:H	1:182:B:ILE:HD13	8	0.68
(1,151)	1:183:A:GLU:H	1:182:A:ILE:HD13	8	0.68
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD21	2	0.68
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD21	2	0.68
(1,106)	1:185:B:LEU:HD21	1:183:A:GLU:H	9	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:185:A:LEU:HD23	1:183:B:GLU:H	10	0.68
(1,2768)	1:194:B:GLN:H	1:194:B:GLN:HB3	1	0.67
(1,2768)	1:194:B:GLN:H	1:194:B:GLN:HB3	3	0.67
(1,2768)	1:194:B:GLN:H	1:194:B:GLN:HB3	5	0.67
(1,2768)	1:194:B:GLN:H	1:194:B:GLN:HB3	6	0.67
(1,2767)	1:194:A:GLN:H	1:194:A:GLN:HB3	1	0.67
(1,2767)	1:194:A:GLN:H	1:194:A:GLN:HB3	3	0.67
(1,2767)	1:194:A:GLN:H	1:194:A:GLN:HB3	5	0.67
(1,2767)	1:194:A:GLN:H	1:194:A:GLN:HB3	6	0.67
(1,2767)	1:194:A:GLN:H	1:194:A:GLN:HB3	8	0.67
(1,2761)	1:175:A:LEU:H	1:175:A:LEU:HD12	3	0.67
(1,2543)	1:185:A:LEU:H	1:185:A:LEU:HD23	4	0.67
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD21	7	0.67
(1,2520)	1:205:B:GLN:H	1:204:B:LEU:HD21	9	0.67
(1,2519)	1:205:A:GLN:H	1:204:A:LEU:HD21	7	0.67
(1,2414)	1:192:B:ASN:HB2	1:191:B:GLU:HA	9	0.67
(1,2405)	1:179:A:TRP:HA	1:182:A:ILE:HG12	4	0.67
(1,2404)	1:183:B:GLU:HA	1:201:B:MET:HB2	2	0.67
(1,2403)	1:183:A:GLU:HA	1:201:A:MET:HB2	2	0.67
(1,2362)	1:196:B:ALA:H	1:194:B:GLN:HB3	8	0.67
(1,2360)	1:200:B:VAL:HG11	1:175:A:LEU:H	5	0.67
(1,2324)	1:204:B:LEU:HD12	1:200:B:VAL:HA	1	0.67
(1,2324)	1:204:B:LEU:HD13	1:200:B:VAL:HA	5	0.67
(1,2324)	1:204:B:LEU:HD13	1:200:B:VAL:HA	6	0.67
(1,2323)	1:204:A:LEU:HD12	1:200:A:VAL:HA	1	0.67
(1,2323)	1:204:A:LEU:HD13	1:200:A:VAL:HA	5	0.67
(1,2323)	1:204:A:LEU:HD13	1:200:A:VAL:HA	6	0.67
(1,2301)	1:188:A:ASN:HB3	1:185:A:LEU:HB3	3	0.67
(1,2271)	1:212:A:LYS:HG2	1:212:A:LYS:HA	7	0.67
(1,2233)	1:200:A:VAL:HA	1:190:A:PHE:HE2	4	0.67
(1,2040)	1:203:B:ARG:H	1:205:B:GLN:HE22	10	0.67
(1,2039)	1:203:A:ARG:H	1:205:A:GLN:HE22	7	0.67
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE1	10	0.67
(1,1818)	1:192:B:ASN:H	1:187:B:LYS:HG2	8	0.67
(1,1817)	1:192:A:ASN:H	1:187:A:LYS:HG2	8	0.67
(1,1121)	1:184:A:ALA:HB3	1:182:A:ILE:H	6	0.67
(1,1105)	1:176:A:THR:HG23	1:179:A:TRP:HD1	8	0.67
(1,1104)	1:179:B:TRP:HE1	1:176:B:THR:HG23	8	0.67
(1,1103)	1:179:A:TRP:HE1	1:176:A:THR:HG23	8	0.67
(1,946)	1:175:B:LEU:HD22	1:199:A:GLN:HB3	5	0.67
(1,706)	1:195:B:ALA:HA	1:198:B:ARG:HG2	2	0.67
(1,705)	1:195:A:ALA:HA	1:198:A:ARG:HG2	2	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB2	4	0.67
(1,253)	1:175:A:LEU:HD11	1:196:B:ALA:HA	3	0.67
(1,160)	1:182:B:ILE:HD11	1:177:B:VAL:HA	4	0.67
(1,159)	1:182:A:ILE:HD11	1:177:A:VAL:HA	4	0.67
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD21	5	0.67
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD11	3	0.67
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD12	7	0.67
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD21	6	0.66
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD21	8	0.66
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD21	9	0.66
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD21	9	0.66
(1,2768)	1:194:B:GLN:H	1:194:B:GLN:HB3	8	0.66
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD23	9	0.66
(1,2574)	1:208:B:TRP:HE1	1:203:A:ARG:HD2	7	0.66
(1,2574)	1:208:B:TRP:HE1	1:203:A:ARG:HD2	8	0.66
(1,2545)	1:181:A:ASP:H	1:181:A:ASP:HB3	4	0.66
(1,2544)	1:185:B:LEU:H	1:185:B:LEU:HD23	7	0.66
(1,2543)	1:185:A:LEU:H	1:185:A:LEU:HD23	7	0.66
(1,2512)	1:176:B:THR:H	1:173:B:GLN:HB3	9	0.66
(1,2511)	1:176:A:THR:H	1:173:A:GLN:HB3	9	0.66
(1,2486)	1:180:B:ASP:H	1:183:B:GLU:HB3	3	0.66
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD23	7	0.66
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD22	9	0.66
(1,2413)	1:192:A:ASN:HB2	1:191:A:GLU:HA	9	0.66
(1,2406)	1:179:B:TRP:HA	1:182:B:ILE:HG12	4	0.66
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG12	1	0.66
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG13	10	0.66
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG12	1	0.66
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG12	2	0.66
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG13	10	0.66
(1,2362)	1:196:B:ALA:H	1:194:B:GLN:HB3	3	0.66
(1,2361)	1:196:A:ALA:H	1:194:A:GLN:HB3	3	0.66
(1,2359)	1:200:A:VAL:HG11	1:175:B:LEU:H	5	0.66
(1,2302)	1:188:B:ASN:HB3	1:185:B:LEU:HB3	2	0.66
(1,2302)	1:188:B:ASN:HB3	1:185:B:LEU:HB3	3	0.66
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG23	3	0.66
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG23	3	0.66
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG22	10	0.66
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG21	2	0.66
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG23	8	0.66
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG21	2	0.66
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG23	8	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1984)	1:173:A:GLN:H	1:173:A:GLN:HB2	3	0.66
(1,1984)	1:173:A:GLN:H	1:173:A:GLN:HB2	4	0.66
(1,1983)	1:173:B:GLN:H	1:173:B:GLN:HB2	3	0.66
(1,1983)	1:173:B:GLN:H	1:173:B:GLN:HB2	4	0.66
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD11	3	0.66
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD12	4	0.66
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD12	4	0.66
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG11	3	0.66
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG13	10	0.66
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG11	3	0.66
(1,1146)	1:211:B:ALA:HA	1:206:A:LYS:HE3	5	0.66
(1,1122)	1:184:B:ALA:HB3	1:182:B:ILE:H	8	0.66
(1,1121)	1:184:A:ALA:HB3	1:182:A:ILE:H	8	0.66
(1,1106)	1:176:B:THR:HG21	1:179:B:TRP:HD1	2	0.66
(1,160)	1:182:B:ILE:HD12	1:177:B:VAL:HA	2	0.66
(1,159)	1:182:A:ILE:HD12	1:177:A:VAL:HA	2	0.66
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD21	5	0.66
(1,114)	1:173:B:GLN:HE21	1:175:B:LEU:HD13	2	0.66
(1,113)	1:173:A:GLN:HE21	1:175:A:LEU:HD13	2	0.66
(1,105)	1:185:A:LEU:HD21	1:183:B:GLU:H	8	0.66
(1,105)	1:185:A:LEU:HD21	1:183:B:GLU:H	9	0.66
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD11	3	0.66
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD12	4	0.66
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD12	7	0.66
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD22	4	0.66
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD22	4	0.66
(1,2762)	1:175:B:LEU:H	1:175:B:LEU:HD12	1	0.65
(1,2761)	1:175:A:LEU:H	1:175:A:LEU:HD12	1	0.65
(1,2645)	1:188:A:ASN:HD22	1:187:A:LYS:HG3	8	0.65
(1,2580)	1:208:B:TRP:HE1	1:175:B:LEU:HD11	7	0.65
(1,2579)	1:208:A:TRP:HE1	1:175:A:LEU:HD11	7	0.65
(1,2573)	1:208:A:TRP:HE1	1:203:B:ARG:HD2	7	0.65
(1,2546)	1:181:B:ASP:H	1:181:B:ASP:HB3	4	0.65
(1,2492)	1:180:B:ASP:H	1:182:B:ILE:HG22	10	0.65
(1,2491)	1:180:A:ASP:H	1:182:A:ILE:HG22	10	0.65
(1,2485)	1:180:A:ASP:H	1:183:A:GLU:HB3	3	0.65
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD22	8	0.65
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD23	7	0.65
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD22	8	0.65
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD22	9	0.65
(1,2413)	1:192:A:ASN:HB2	1:191:A:GLU:HA	6	0.65
(1,2406)	1:179:B:TRP:HA	1:182:B:ILE:HG12	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2406)	1:179:B:TRP:HA	1:182:B:ILE:HG12	6	0.65
(1,2405)	1:179:A:TRP:HA	1:182:A:ILE:HG12	5	0.65
(1,2401)	1:208:A:TRP:HA	1:203:B:ARG:HB3	5	0.65
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG12	2	0.65
(1,2323)	1:204:A:LEU:HD13	1:200:A:VAL:HA	8	0.65
(1,2301)	1:188:A:ASN:HB3	1:185:A:LEU:HB3	2	0.65
(1,2272)	1:212:B:LYS:HG2	1:212:B:LYS:HA	4	0.65
(1,2271)	1:212:A:LYS:HG2	1:212:A:LYS:HA	4	0.65
(1,2188)	1:193:B:ASP:H	1:192:B:ASN:HB2	5	0.65
(1,2187)	1:193:A:ASP:H	1:192:A:ASN:HB2	5	0.65
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG22	10	0.65
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG23	5	0.65
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG23	5	0.65
(1,1770)	1:175:B:LEU:H	1:175:B:LEU:HB3	7	0.65
(1,1769)	1:175:A:LEU:H	1:175:A:LEU:HB3	7	0.65
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD11	3	0.65
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG11	4	0.65
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG13	10	0.65
(1,1121)	1:184:A:ALA:HB2	1:182:A:ILE:H	4	0.65
(1,971)	1:204:A:LEU:HD22	1:182:B:ILE:HD12	6	0.65
(1,868)	1:188:B:ASN:HB3	1:189:B:ASN:HB2	8	0.65
(1,867)	1:188:A:ASN:HB3	1:189:A:ASN:HB2	8	0.65
(1,766)	1:174:B:GLU:HA	1:174:B:GLU:HG2	8	0.65
(1,644)	1:199:B:GLN:H	1:198:B:ARG:HD3	10	0.65
(1,254)	1:175:B:LEU:HD11	1:196:A:ALA:HA	2	0.65
(1,159)	1:182:A:ILE:HD11	1:177:A:VAL:HA	1	0.65
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG23	2	0.65
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG23	2	0.65
(1,106)	1:185:B:LEU:HD21	1:183:A:GLU:H	8	0.65
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD12	4	0.65
(1,34)	1:205:B:GLN:HE22	1:201:B:MET:HE1	2	0.65
(1,33)	1:205:A:GLN:HE22	1:201:A:MET:HE1	2	0.65
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD21	3	0.64
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG21	1	0.64
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG22	8	0.64
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG21	1	0.64
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG22	8	0.64
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB1	9	0.64
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB1	9	0.64
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD22	3	0.64
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD21	4	0.64
(1,2646)	1:188:B:ASN:HD22	1:187:B:LYS:HG3	8	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD22	2	0.64
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD23	7	0.64
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD23	9	0.64
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD23	7	0.64
(1,2414)	1:192:B:ASN:HB2	1:191:B:GLU:HA	6	0.64
(1,2406)	1:179:B:TRP:HA	1:182:B:ILE:HG12	8	0.64
(1,2405)	1:179:A:TRP:HA	1:182:A:ILE:HG12	6	0.64
(1,2402)	1:208:B:TRP:HA	1:203:A:ARG:HB3	5	0.64
(1,2368)	1:185:B:LEU:HG	1:185:B:LEU:H	4	0.64
(1,2368)	1:185:B:LEU:HG	1:185:B:LEU:H	8	0.64
(1,2324)	1:204:B:LEU:HD13	1:200:B:VAL:HA	8	0.64
(1,2298)	1:197:B:VAL:HA	1:186:B:LEU:HB2	7	0.64
(1,2297)	1:197:A:VAL:HA	1:186:A:LEU:HB2	7	0.64
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD11	1	0.64
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD11	1	0.64
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG23	1	0.64
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG23	5	0.64
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG21	7	0.64
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG23	1	0.64
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG21	7	0.64
(1,2127)	1:185:A:LEU:HD12	1:178:B:PRO:HB2	3	0.64
(1,2096)	1:175:B:LEU:HD13	1:199:A:GLN:HE22	3	0.64
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG22	4	0.64
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG22	4	0.64
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG23	7	0.64
(1,1794)	1:193:B:ASP:H	1:188:B:ASN:HA	7	0.64
(1,1793)	1:193:A:ASP:H	1:188:A:ASN:HA	7	0.64
(1,1770)	1:175:B:LEU:H	1:175:B:LEU:HB3	8	0.64
(1,1770)	1:175:B:LEU:H	1:175:B:LEU:HB3	10	0.64
(1,1769)	1:175:A:LEU:H	1:175:A:LEU:HB3	8	0.64
(1,1769)	1:175:A:LEU:H	1:175:A:LEU:HB3	10	0.64
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB2	10	0.64
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG12	2	0.64
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG11	4	0.64
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG12	7	0.64
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG12	7	0.64
(1,1123)	1:211:A:ALA:HB2	1:204:B:LEU:H	8	0.64
(1,1122)	1:184:B:ALA:HB2	1:182:B:ILE:H	1	0.64
(1,1122)	1:184:B:ALA:HB2	1:182:B:ILE:H	4	0.64
(1,1121)	1:184:A:ALA:HB2	1:182:A:ILE:H	1	0.64
(1,1104)	1:179:B:TRP:HE1	1:176:B:THR:HG21	1	0.64
(1,1103)	1:179:A:TRP:HE1	1:176:A:THR:HG21	1	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,972)	1:204:B:LEU:HD23	1:182:A:ILE:HD13	3	0.64
(1,765)	1:174:A:GLU:HA	1:174:A:GLU:HG2	8	0.64
(1,765)	1:174:A:GLU:HA	1:174:A:GLU:HG2	9	0.64
(1,643)	1:199:A:GLN:H	1:198:A:ARG:HD3	10	0.64
(1,346)	1:191:B:GLU:H	1:191:B:GLU:HG2	9	0.64
(1,345)	1:191:A:GLU:H	1:191:A:GLU:HG2	9	0.64
(1,262)	1:175:B:LEU:HD13	1:199:A:GLN:HG3	3	0.64
(1,160)	1:182:B:ILE:HD11	1:177:B:VAL:HA	1	0.64
(1,105)	1:185:A:LEU:HD21	1:183:B:GLU:H	2	0.64
(1,2710)	1:199:B:GLN:HE22	1:175:A:LEU:HA	7	0.63
(1,2582)	1:179:B:TRP:HE1	1:204:A:LEU:HG	2	0.63
(1,2582)	1:179:B:TRP:HE1	1:204:A:LEU:HG	7	0.63
(1,2581)	1:179:A:TRP:HE1	1:204:B:LEU:HG	2	0.63
(1,2581)	1:179:A:TRP:HE1	1:204:B:LEU:HG	7	0.63
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD21	10	0.63
(1,2544)	1:185:B:LEU:H	1:185:A:LEU:HD23	3	0.63
(1,2543)	1:185:A:LEU:H	1:185:B:LEU:HD23	3	0.63
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG12	5	0.63
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD23	4	0.63
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD21	10	0.63
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD23	4	0.63
(1,2405)	1:179:A:TRP:HA	1:182:A:ILE:HG12	8	0.63
(1,2368)	1:185:B:LEU:HG	1:185:B:LEU:H	1	0.63
(1,2368)	1:185:B:LEU:HG	1:185:B:LEU:H	2	0.63
(1,2368)	1:185:B:LEU:HG	1:185:B:LEU:H	3	0.63
(1,2368)	1:185:B:LEU:HG	1:185:B:LEU:H	5	0.63
(1,2368)	1:185:B:LEU:HG	1:185:B:LEU:H	6	0.63
(1,2368)	1:185:B:LEU:HG	1:185:B:LEU:H	7	0.63
(1,2368)	1:185:B:LEU:HG	1:185:B:LEU:H	9	0.63
(1,2368)	1:185:B:LEU:HG	1:185:B:LEU:H	10	0.63
(1,2367)	1:185:A:LEU:HG	1:185:A:LEU:H	1	0.63
(1,2367)	1:185:A:LEU:HG	1:185:A:LEU:H	2	0.63
(1,2367)	1:185:A:LEU:HG	1:185:A:LEU:H	3	0.63
(1,2367)	1:185:A:LEU:HG	1:185:A:LEU:H	4	0.63
(1,2367)	1:185:A:LEU:HG	1:185:A:LEU:H	5	0.63
(1,2367)	1:185:A:LEU:HG	1:185:A:LEU:H	6	0.63
(1,2367)	1:185:A:LEU:HG	1:185:A:LEU:H	7	0.63
(1,2367)	1:185:A:LEU:HG	1:185:A:LEU:H	8	0.63
(1,2367)	1:185:A:LEU:HG	1:185:A:LEU:H	9	0.63
(1,2367)	1:185:A:LEU:HG	1:185:A:LEU:H	10	0.63
(1,2302)	1:188:B:ASN:HB3	1:185:B:LEU:HB3	5	0.63
(1,2301)	1:188:A:ASN:HB3	1:185:A:LEU:HB3	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG21	6	0.63
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG23	5	0.63
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG21	6	0.63
(1,2102)	1:204:B:LEU:HD11	1:179:B:TRP:HZ3	7	0.63
(1,2101)	1:204:A:LEU:HD11	1:179:A:TRP:HZ3	7	0.63
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG23	6	0.63
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG23	7	0.63
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG23	6	0.63
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB3	8	0.63
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB3	8	0.63
(1,1770)	1:175:B:LEU:H	1:175:B:LEU:HB3	6	0.63
(1,1770)	1:175:B:LEU:H	1:175:B:LEU:HB3	9	0.63
(1,1769)	1:175:A:LEU:H	1:175:A:LEU:HB3	6	0.63
(1,1769)	1:175:A:LEU:H	1:175:A:LEU:HB3	9	0.63
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB2	10	0.63
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG12	1	0.63
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG12	2	0.63
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD11	3	0.63
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD13	4	0.63
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD11	3	0.63
(1,972)	1:204:B:LEU:HD21	1:182:A:ILE:HD13	2	0.63
(1,946)	1:175:B:LEU:HD23	1:199:A:GLN:HB3	3	0.63
(1,945)	1:175:A:LEU:HD22	1:199:B:GLN:HB3	2	0.63
(1,766)	1:174:B:GLU:HA	1:174:B:GLU:HG2	9	0.63
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG11	5	0.63
(1,706)	1:195:B:ALA:HA	1:198:B:ARG:HG2	8	0.63
(1,705)	1:195:A:ALA:HA	1:198:A:ARG:HG2	8	0.63
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB2	2	0.63
(1,654)	1:203:B:ARG:HD3	1:211:A:ALA:HB3	9	0.63
(1,419)	1:193:A:ASP:H	1:193:A:ASP:HB3	5	0.63
(1,398)	1:175:B:LEU:HB2	1:190:A:PHE:HZ	3	0.63
(1,154)	1:182:B:ILE:H	1:182:B:ILE:HD13	8	0.63
(1,153)	1:182:A:ILE:H	1:182:A:ILE:HD13	8	0.63
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG21	5	0.63
(1,106)	1:185:B:LEU:HD21	1:183:A:GLU:H	1	0.63
(1,106)	1:185:B:LEU:HD21	1:183:A:GLU:H	6	0.63
(1,105)	1:185:A:LEU:HD21	1:183:B:GLU:H	1	0.63
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD23	2	0.63
(1,34)	1:205:B:GLN:HE22	1:201:B:MET:HE1	8	0.63
(1,33)	1:205:A:GLN:HE22	1:201:A:MET:HE1	8	0.63
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD21	3	0.62
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG22	4	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG22	4	0.62
(1,2808)	1:185:B:LEU:H	1:182:A:ILE:HD11	4	0.62
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD13	3	0.62
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD13	5	0.62
(1,2674)	1:202:B:GLU:H	1:179:B:TRP:HE3	7	0.62
(1,2673)	1:202:A:GLU:H	1:179:A:TRP:HE3	7	0.62
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD21	8	0.62
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD22	2	0.62
(1,2546)	1:181:B:ASP:H	1:180:B:ASP:HB3	10	0.62
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD22	3	0.62
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD22	3	0.62
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD21	10	0.62
(1,2239)	1:187:A:LYS:HA	1:197:A:VAL:H	3	0.62
(1,2138)	1:187:B:LYS:HD3	1:184:B:ALA:HA	10	0.62
(1,2128)	1:185:B:LEU:HD12	1:178:A:PRO:HB2	3	0.62
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG22	7	0.62
(1,2095)	1:175:A:LEU:HD13	1:199:B:GLN:HE22	3	0.62
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB2	6	0.62
(1,2040)	1:203:B:ARG:H	1:205:B:GLN:HE22	2	0.62
(1,1818)	1:192:B:ASN:H	1:187:B:LYS:HG2	6	0.62
(1,1817)	1:192:A:ASN:H	1:187:A:LYS:HG2	6	0.62
(1,1480)	1:179:B:TRP:HE1	1:201:B:MET:HE1	3	0.62
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB3	3	0.62
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB1	7	0.62
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB3	3	0.62
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB1	7	0.62
(1,1384)	1:180:B:ASP:H	1:180:B:ASP:HB3	10	0.62
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG12	1	0.62
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD11	8	0.62
(1,971)	1:204:A:LEU:HD23	1:182:B:ILE:HD13	3	0.62
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB2	2	0.62
(1,653)	1:203:A:ARG:HD3	1:211:B:ALA:HB3	9	0.62
(1,420)	1:193:B:ASP:H	1:193:B:ASP:HB3	5	0.62
(1,397)	1:175:A:LEU:HB2	1:190:B:PHE:HZ	3	0.62
(1,346)	1:191:B:GLU:H	1:191:B:GLU:HG2	5	0.62
(1,253)	1:175:A:LEU:HD11	1:196:B:ALA:HA	2	0.62
(1,106)	1:185:B:LEU:HD21	1:183:A:GLU:H	2	0.62
(1,105)	1:185:A:LEU:HD21	1:183:B:GLU:H	6	0.62
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD23	2	0.62
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG21	6	0.61
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG21	6	0.61
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG22	7	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD22	3	0.61
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD13	5	0.61
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD13	3	0.61
(1,2582)	1:179:B:TRP:HE1	1:204:A:LEU:HG	8	0.61
(1,2581)	1:179:A:TRP:HE1	1:204:B:LEU:HG	4	0.61
(1,2581)	1:179:A:TRP:HE1	1:204:B:LEU:HG	8	0.61
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD21	10	0.61
(1,2545)	1:181:A:ASP:H	1:180:A:ASP:HB3	10	0.61
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG12	9	0.61
(1,2414)	1:192:B:ASN:HB2	1:191:B:GLU:HA	7	0.61
(1,2413)	1:192:A:ASN:HB2	1:191:A:GLU:HA	7	0.61
(1,2376)	1:202:B:GLU:H	1:200:B:VAL:HG13	9	0.61
(1,2375)	1:202:A:GLU:H	1:200:A:VAL:HG13	9	0.61
(1,2362)	1:196:B:ALA:H	1:194:B:GLN:HB3	2	0.61
(1,2361)	1:196:A:ALA:H	1:194:A:GLN:HB3	2	0.61
(1,2332)	1:212:B:LYS:HB3	1:211:B:ALA:H	7	0.61
(1,2332)	1:212:B:LYS:HB3	1:211:B:ALA:H	10	0.61
(1,2331)	1:212:A:LYS:HB3	1:211:A:ALA:H	7	0.61
(1,2331)	1:212:A:LYS:HB3	1:211:A:ALA:H	10	0.61
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG23	4	0.61
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG23	8	0.61
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG23	10	0.61
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG23	4	0.61
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG23	8	0.61
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG23	10	0.61
(1,2240)	1:187:B:LYS:HA	1:197:B:VAL:H	1	0.61
(1,2240)	1:187:B:LYS:HA	1:197:B:VAL:H	3	0.61
(1,2240)	1:187:B:LYS:HA	1:197:B:VAL:H	4	0.61
(1,2240)	1:187:B:LYS:HA	1:197:B:VAL:H	7	0.61
(1,2239)	1:187:A:LYS:HA	1:197:A:VAL:H	1	0.61
(1,2239)	1:187:A:LYS:HA	1:197:A:VAL:H	4	0.61
(1,2239)	1:187:A:LYS:HA	1:197:A:VAL:H	6	0.61
(1,2239)	1:187:A:LYS:HA	1:197:A:VAL:H	8	0.61
(1,2137)	1:187:A:LYS:HD3	1:184:A:ALA:HA	10	0.61
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG22	7	0.61
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB2	6	0.61
(1,2039)	1:203:A:ARG:H	1:205:A:GLN:HE22	2	0.61
(1,2039)	1:203:A:ARG:H	1:205:A:GLN:HE22	3	0.61
(1,1983)	1:173:B:GLN:H	1:173:B:GLN:HB2	7	0.61
(1,1818)	1:192:B:ASN:H	1:187:B:LYS:HG2	1	0.61
(1,1817)	1:192:A:ASN:H	1:187:A:LYS:HG2	1	0.61
(1,1800)	1:193:B:ASP:H	1:192:B:ASN:HB2	7	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1799)	1:193:A:ASP:H	1:192:A:ASN:HB2	7	0.61
(1,1479)	1:179:A:TRP:HE1	1:201:A:MET:HE1	3	0.61
(1,1384)	1:180:B:ASP:H	1:180:B:ASP:HB3	4	0.61
(1,1384)	1:180:B:ASP:H	1:180:B:ASP:HB3	5	0.61
(1,1383)	1:180:A:ASP:H	1:180:A:ASP:HB3	4	0.61
(1,1383)	1:180:A:ASP:H	1:180:A:ASP:HB3	10	0.61
(1,1182)	1:199:B:GLN:HA	1:200:B:VAL:HG13	5	0.61
(1,1122)	1:184:B:ALA:HB2	1:182:B:ILE:H	5	0.61
(1,1122)	1:184:B:ALA:HB2	1:182:B:ILE:H	7	0.61
(1,1121)	1:184:A:ALA:HB2	1:182:A:ILE:H	5	0.61
(1,1121)	1:184:A:ALA:HB2	1:182:A:ILE:H	7	0.61
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD11	1	0.61
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD11	8	0.61
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD11	1	0.61
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD13	4	0.61
(1,946)	1:175:B:LEU:HD22	1:199:A:GLN:HB3	2	0.61
(1,945)	1:175:A:LEU:HD23	1:199:B:GLN:HB3	3	0.61
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG11	5	0.61
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG11	9	0.61
(1,394)	1:176:B:THR:H	1:175:B:LEU:HB2	9	0.61
(1,393)	1:176:A:THR:H	1:175:A:LEU:HB2	9	0.61
(1,345)	1:191:A:GLU:H	1:191:A:GLU:HG2	5	0.61
(1,312)	1:173:B:GLN:HB2	1:173:B:GLN:H	6	0.61
(1,311)	1:173:A:GLN:HB2	1:173:A:GLN:H	6	0.61
(1,261)	1:175:A:LEU:HD13	1:199:B:GLN:HG3	3	0.61
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG21	5	0.61
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB1	6	0.61
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG22	7	0.6
(1,2709)	1:199:A:GLN:HE22	1:175:B:LEU:HA	7	0.6
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD13	8	0.6
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD13	8	0.6
(1,2582)	1:179:B:TRP:HE1	1:204:A:LEU:HG	4	0.6
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD21	8	0.6
(1,2573)	1:208:A:TRP:HE1	1:203:B:ARG:HD2	5	0.6
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD12	4	0.6
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG12	5	0.6
(1,2416)	1:189:B:ASN:HA	1:186:B:LEU:HA	7	0.6
(1,2415)	1:189:A:ASN:HA	1:186:A:LEU:HA	7	0.6
(1,2406)	1:179:B:TRP:HA	1:182:B:ILE:HG12	2	0.6
(1,2406)	1:179:B:TRP:HA	1:182:B:ILE:HG12	3	0.6
(1,2405)	1:179:A:TRP:HA	1:182:A:ILE:HG12	3	0.6
(1,2404)	1:183:B:GLU:HA	1:201:B:MET:HB2	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2403)	1:183:A:GLU:HA	1:201:A:MET:HB2	5	0.6
(1,2314)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	10	0.6
(1,2313)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	10	0.6
(1,2240)	1:187:B:LYS:HA	1:197:B:VAL:H	6	0.6
(1,2240)	1:187:B:LYS:HA	1:197:B:VAL:H	8	0.6
(1,2239)	1:187:A:LYS:HA	1:197:A:VAL:H	7	0.6
(1,2112)	1:184:B:ALA:H	1:182:B:ILE:HG21	9	0.6
(1,2111)	1:184:A:ALA:H	1:182:A:ILE:HG21	9	0.6
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG21	3	0.6
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG21	3	0.6
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD13	7	0.6
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD13	7	0.6
(1,2040)	1:203:B:ARG:H	1:205:B:GLN:HE22	3	0.6
(1,1984)	1:173:A:GLN:H	1:173:A:GLN:HB2	7	0.6
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB3	9	0.6
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB3	9	0.6
(1,1384)	1:180:B:ASP:H	1:180:B:ASP:HB3	3	0.6
(1,1383)	1:180:A:ASP:H	1:180:A:ASP:HB3	3	0.6
(1,1383)	1:180:A:ASP:H	1:180:A:ASP:HB3	5	0.6
(1,1181)	1:199:A:GLN:HA	1:200:A:VAL:HG13	5	0.6
(1,1103)	1:179:A:TRP:HE1	1:176:A:THR:HG23	3	0.6
(1,972)	1:204:B:LEU:HD22	1:182:A:ILE:HD12	6	0.6
(1,971)	1:204:A:LEU:HD21	1:182:B:ILE:HD13	2	0.6
(1,918)	1:173:B:GLN:HG2	1:175:B:LEU:HD12	10	0.6
(1,917)	1:173:A:GLN:HG2	1:175:A:LEU:HD12	10	0.6
(1,860)	1:200:B:VAL:HA	1:175:A:LEU:HB3	8	0.6
(1,644)	1:199:B:GLN:H	1:198:B:ARG:HD3	8	0.6
(1,643)	1:199:A:GLN:H	1:198:A:ARG:HD3	8	0.6
(1,420)	1:193:B:ASP:H	1:193:B:ASP:HB3	2	0.6
(1,419)	1:193:A:ASP:H	1:193:A:ASP:HB3	2	0.6
(1,394)	1:176:B:THR:H	1:175:B:LEU:HB2	10	0.6
(1,393)	1:176:A:THR:H	1:175:A:LEU:HB2	10	0.6
(1,173)	1:211:A:ALA:HB3	1:203:B:ARG:HD3	9	0.6
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB1	6	0.6
(1,2850)	1:177:B:VAL:H	1:204:A:LEU:HD23	6	0.59
(1,2849)	1:177:A:VAL:H	1:204:B:LEU:HD23	6	0.59
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG23	3	0.59
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG23	3	0.59
(1,2807)	1:185:A:LEU:H	1:182:B:ILE:HD11	4	0.59
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD21	7	0.59
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD11	2	0.59
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD12	7	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:185:B:LEU:H	1:185:A:LEU:HD22	10	0.59
(1,2543)	1:185:A:LEU:H	1:185:B:LEU:HD22	10	0.59
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD11	8	0.59
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD12	2	0.59
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD12	2	0.59
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD12	4	0.59
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG11	2	0.59
(1,2485)	1:180:A:ASP:H	1:201:A:MET:HE1	9	0.59
(1,2405)	1:179:A:TRP:HA	1:182:A:ILE:HG12	2	0.59
(1,2402)	1:208:B:TRP:HA	1:203:A:ARG:HB3	1	0.59
(1,2314)	1:182:B:ILE:HG21	1:182:B:ILE:HG13	3	0.59
(1,2314)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	7	0.59
(1,2314)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	8	0.59
(1,2314)	1:182:B:ILE:HG22	1:182:B:ILE:HG13	9	0.59
(1,2313)	1:182:A:ILE:HG21	1:182:A:ILE:HG13	3	0.59
(1,2313)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	4	0.59
(1,2313)	1:182:A:ILE:HG22	1:182:A:ILE:HG13	5	0.59
(1,2313)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	7	0.59
(1,2313)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	8	0.59
(1,2313)	1:182:A:ILE:HG22	1:182:A:ILE:HG13	9	0.59
(1,2022)	1:179:B:TRP:HE1	1:205:B:GLN:HE22	5	0.59
(1,2021)	1:179:A:TRP:HE1	1:205:A:GLN:HE22	5	0.59
(1,2020)	1:205:B:GLN:HE22	1:179:B:TRP:HD1	1	0.59
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE1	9	0.59
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD12	2	0.59
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD12	2	0.59
(1,1104)	1:179:B:TRP:HE1	1:176:B:THR:HG23	3	0.59
(1,1074)	1:192:B:ASN:H	1:187:B:LYS:HG3	5	0.59
(1,1073)	1:192:A:ASN:H	1:187:A:LYS:HG3	5	0.59
(1,859)	1:200:A:VAL:HA	1:175:B:LEU:HB3	8	0.59
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB3	10	0.59
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB3	10	0.59
(1,420)	1:193:B:ASP:H	1:193:B:ASP:HB3	1	0.59
(1,420)	1:193:B:ASP:H	1:193:B:ASP:HB3	3	0.59
(1,420)	1:193:B:ASP:H	1:193:B:ASP:HB3	6	0.59
(1,420)	1:193:B:ASP:H	1:193:B:ASP:HB3	8	0.59
(1,420)	1:193:B:ASP:H	1:193:B:ASP:HB3	9	0.59
(1,419)	1:193:A:ASP:H	1:193:A:ASP:HB3	1	0.59
(1,419)	1:193:A:ASP:H	1:193:A:ASP:HB3	3	0.59
(1,419)	1:193:A:ASP:H	1:193:A:ASP:HB3	6	0.59
(1,419)	1:193:A:ASP:H	1:193:A:ASP:HB3	8	0.59
(1,419)	1:193:A:ASP:H	1:193:A:ASP:HB3	9	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:211:B:ALA:HB3	1:203:A:ARG:HD3	9	0.59
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD12	2	0.59
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD12	2	0.59
(1,54)	1:195:B:ALA:HB3	1:199:B:GLN:H	9	0.59
(1,51)	1:195:A:ALA:HB2	1:194:A:GLN:H	7	0.59
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG22	2	0.58
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG21	5	0.58
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG22	2	0.58
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG21	5	0.58
(1,2790)	1:189:B:ASN:H	1:191:B:GLU:HA	7	0.58
(1,2789)	1:189:A:ASN:H	1:191:A:GLU:HA	7	0.58
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD21	7	0.58
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB1	3	0.58
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB1	3	0.58
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB1	10	0.58
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD12	7	0.58
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD12	1	0.58
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD11	2	0.58
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD12	7	0.58
(1,2561)	1:209:A:SER:H	1:211:A:ALA:HB1	10	0.58
(1,2546)	1:181:B:ASP:H	1:180:B:ASP:HB3	3	0.58
(1,2545)	1:181:A:ASP:H	1:180:A:ASP:HB3	3	0.58
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD11	3	0.58
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD13	7	0.58
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD11	3	0.58
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD13	7	0.58
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG11	2	0.58
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG11	7	0.58
(1,2448)	1:187:B:LYS:H	1:185:B:LEU:HD22	1	0.58
(1,2404)	1:183:B:GLU:HA	1:201:B:MET:HB2	1	0.58
(1,2403)	1:183:A:GLU:HA	1:201:A:MET:HB2	1	0.58
(1,2401)	1:208:A:TRP:HA	1:203:B:ARG:HB3	1	0.58
(1,2374)	1:176:B:THR:HG21	1:190:A:PHE:HZ	3	0.58
(1,2314)	1:182:B:ILE:HG22	1:182:B:ILE:HG13	1	0.58
(1,2314)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	2	0.58
(1,2314)	1:182:B:ILE:HG23	1:182:B:ILE:HG13	4	0.58
(1,2314)	1:182:B:ILE:HG22	1:182:B:ILE:HG13	5	0.58
(1,2314)	1:182:B:ILE:HG22	1:182:B:ILE:HG13	6	0.58
(1,2313)	1:182:A:ILE:HG22	1:182:A:ILE:HG13	1	0.58
(1,2313)	1:182:A:ILE:HG23	1:182:A:ILE:HG13	2	0.58
(1,2313)	1:182:A:ILE:HG22	1:182:A:ILE:HG13	6	0.58
(1,2302)	1:188:B:ASN:HB3	1:185:B:LEU:HB3	6	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2301)	1:188:A:ASN:HB3	1:185:A:LEU:HB3	6	0.58
(1,2298)	1:200:B:VAL:HG13	1:197:B:VAL:HA	5	0.58
(1,2228)	1:208:B:TRP:HA	1:179:B:TRP:HH2	1	0.58
(1,2227)	1:208:A:TRP:HA	1:179:A:TRP:HH2	1	0.58
(1,2128)	1:185:B:LEU:HD13	1:189:B:ASN:HB2	8	0.58
(1,2102)	1:204:B:LEU:HD13	1:179:B:TRP:HZ3	9	0.58
(1,2070)	1:194:B:GLN:H	1:196:B:ALA:HB1	2	0.58
(1,2069)	1:194:A:GLN:H	1:196:A:ALA:HB1	2	0.58
(1,2022)	1:179:B:TRP:HE1	1:205:B:GLN:HE22	7	0.58
(1,2021)	1:179:A:TRP:HE1	1:205:A:GLN:HE22	7	0.58
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE1	9	0.58
(1,1579)	1:188:A:ASN:HD22	1:185:A:LEU:HA	9	0.58
(1,1429)	1:211:A:ALA:H	1:206:B:LYS:HE3	8	0.58
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD11	6	0.58
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD12	10	0.58
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD12	10	0.58
(1,1122)	1:184:B:ALA:HB3	1:182:B:ILE:H	2	0.58
(1,1122)	1:184:B:ALA:HB2	1:182:B:ILE:H	9	0.58
(1,1121)	1:184:A:ALA:HB3	1:182:A:ILE:H	2	0.58
(1,972)	1:204:B:LEU:HD22	1:182:A:ILE:HD12	1	0.58
(1,971)	1:204:A:LEU:HD22	1:182:B:ILE:HD12	1	0.58
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG11	9	0.58
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB1	8	0.58
(1,420)	1:193:B:ASP:H	1:193:B:ASP:HB3	10	0.58
(1,419)	1:193:A:ASP:H	1:193:A:ASP:HB3	10	0.58
(1,54)	1:195:B:ALA:HB3	1:199:B:GLN:H	3	0.58
(1,53)	1:195:A:ALA:HB3	1:199:A:GLN:H	3	0.58
(1,53)	1:195:A:ALA:HB3	1:199:A:GLN:H	9	0.58
(1,52)	1:195:B:ALA:HB2	1:194:B:GLN:H	7	0.58
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD22	4	0.57
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD21	9	0.57
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB1	10	0.57
(1,2745)	1:195:A:ALA:H	1:197:A:VAL:HG22	10	0.57
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD12	7	0.57
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD12	1	0.57
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD23	1	0.57
(1,2574)	1:208:B:TRP:HE1	1:203:A:ARG:HD2	5	0.57
(1,2562)	1:209:B:SER:H	1:211:B:ALA:HB1	10	0.57
(1,2543)	1:185:A:LEU:H	1:185:B:LEU:HD23	8	0.57
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD11	6	0.57
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG11	7	0.57
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG12	9	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2486)	1:180:B:ASP:H	1:201:B:MET:HE1	9	0.57
(1,2447)	1:187:A:LYS:H	1:185:A:LEU:HD22	1	0.57
(1,2406)	1:179:B:TRP:HA	1:182:B:ILE:HG12	10	0.57
(1,2405)	1:179:A:TRP:HA	1:182:A:ILE:HG12	10	0.57
(1,2297)	1:200:A:VAL:HG13	1:197:A:VAL:HA	5	0.57
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG21	2	0.57
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG21	2	0.57
(1,2240)	1:187:B:LYS:HA	1:197:B:VAL:H	10	0.57
(1,2239)	1:187:A:LYS:HA	1:197:A:VAL:H	10	0.57
(1,2127)	1:185:A:LEU:HD13	1:189:A:ASN:HB2	8	0.57
(1,2101)	1:204:A:LEU:HD13	1:179:A:TRP:HZ3	9	0.57
(1,2019)	1:205:A:GLN:HE22	1:179:A:TRP:HD1	1	0.57
(1,1693)	1:189:A:ASN:HD22	1:182:B:ILE:HD12	7	0.57
(1,1580)	1:188:B:ASN:HD22	1:185:B:LEU:HA	9	0.57
(1,1580)	1:188:B:ASN:HD22	1:185:B:LEU:HA	10	0.57
(1,1579)	1:188:A:ASN:HD22	1:185:A:LEU:HA	10	0.57
(1,1430)	1:211:B:ALA:H	1:206:A:LYS:HE3	8	0.57
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD11	6	0.57
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB1	6	0.57
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB1	6	0.57
(1,1144)	1:193:B:ASP:H	1:190:B:PHE:HA	7	0.57
(1,1143)	1:193:A:ASP:H	1:190:A:PHE:HA	7	0.57
(1,1121)	1:184:A:ALA:HB2	1:182:A:ILE:H	9	0.57
(1,1116)	1:175:B:LEU:HD21	1:199:A:GLN:H	6	0.57
(1,832)	1:182:B:ILE:HG23	1:179:B:TRP:HA	8	0.57
(1,831)	1:182:A:ILE:HG23	1:179:A:TRP:HA	8	0.57
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB1	8	0.57
(1,397)	1:175:A:LEU:HB2	1:190:B:PHE:HZ	10	0.57
(1,394)	1:176:B:THR:H	1:175:B:LEU:HB2	2	0.57
(1,393)	1:176:A:THR:H	1:175:A:LEU:HB2	2	0.57
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD21	3	0.57
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD22	7	0.57
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD21	3	0.57
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD22	7	0.57
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD13	1	0.57
(1,94)	1:175:B:LEU:HD23	1:200:A:VAL:H	6	0.57
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG23	2	0.57
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG23	2	0.57
(1,54)	1:195:B:ALA:HB2	1:199:B:GLN:H	10	0.57
(1,53)	1:195:A:ALA:HB2	1:199:A:GLN:H	10	0.57
(1,26)	1:201:B:MET:HE2	1:179:B:TRP:HB3	3	0.57
(1,25)	1:201:A:MET:HE2	1:179:A:TRP:HB3	3	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:201:B:MET:HE1	1:183:B:GLU:HA	10	0.57
(1,23)	1:201:A:MET:HE1	1:183:A:GLU:HA	10	0.57
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD21	2	0.56
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD21	9	0.56
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG22	7	0.56
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD23	2	0.56
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD23	2	0.56
(1,2746)	1:195:B:ALA:H	1:197:B:VAL:HG22	10	0.56
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD22	5	0.56
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD21	2	0.56
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD11	4	0.56
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD11	4	0.56
(1,2668)	1:205:B:GLN:H	1:202:B:GLU:HB2	10	0.56
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD23	1	0.56
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD22	4	0.56
(1,2574)	1:208:B:TRP:HE1	1:203:A:ARG:HD2	6	0.56
(1,2544)	1:185:B:LEU:H	1:185:A:LEU:HD23	8	0.56
(1,2543)	1:185:A:LEU:H	1:185:B:LEU:HD23	5	0.56
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD22	1	0.56
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD22	1	0.56
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD11	8	0.56
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD11	1	0.56
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD12	5	0.56
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD11	1	0.56
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD12	5	0.56
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD11	6	0.56
(1,2486)	1:180:B:ASP:H	1:183:B:GLU:HB3	6	0.56
(1,2485)	1:180:A:ASP:H	1:183:A:GLU:HB3	6	0.56
(1,2302)	1:188:B:ASN:HB3	1:185:B:LEU:HB3	9	0.56
(1,2301)	1:188:A:ASN:HB3	1:185:A:LEU:HB3	9	0.56
(1,2239)	1:187:A:LYS:HA	1:197:A:VAL:H	5	0.56
(1,2128)	1:185:B:LEU:HD13	1:178:A:PRO:HB2	4	0.56
(1,2126)	1:186:B:LEU:HD11	1:178:A:PRO:HG2	3	0.56
(1,2125)	1:186:A:LEU:HD11	1:178:B:PRO:HG2	3	0.56
(1,1694)	1:189:B:ASN:HD22	1:182:A:ILE:HD12	7	0.56
(1,942)	1:175:B:LEU:HD23	1:200:A:VAL:HG11	6	0.56
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG12	3	0.56
(1,705)	1:195:A:ALA:HA	1:198:A:ARG:HG2	4	0.56
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB3	1	0.56
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB1	3	0.56
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB2	7	0.56
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB3	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB1	3	0.56
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB2	7	0.56
(1,394)	1:176:B:THR:H	1:175:B:LEU:HB2	4	0.56
(1,320)	1:173:B:GLN:HG3	1:173:B:GLN:H	7	0.56
(1,319)	1:173:A:GLN:HG3	1:173:A:GLN:H	7	0.56
(1,254)	1:175:B:LEU:HD13	1:196:A:ALA:HA	1	0.56
(1,253)	1:175:A:LEU:HD13	1:196:B:ALA:HA	1	0.56
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD13	1	0.56
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB3	7	0.56
(1,54)	1:195:B:ALA:HB1	1:199:B:GLN:H	6	0.56
(1,53)	1:195:A:ALA:HB1	1:199:A:GLN:H	6	0.56
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG21	9	0.56
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG21	9	0.56
(1,2873)	1:204:A:LEU:H	1:182:B:ILE:HD12	4	0.55
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG22	7	0.55
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD12	3	0.55
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD12	3	0.55
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD11	9	0.55
(1,2667)	1:205:A:GLN:H	1:202:A:GLU:HB2	10	0.55
(1,2573)	1:208:A:TRP:HE1	1:203:B:ARG:HD2	2	0.55
(1,2546)	1:181:B:ASP:H	1:180:B:ASP:HB3	5	0.55
(1,2545)	1:181:A:ASP:H	1:180:A:ASP:HB3	5	0.55
(1,2544)	1:185:B:LEU:H	1:185:A:LEU:HD23	1	0.55
(1,2544)	1:185:B:LEU:H	1:185:A:LEU:HD23	5	0.55
(1,2543)	1:185:A:LEU:H	1:185:B:LEU:HD23	1	0.55
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD23	9	0.55
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD21	7	0.55
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD23	9	0.55
(1,2486)	1:180:B:ASP:H	1:183:B:GLU:HB3	4	0.55
(1,2485)	1:180:A:ASP:H	1:183:A:GLU:HB3	4	0.55
(1,2402)	1:208:B:TRP:HA	1:203:A:ARG:HB3	8	0.55
(1,2373)	1:176:A:THR:HG21	1:190:B:PHE:HZ	3	0.55
(1,2322)	1:197:B:VAL:HG12	1:187:B:LYS:HG3	4	0.55
(1,2321)	1:197:A:VAL:HG12	1:187:A:LYS:HG3	4	0.55
(1,2298)	1:200:B:VAL:HG12	1:197:B:VAL:HA	1	0.55
(1,2298)	1:197:B:VAL:HA	1:186:B:LEU:HB2	10	0.55
(1,2297)	1:200:A:VAL:HG12	1:197:A:VAL:HA	1	0.55
(1,2297)	1:197:A:VAL:HA	1:186:A:LEU:HB2	10	0.55
(1,2264)	1:181:B:ASP:HA	1:185:A:LEU:HD12	10	0.55
(1,2263)	1:181:A:ASP:HA	1:185:B:LEU:HD12	10	0.55
(1,2240)	1:187:B:LYS:HA	1:197:B:VAL:H	5	0.55
(1,2228)	1:208:B:TRP:HA	1:179:B:TRP:HH2	5	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2227)	1:208:A:TRP:HA	1:179:A:TRP:HH2	5	0.55
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD21	7	0.55
(1,2125)	1:186:A:LEU:HD13	1:178:B:PRO:HG2	4	0.55
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG22	9	0.55
(1,2021)	1:179:A:TRP:HE1	1:205:A:GLN:HE22	8	0.55
(1,1814)	1:192:B:ASN:H	1:191:B:GLU:HB3	1	0.55
(1,1813)	1:192:A:ASN:H	1:191:A:GLU:HB3	1	0.55
(1,1557)	1:173:A:GLN:HE21	1:200:B:VAL:HG12	4	0.55
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD11	9	0.55
(1,1191)	1:188:A:ASN:HA	1:191:A:GLU:HG2	1	0.55
(1,1171)	1:209:A:SER:HB3	1:210:A:LEU:HD23	5	0.55
(1,1115)	1:175:A:LEU:HD21	1:199:B:GLN:H	6	0.55
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD11	2	0.55
(1,941)	1:175:A:LEU:HD23	1:200:B:VAL:HG11	6	0.55
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG13	1	0.55
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG13	1	0.55
(1,706)	1:195:B:ALA:HA	1:198:B:ARG:HG2	4	0.55
(1,393)	1:176:A:THR:H	1:175:A:LEU:HB2	4	0.55
(1,122)	1:199:B:GLN:H	1:198:B:ARG:HG2	10	0.55
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB3	7	0.55
(1,51)	1:195:A:ALA:HB2	1:194:A:GLN:H	4	0.55
(1,2874)	1:204:B:LEU:H	1:182:A:ILE:HD13	5	0.54
(1,2873)	1:204:A:LEU:H	1:182:B:ILE:HD13	5	0.54
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD22	4	0.54
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD21	2	0.54
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB1	1	0.54
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB1	1	0.54
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD21	2	0.54
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD11	9	0.54
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD12	10	0.54
(1,2582)	1:179:B:TRP:HE1	1:204:A:LEU:HG	5	0.54
(1,2581)	1:179:A:TRP:HE1	1:204:B:LEU:HG	5	0.54
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD22	4	0.54
(1,2574)	1:208:B:TRP:HE1	1:203:A:ARG:HD2	2	0.54
(1,2562)	1:209:B:SER:H	1:206:B:LYS:HG3	2	0.54
(1,2561)	1:209:A:SER:H	1:206:A:LYS:HG3	2	0.54
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD21	4	0.54
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD23	7	0.54
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD21	4	0.54
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD13	4	0.54
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD11	9	0.54
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD12	10	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG11	1	0.54
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG11	1	0.54
(1,2406)	1:179:B:TRP:HA	1:182:B:ILE:HG12	9	0.54
(1,2405)	1:179:A:TRP:HA	1:182:A:ILE:HG12	9	0.54
(1,2404)	1:183:B:GLU:HA	1:201:B:MET:HB2	6	0.54
(1,2403)	1:183:A:GLU:HA	1:201:A:MET:HB2	6	0.54
(1,2401)	1:208:A:TRP:HA	1:203:B:ARG:HB3	9	0.54
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD13	9	0.54
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD13	9	0.54
(1,2302)	1:188:B:ASN:HB3	1:185:B:LEU:HB3	10	0.54
(1,2301)	1:188:A:ASN:HB3	1:185:A:LEU:HB3	10	0.54
(1,2228)	1:208:B:TRP:HA	1:179:B:TRP:HH2	2	0.54
(1,2228)	1:208:B:TRP:HA	1:179:B:TRP:HH2	6	0.54
(1,2227)	1:208:A:TRP:HA	1:179:A:TRP:HH2	2	0.54
(1,2227)	1:208:A:TRP:HA	1:179:A:TRP:HH2	6	0.54
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD21	7	0.54
(1,2126)	1:186:B:LEU:HD13	1:178:A:PRO:HG2	4	0.54
(1,2126)	1:186:B:LEU:HD11	1:178:A:PRO:HG2	8	0.54
(1,2096)	1:175:B:LEU:HD13	1:199:A:GLN:HE22	1	0.54
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG22	9	0.54
(1,2022)	1:179:B:TRP:HE1	1:205:B:GLN:HE22	8	0.54
(1,1813)	1:192:A:ASN:H	1:191:A:GLU:HB3	6	0.54
(1,1429)	1:211:A:ALA:H	1:206:B:LYS:HE3	2	0.54
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD11	1	0.54
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD11	9	0.54
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD11	1	0.54
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB2	5	0.54
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB2	5	0.54
(1,1192)	1:188:B:ASN:HA	1:191:B:GLU:HG2	1	0.54
(1,1172)	1:209:B:SER:HB3	1:210:B:LEU:HD23	5	0.54
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD13	6	0.54
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG12	4	0.54
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG12	3	0.54
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG12	4	0.54
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB3	5	0.54
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB2	6	0.54
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB3	5	0.54
(1,186)	1:184:B:ALA:HB1	1:187:B:LYS:HE2	9	0.54
(1,160)	1:182:B:ILE:HD11	1:177:B:VAL:HA	8	0.54
(1,159)	1:182:A:ILE:HD11	1:177:A:VAL:HA	8	0.54
(1,121)	1:199:A:GLN:H	1:198:A:ARG:HG2	10	0.54
(1,110)	1:210:B:LEU:HD11	1:212:A:LYS:H	3	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:210:B:LEU:HD12	1:212:A:LYS:H	4	0.54
(1,109)	1:210:A:LEU:HD11	1:212:B:LYS:H	3	0.54
(1,109)	1:210:A:LEU:HD12	1:212:B:LYS:H	4	0.54
(1,93)	1:175:A:LEU:HD23	1:200:B:VAL:H	6	0.54
(1,54)	1:195:B:ALA:HB1	1:199:B:GLN:H	7	0.54
(1,53)	1:195:A:ALA:HB1	1:199:A:GLN:H	7	0.54
(1,52)	1:195:B:ALA:HB2	1:194:B:GLN:H	4	0.54
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG21	9	0.53
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG21	9	0.53
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB2	7	0.53
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD21	10	0.53
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD22	5	0.53
(1,2711)	1:199:A:GLN:HE22	1:199:A:GLN:HA	4	0.53
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD11	4	0.53
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD13	6	0.53
(1,2684)	1:203:B:ARG:H	1:204:B:LEU:HD12	10	0.53
(1,2683)	1:203:A:ARG:H	1:204:A:LEU:HD13	6	0.53
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD22	5	0.53
(1,2543)	1:185:A:LEU:H	1:185:B:LEU:HD23	2	0.53
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD22	10	0.53
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD22	10	0.53
(1,2530)	1:210:B:LEU:H	1:210:B:LEU:HD13	8	0.53
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD13	8	0.53
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD11	9	0.53
(1,2529)	1:210:A:LEU:H	1:210:A:LEU:HD12	10	0.53
(1,2511)	1:176:A:THR:H	1:173:A:GLN:HB3	7	0.53
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG13	6	0.53
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG13	4	0.53
(1,2406)	1:179:B:TRP:HA	1:182:B:ILE:HG12	7	0.53
(1,2405)	1:179:A:TRP:HA	1:182:A:ILE:HG12	7	0.53
(1,2359)	1:200:A:VAL:HG12	1:175:B:LEU:H	3	0.53
(1,2262)	1:186:B:LEU:HA	1:200:B:VAL:HG21	9	0.53
(1,2261)	1:186:A:LEU:HA	1:200:A:VAL:HG21	9	0.53
(1,2129)	1:185:A:LEU:HD21	1:185:A:LEU:HA	7	0.53
(1,2125)	1:186:A:LEU:HD11	1:178:B:PRO:HG2	8	0.53
(1,2095)	1:175:A:LEU:HD13	1:199:B:GLN:HE22	1	0.53
(1,2089)	1:191:A:GLU:H	1:197:A:VAL:HG23	10	0.53
(1,2020)	1:205:B:GLN:HE22	1:179:B:TRP:HD1	4	0.53
(1,1814)	1:192:B:ASN:H	1:191:B:GLU:HB3	2	0.53
(1,1814)	1:192:B:ASN:H	1:191:B:GLU:HB3	3	0.53
(1,1814)	1:192:B:ASN:H	1:191:B:GLU:HB3	4	0.53
(1,1814)	1:192:B:ASN:H	1:191:B:GLU:HB3	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1814)	1:192:B:ASN:H	1:191:B:GLU:HB3	9	0.53
(1,1813)	1:192:A:ASN:H	1:191:A:GLU:HB3	2	0.53
(1,1813)	1:192:A:ASN:H	1:191:A:GLU:HB3	3	0.53
(1,1813)	1:192:A:ASN:H	1:191:A:GLU:HB3	4	0.53
(1,1813)	1:192:A:ASN:H	1:191:A:GLU:HB3	9	0.53
(1,1480)	1:179:B:TRP:HE1	1:201:B:MET:HE2	10	0.53
(1,1471)	1:208:A:TRP:HE1	1:208:A:TRP:HB2	9	0.53
(1,1430)	1:211:B:ALA:H	1:206:A:LYS:HE3	2	0.53
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD13	10	0.53
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD13	10	0.53
(1,1408)	1:212:B:LYS:H	1:203:A:ARG:HD3	5	0.53
(1,1407)	1:212:A:LYS:H	1:203:B:ARG:HD3	5	0.53
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB3	8	0.53
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG12	7	0.53
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG12	7	0.53
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD11	2	0.53
(1,692)	1:196:B:ALA:HA	1:195:B:ALA:HB1	9	0.53
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB2	6	0.53
(1,398)	1:175:B:LEU:HB2	1:190:A:PHE:HZ	10	0.53
(1,394)	1:176:B:THR:H	1:175:B:LEU:HB2	1	0.53
(1,393)	1:176:A:THR:H	1:175:A:LEU:HB2	1	0.53
(1,311)	1:173:A:GLN:HB2	1:173:A:GLN:H	3	0.53
(1,311)	1:173:A:GLN:HB2	1:173:A:GLN:H	4	0.53
(1,295)	1:185:A:LEU:HD22	1:182:B:ILE:HD11	8	0.53
(1,262)	1:175:B:LEU:HD12	1:199:A:GLN:HG3	7	0.53
(1,261)	1:175:A:LEU:HD12	1:199:B:GLN:HG3	7	0.53
(1,261)	1:175:A:LEU:HD13	1:199:B:GLN:HG3	10	0.53
(1,185)	1:184:A:ALA:HB1	1:187:A:LYS:HE2	9	0.53
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG23	4	0.53
(1,122)	1:199:B:GLN:H	1:198:B:ARG:HG2	7	0.53
(1,122)	1:199:B:GLN:H	1:198:B:ARG:HG2	9	0.53
(1,121)	1:199:A:GLN:H	1:198:A:ARG:HG2	7	0.53
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD22	8	0.53
(1,52)	1:195:B:ALA:HB3	1:194:B:GLN:H	10	0.53
(1,2874)	1:204:B:LEU:H	1:182:A:ILE:HD12	8	0.52
(1,2826)	1:182:B:ILE:H	1:182:B:ILE:HG22	10	0.52
(1,2825)	1:182:A:ILE:H	1:182:A:ILE:HG22	10	0.52
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB2	7	0.52
(1,2772)	1:175:B:LEU:H	1:190:A:PHE:HZ	5	0.52
(1,2771)	1:175:A:LEU:H	1:190:B:PHE:HZ	5	0.52
(1,2712)	1:199:B:GLN:HE22	1:199:B:GLN:HA	4	0.52
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD12	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD11	10	0.52
(1,2670)	1:202:B:GLU:H	1:179:B:TRP:HZ3	1	0.52
(1,2669)	1:202:A:GLU:H	1:179:A:TRP:HZ3	1	0.52
(1,2668)	1:205:B:GLN:H	1:202:B:GLU:HB2	9	0.52
(1,2667)	1:205:A:GLN:H	1:202:A:GLU:HB2	9	0.52
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD12	2	0.52
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD22	5	0.52
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD23	6	0.52
(1,2573)	1:208:A:TRP:HE1	1:203:B:ARG:HD2	6	0.52
(1,2544)	1:185:B:LEU:H	1:185:A:LEU:HD23	2	0.52
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD21	3	0.52
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD21	6	0.52
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD21	8	0.52
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD21	3	0.52
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD21	6	0.52
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG13	4	0.52
(1,2485)	1:180:A:ASP:H	1:183:A:GLU:HB3	8	0.52
(1,2414)	1:192:B:ASN:HB2	1:191:B:GLU:HA	1	0.52
(1,2413)	1:192:A:ASN:HB2	1:191:A:GLU:HA	1	0.52
(1,2402)	1:208:B:TRP:HA	1:203:A:ARG:HB3	2	0.52
(1,2401)	1:208:A:TRP:HA	1:203:B:ARG:HB3	4	0.52
(1,2401)	1:208:A:TRP:HA	1:203:B:ARG:HB3	6	0.52
(1,2401)	1:208:A:TRP:HA	1:203:B:ARG:HB3	8	0.52
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG13	1	0.52
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG13	6	0.52
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG13	1	0.52
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG13	6	0.52
(1,2372)	1:186:B:LEU:HD12	1:177:A:VAL:H	7	0.52
(1,2371)	1:186:A:LEU:HD12	1:177:B:VAL:H	7	0.52
(1,2332)	1:212:B:LYS:HB3	1:211:B:ALA:H	1	0.52
(1,2332)	1:212:B:LYS:HB3	1:211:B:ALA:H	4	0.52
(1,2331)	1:212:A:LYS:HB3	1:211:A:ALA:H	1	0.52
(1,2331)	1:212:A:LYS:HB3	1:211:A:ALA:H	4	0.52
(1,2240)	1:187:B:LYS:HA	1:197:B:VAL:H	9	0.52
(1,2239)	1:187:A:LYS:HA	1:197:A:VAL:H	9	0.52
(1,2232)	1:187:B:LYS:H	1:197:B:VAL:HA	8	0.52
(1,2231)	1:187:A:LYS:H	1:197:A:VAL:HA	8	0.52
(1,2228)	1:208:B:TRP:HA	1:179:B:TRP:HH2	9	0.52
(1,2227)	1:208:A:TRP:HA	1:179:A:TRP:HH2	9	0.52
(1,2130)	1:185:B:LEU:HD21	1:185:B:LEU:HA	7	0.52
(1,2127)	1:185:A:LEU:HD13	1:178:B:PRO:HB2	4	0.52
(1,2126)	1:186:B:LEU:HD11	1:178:A:PRO:HG2	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2125)	1:186:A:LEU:HD11	1:178:B:PRO:HG2	1	0.52
(1,2090)	1:191:B:GLU:H	1:197:B:VAL:HG23	10	0.52
(1,2053)	1:199:A:GLN:H	1:199:A:GLN:HB3	3	0.52
(1,2019)	1:205:A:GLN:HE22	1:179:A:TRP:HD1	4	0.52
(1,1814)	1:192:B:ASN:H	1:191:B:GLU:HB3	8	0.52
(1,1814)	1:192:B:ASN:H	1:191:B:GLU:HB3	10	0.52
(1,1813)	1:192:A:ASN:H	1:191:A:GLU:HB3	8	0.52
(1,1813)	1:192:A:ASN:H	1:191:A:GLU:HB3	10	0.52
(1,1793)	1:193:A:ASP:H	1:188:A:ASN:HA	5	0.52
(1,1782)	1:175:B:LEU:H	1:177:B:VAL:HG22	6	0.52
(1,1781)	1:175:A:LEU:H	1:177:A:VAL:HG22	6	0.52
(1,1479)	1:179:A:TRP:HE1	1:201:A:MET:HE2	10	0.52
(1,1472)	1:208:B:TRP:HE1	1:208:B:TRP:HB2	5	0.52
(1,1472)	1:208:B:TRP:HE1	1:208:B:TRP:HB2	6	0.52
(1,1472)	1:208:B:TRP:HE1	1:208:B:TRP:HB2	7	0.52
(1,1472)	1:208:B:TRP:HE1	1:208:B:TRP:HB2	8	0.52
(1,1472)	1:208:B:TRP:HE1	1:208:B:TRP:HB2	9	0.52
(1,1472)	1:208:B:TRP:HE1	1:208:B:TRP:HB2	10	0.52
(1,1471)	1:208:A:TRP:HE1	1:208:A:TRP:HB2	4	0.52
(1,1471)	1:208:A:TRP:HE1	1:208:A:TRP:HB2	5	0.52
(1,1471)	1:208:A:TRP:HE1	1:208:A:TRP:HB2	6	0.52
(1,1471)	1:208:A:TRP:HE1	1:208:A:TRP:HB2	7	0.52
(1,1471)	1:208:A:TRP:HE1	1:208:A:TRP:HB2	8	0.52
(1,1471)	1:208:A:TRP:HE1	1:208:A:TRP:HB2	10	0.52
(1,1466)	1:208:B:TRP:HE1	1:173:B:GLN:H	10	0.52
(1,1465)	1:208:A:TRP:HE1	1:173:A:GLN:H	10	0.52
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB2	1	0.52
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB2	1	0.52
(1,1103)	1:179:A:TRP:HE1	1:176:A:THR:HG21	2	0.52
(1,971)	1:204:A:LEU:HD23	1:182:B:ILE:HD12	10	0.52
(1,723)	1:190:A:PHE:HA	1:191:A:GLU:HG2	7	0.52
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG13	2	0.52
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG13	2	0.52
(1,691)	1:196:A:ALA:HA	1:195:A:ALA:HB1	9	0.52
(1,397)	1:175:A:LEU:HB2	1:190:B:PHE:HZ	6	0.52
(1,348)	1:202:B:GLU:H	1:202:B:GLU:HG2	9	0.52
(1,347)	1:202:A:GLU:H	1:202:A:GLU:HG2	9	0.52
(1,312)	1:173:B:GLN:HB2	1:173:B:GLN:H	3	0.52
(1,312)	1:173:B:GLN:HB2	1:173:B:GLN:H	4	0.52
(1,296)	1:185:B:LEU:HD22	1:182:A:ILE:HD13	9	0.52
(1,262)	1:175:B:LEU:HD11	1:199:A:GLN:HG3	2	0.52
(1,262)	1:175:B:LEU:HD13	1:199:A:GLN:HG3	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:210:B:LEU:HD12	1:211:A:ALA:HA	3	0.52
(1,217)	1:210:A:LEU:HD12	1:211:B:ALA:HA	3	0.52
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG21	9	0.52
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG21	9	0.52
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG23	1	0.52
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG23	4	0.52
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG23	1	0.52
(1,122)	1:199:B:GLN:H	1:198:B:ARG:HG2	3	0.52
(1,121)	1:199:A:GLN:H	1:198:A:ARG:HG2	9	0.52
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD22	8	0.52
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB2	1	0.52
(1,54)	1:195:B:ALA:HB2	1:199:B:GLN:H	1	0.52
(1,53)	1:195:A:ALA:HB2	1:199:A:GLN:H	1	0.52
(1,51)	1:195:A:ALA:HB3	1:194:A:GLN:H	10	0.52
(1,2874)	1:204:B:LEU:H	1:182:A:ILE:HD12	4	0.51
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD21	1	0.51
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD21	1	0.51
(1,2740)	1:196:B:ALA:H	1:197:B:VAL:HB	8	0.51
(1,2739)	1:196:A:ALA:H	1:197:A:VAL:HB	8	0.51
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD11	1	0.51
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD11	4	0.51
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD11	10	0.51
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD11	1	0.51
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD12	5	0.51
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD12	2	0.51
(1,2582)	1:179:B:TRP:HE1	1:204:A:LEU:HG	3	0.51
(1,2581)	1:179:A:TRP:HE1	1:204:B:LEU:HG	3	0.51
(1,2562)	1:209:B:SER:H	1:206:B:LYS:HG3	8	0.51
(1,2561)	1:209:A:SER:H	1:206:A:LYS:HG3	8	0.51
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD23	5	0.51
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD23	5	0.51
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD21	8	0.51
(1,2512)	1:176:B:THR:H	1:173:B:GLN:HB3	7	0.51
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG13	6	0.51
(1,2486)	1:180:B:ASP:H	1:183:B:GLU:HB3	8	0.51
(1,2404)	1:183:B:GLU:HA	1:201:B:MET:HB2	8	0.51
(1,2403)	1:183:A:GLU:HA	1:201:A:MET:HB2	8	0.51
(1,2402)	1:208:B:TRP:HA	1:203:A:ARG:HB3	3	0.51
(1,2402)	1:208:B:TRP:HA	1:203:A:ARG:HB3	6	0.51
(1,2402)	1:208:B:TRP:HA	1:203:A:ARG:HB3	7	0.51
(1,2402)	1:208:B:TRP:HA	1:203:A:ARG:HB3	9	0.51
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG11	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG11	10	0.51
(1,2372)	1:186:B:LEU:HD12	1:177:A:VAL:H	5	0.51
(1,2174)	1:203:B:ARG:HD2	1:208:A:TRP:HZ3	8	0.51
(1,2130)	1:185:B:LEU:HD23	1:185:B:LEU:HA	3	0.51
(1,2129)	1:185:A:LEU:HD23	1:185:A:LEU:HA	3	0.51
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD11	2	0.51
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD11	2	0.51
(1,2054)	1:199:B:GLN:H	1:199:B:GLN:HB3	3	0.51
(1,2054)	1:199:B:GLN:H	1:199:B:GLN:HB3	4	0.51
(1,2054)	1:199:B:GLN:H	1:199:B:GLN:HB3	7	0.51
(1,2054)	1:199:B:GLN:H	1:199:B:GLN:HB3	9	0.51
(1,2054)	1:199:B:GLN:H	1:199:B:GLN:HB3	10	0.51
(1,2053)	1:199:A:GLN:H	1:199:A:GLN:HB3	4	0.51
(1,2053)	1:199:A:GLN:H	1:199:A:GLN:HB3	7	0.51
(1,2053)	1:199:A:GLN:H	1:199:A:GLN:HB3	9	0.51
(1,1814)	1:192:B:ASN:H	1:191:B:GLU:HB3	5	0.51
(1,1813)	1:192:A:ASN:H	1:191:A:GLU:HB3	5	0.51
(1,1794)	1:193:B:ASP:H	1:188:B:ASN:HA	5	0.51
(1,1738)	1:195:B:ALA:H	1:194:B:GLN:HB3	7	0.51
(1,1737)	1:195:A:ALA:H	1:194:A:GLN:HB3	7	0.51
(1,1553)	1:173:A:GLN:HE21	1:175:A:LEU:HB3	8	0.51
(1,1472)	1:208:B:TRP:HE1	1:208:B:TRP:HB2	1	0.51
(1,1472)	1:208:B:TRP:HE1	1:208:B:TRP:HB2	2	0.51
(1,1472)	1:208:B:TRP:HE1	1:208:B:TRP:HB2	4	0.51
(1,1471)	1:208:A:TRP:HE1	1:208:A:TRP:HB2	1	0.51
(1,1471)	1:208:A:TRP:HE1	1:208:A:TRP:HB2	2	0.51
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD11	3	0.51
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD13	6	0.51
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD11	3	0.51
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD13	6	0.51
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB3	8	0.51
(1,1106)	1:176:B:THR:HG21	1:179:B:TRP:HD1	5	0.51
(1,1105)	1:176:A:THR:HG21	1:179:A:TRP:HD1	5	0.51
(1,1104)	1:179:B:TRP:HE1	1:176:B:THR:HG21	2	0.51
(1,1050)	1:212:B:LYS:HB3	1:212:B:LYS:HE3	2	0.51
(1,1049)	1:212:A:LYS:HB3	1:212:A:LYS:HE3	2	0.51
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD13	5	0.51
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD13	6	0.51
(1,831)	1:182:A:ILE:HG23	1:179:A:TRP:HA	4	0.51
(1,724)	1:190:B:PHE:HA	1:191:B:GLU:HG2	7	0.51
(1,397)	1:175:A:LEU:HB2	1:190:B:PHE:HZ	9	0.51
(1,394)	1:176:B:THR:H	1:175:B:LEU:HB2	5	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:176:A:THR:H	1:175:A:LEU:HB2	5	0.51
(1,261)	1:175:A:LEU:HD11	1:199:B:GLN:HG3	2	0.51
(1,261)	1:175:A:LEU:HD12	1:199:B:GLN:HG3	4	0.51
(1,253)	1:175:A:LEU:HD13	1:196:B:ALA:HA	5	0.51
(1,122)	1:199:B:GLN:H	1:198:B:ARG:HG2	4	0.51
(1,122)	1:199:B:GLN:H	1:198:B:ARG:HG2	6	0.51
(1,121)	1:199:A:GLN:H	1:198:A:ARG:HG2	3	0.51
(1,121)	1:199:A:GLN:H	1:198:A:ARG:HG2	4	0.51
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG22	6	0.51
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG22	8	0.51
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG22	8	0.51
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB2	1	0.51
(1,54)	1:195:B:ALA:HB2	1:199:B:GLN:H	5	0.51
(1,53)	1:195:A:ALA:HB2	1:199:A:GLN:H	5	0.51
(1,53)	1:195:A:ALA:HB3	1:199:A:GLN:H	8	0.51
(1,2861)	1:173:B:GLN:H	1:212:B:LYS:HG2	6	0.5
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD22	7	0.5
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD22	6	0.5
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD22	6	0.5
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD21	1	0.5
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD21	1	0.5
(1,2739)	1:196:A:ALA:H	1:197:A:VAL:HB	5	0.5
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD23	6	0.5
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD13	4	0.5
(1,2401)	1:208:A:TRP:HA	1:203:B:ARG:HB3	2	0.5
(1,2401)	1:208:A:TRP:HA	1:203:B:ARG:HB3	7	0.5
(1,2371)	1:186:A:LEU:HD12	1:177:B:VAL:H	5	0.5
(1,2240)	1:187:B:LYS:HA	1:197:B:VAL:H	2	0.5
(1,2239)	1:187:A:LYS:HA	1:197:A:VAL:H	2	0.5
(1,2228)	1:208:B:TRP:HA	1:179:B:TRP:HH2	8	0.5
(1,2227)	1:208:A:TRP:HA	1:179:A:TRP:HH2	8	0.5
(1,2166)	1:189:B:ASN:HB3	1:185:B:LEU:HG	9	0.5
(1,2130)	1:185:B:LEU:HD23	1:185:B:LEU:HA	1	0.5
(1,2130)	1:185:B:LEU:HD23	1:185:B:LEU:HA	2	0.5
(1,2130)	1:185:B:LEU:HD21	1:185:B:LEU:HA	4	0.5
(1,2130)	1:185:B:LEU:HD23	1:185:B:LEU:HA	5	0.5
(1,2130)	1:185:B:LEU:HD23	1:185:B:LEU:HA	9	0.5
(1,2130)	1:185:B:LEU:HD22	1:185:B:LEU:HA	10	0.5
(1,2129)	1:185:A:LEU:HD23	1:185:A:LEU:HA	1	0.5
(1,2129)	1:185:A:LEU:HD23	1:185:A:LEU:HA	2	0.5
(1,2129)	1:185:A:LEU:HD21	1:185:A:LEU:HA	4	0.5
(1,2129)	1:185:A:LEU:HD23	1:185:A:LEU:HA	5	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2129)	1:185:A:LEU:HD22	1:185:A:LEU:HA	10	0.5
(1,2127)	1:185:A:LEU:HD13	1:178:B:PRO:HB2	2	0.5
(1,2127)	1:185:A:LEU:HD12	1:189:A:ASN:HB2	6	0.5
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD13	5	0.5
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD11	1	0.5
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD13	5	0.5
(1,2054)	1:199:B:GLN:H	1:199:B:GLN:HB3	2	0.5
(1,2054)	1:199:B:GLN:H	1:199:B:GLN:HB3	5	0.5
(1,2054)	1:199:B:GLN:H	1:199:B:GLN:HB3	6	0.5
(1,2054)	1:199:B:GLN:H	1:199:B:GLN:HB3	8	0.5
(1,2053)	1:199:A:GLN:H	1:199:A:GLN:HB3	2	0.5
(1,2053)	1:199:A:GLN:H	1:199:A:GLN:HB3	5	0.5
(1,2053)	1:199:A:GLN:H	1:199:A:GLN:HB3	6	0.5
(1,2053)	1:199:A:GLN:H	1:199:A:GLN:HB3	8	0.5
(1,2053)	1:199:A:GLN:H	1:199:A:GLN:HB3	10	0.5
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG11	5	0.5
(1,1732)	1:195:B:ALA:H	1:198:B:ARG:HD3	10	0.5
(1,1558)	1:173:B:GLN:HE21	1:200:A:VAL:HG12	4	0.5
(1,1554)	1:173:B:GLN:HE21	1:175:B:LEU:HB3	8	0.5
(1,1471)	1:208:A:TRP:HE1	1:208:A:TRP:HB2	3	0.5
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD12	9	0.5
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD12	9	0.5
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD12	5	0.5
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG13	9	0.5
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG13	9	0.5
(1,1106)	1:176:B:THR:HG22	1:179:B:TRP:HD1	4	0.5
(1,1105)	1:176:A:THR:HG22	1:179:A:TRP:HD1	4	0.5
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD13	5	0.5
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD13	10	0.5
(1,832)	1:182:B:ILE:HG22	1:179:B:TRP:HA	1	0.5
(1,832)	1:182:B:ILE:HG23	1:179:B:TRP:HA	4	0.5
(1,394)	1:176:B:THR:H	1:175:B:LEU:HB2	3	0.5
(1,393)	1:176:A:THR:H	1:175:A:LEU:HB2	3	0.5
(1,295)	1:185:A:LEU:HD23	1:182:B:ILE:HD12	7	0.5
(1,295)	1:185:A:LEU:HD22	1:182:B:ILE:HD13	9	0.5
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD21	1	0.5
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD21	1	0.5
(1,122)	1:199:B:GLN:H	1:198:B:ARG:HG2	5	0.5
(1,121)	1:199:A:GLN:H	1:198:A:ARG:HG2	5	0.5
(1,121)	1:199:A:GLN:H	1:198:A:ARG:HG2	6	0.5
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG23	3	0.5
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG23	3	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG22	6	0.5
(1,54)	1:195:B:ALA:HB3	1:199:B:GLN:H	8	0.5
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG22	7	0.5
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG22	7	0.5
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG13	4	0.5
(1,2873)	1:204:A:LEU:H	1:182:B:ILE:HD12	8	0.49
(1,2862)	1:173:A:GLN:H	1:212:A:LYS:HG2	6	0.49
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD22	7	0.49
(1,2841)	1:179:A:TRP:H	1:185:B:LEU:HD23	10	0.49
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB2	6	0.49
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB2	6	0.49
(1,2776)	1:193:B:ASP:H	1:195:B:ALA:HB3	5	0.49
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD21	10	0.49
(1,2740)	1:196:B:ALA:H	1:197:B:VAL:HB	1	0.49
(1,2740)	1:196:B:ALA:H	1:197:B:VAL:HB	5	0.49
(1,2739)	1:196:A:ALA:H	1:197:A:VAL:HB	1	0.49
(1,2739)	1:196:A:ALA:H	1:197:A:VAL:HB	6	0.49
(1,2562)	1:209:B:SER:H	1:206:B:LYS:HG3	7	0.49
(1,2561)	1:209:A:SER:H	1:206:A:LYS:HG3	7	0.49
(1,2544)	1:185:B:LEU:H	1:185:A:LEU:HD23	6	0.49
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD11	5	0.49
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD13	6	0.49
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD11	5	0.49
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD13	6	0.49
(1,2406)	1:179:B:TRP:HA	1:182:B:ILE:HG12	1	0.49
(1,2402)	1:208:B:TRP:HA	1:203:A:ARG:HB3	4	0.49
(1,2401)	1:208:A:TRP:HA	1:203:B:ARG:HB3	3	0.49
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG13	2	0.49
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG13	2	0.49
(1,2372)	1:186:B:LEU:HD12	1:177:A:VAL:H	6	0.49
(1,2372)	1:186:B:LEU:HD11	1:177:A:VAL:H	9	0.49
(1,2360)	1:200:B:VAL:HG13	1:175:A:LEU:H	1	0.49
(1,2360)	1:200:B:VAL:HG12	1:175:A:LEU:H	3	0.49
(1,2359)	1:200:A:VAL:HG13	1:175:B:LEU:H	1	0.49
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD12	7	0.49
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD12	7	0.49
(1,2298)	1:200:B:VAL:HG11	1:197:B:VAL:HA	6	0.49
(1,2297)	1:200:A:VAL:HG11	1:197:A:VAL:HA	6	0.49
(1,2227)	1:208:A:TRP:HA	1:179:A:TRP:HH2	3	0.49
(1,2166)	1:189:B:ASN:HB3	1:185:B:LEU:HG	3	0.49
(1,2165)	1:189:A:ASN:HB3	1:185:A:LEU:HG	3	0.49
(1,2165)	1:189:A:ASN:HB3	1:185:A:LEU:HG	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2165)	1:189:A:ASN:HB3	1:185:A:LEU:HG	9	0.49
(1,2130)	1:185:B:LEU:HD23	1:185:B:LEU:HA	6	0.49
(1,2130)	1:185:B:LEU:HD23	1:185:B:LEU:HA	8	0.49
(1,2129)	1:185:A:LEU:HD23	1:185:A:LEU:HA	6	0.49
(1,2129)	1:185:A:LEU:HD23	1:185:A:LEU:HA	8	0.49
(1,2129)	1:185:A:LEU:HD23	1:185:A:LEU:HA	9	0.49
(1,2094)	1:185:B:LEU:HD21	1:181:A:ASP:H	9	0.49
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD11	1	0.49
(1,2075)	1:210:A:LEU:HD12	1:211:B:ALA:H	4	0.49
(1,2054)	1:199:B:GLN:H	1:199:B:GLN:HB3	1	0.49
(1,2053)	1:199:A:GLN:H	1:199:A:GLN:HB3	1	0.49
(1,2020)	1:205:B:GLN:HE22	1:179:B:TRP:HD1	10	0.49
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG11	5	0.49
(1,1738)	1:195:B:ALA:H	1:194:B:GLN:HB3	10	0.49
(1,1731)	1:195:A:ALA:H	1:198:A:ARG:HD3	10	0.49
(1,1472)	1:208:B:TRP:HE1	1:208:B:TRP:HB2	3	0.49
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD12	5	0.49
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD23	2	0.49
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD23	2	0.49
(1,1298)	1:191:B:GLU:H	1:187:B:LYS:HG3	1	0.49
(1,1297)	1:191:A:GLU:H	1:187:A:LYS:HG3	1	0.49
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG13	10	0.49
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG13	10	0.49
(1,1050)	1:212:B:LYS:HB3	1:212:B:LYS:HE3	5	0.49
(1,1049)	1:212:A:LYS:HB3	1:212:A:LYS:HE3	5	0.49
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD12	9	0.49
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD13	10	0.49
(1,972)	1:204:B:LEU:HD23	1:182:A:ILE:HD12	10	0.49
(1,832)	1:182:B:ILE:HG22	1:179:B:TRP:HA	6	0.49
(1,831)	1:182:A:ILE:HG22	1:179:A:TRP:HA	1	0.49
(1,831)	1:182:A:ILE:HG22	1:179:A:TRP:HA	6	0.49
(1,772)	1:173:B:GLN:HA	1:173:B:GLN:HG3	6	0.49
(1,771)	1:173:A:GLN:HA	1:173:A:GLN:HG3	6	0.49
(1,398)	1:175:B:LEU:HB2	1:190:A:PHE:HZ	9	0.49
(1,394)	1:176:B:THR:H	1:175:B:LEU:HB2	6	0.49
(1,393)	1:176:A:THR:H	1:175:A:LEU:HB2	6	0.49
(1,393)	1:176:A:THR:H	1:175:A:LEU:HB2	8	0.49
(1,348)	1:202:B:GLU:H	1:202:B:GLU:HG2	2	0.49
(1,348)	1:202:B:GLU:H	1:202:B:GLU:HG2	8	0.49
(1,347)	1:202:A:GLU:H	1:202:A:GLU:HG2	2	0.49
(1,347)	1:202:A:GLU:H	1:202:A:GLU:HG2	8	0.49
(1,296)	1:185:B:LEU:HD23	1:182:A:ILE:HD12	7	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,262)	1:175:B:LEU:HD12	1:199:A:GLN:HG3	4	0.49
(1,254)	1:175:B:LEU:HD13	1:196:A:ALA:HA	5	0.49
(1,253)	1:175:A:LEU:HD12	1:196:B:ALA:HA	4	0.49
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG22	10	0.49
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG22	10	0.49
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG21	9	0.49
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG21	9	0.49
(1,51)	1:195:A:ALA:HB3	1:194:A:GLN:H	1	0.49
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG13	4	0.49
(1,2873)	1:204:A:LEU:H	1:182:B:ILE:HD12	6	0.48
(1,2842)	1:179:B:TRP:H	1:185:A:LEU:HD23	10	0.48
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB2	4	0.48
(1,2775)	1:193:A:ASP:H	1:195:A:ALA:HB3	5	0.48
(1,2740)	1:196:B:ALA:H	1:197:B:VAL:HB	6	0.48
(1,2740)	1:196:B:ALA:H	1:197:B:VAL:HB	9	0.48
(1,2670)	1:202:B:GLU:H	1:179:B:TRP:HZ3	4	0.48
(1,2670)	1:202:B:GLU:H	1:179:B:TRP:HZ3	5	0.48
(1,2669)	1:202:A:GLU:H	1:179:A:TRP:HZ3	4	0.48
(1,2580)	1:208:B:TRP:HE1	1:175:B:LEU:HD11	6	0.48
(1,2579)	1:208:A:TRP:HE1	1:175:A:LEU:HD11	6	0.48
(1,2578)	1:208:B:TRP:HE1	1:204:A:LEU:HD21	3	0.48
(1,2574)	1:208:B:TRP:HE1	1:203:A:ARG:HD2	3	0.48
(1,2562)	1:209:B:SER:H	1:206:B:LYS:HG3	1	0.48
(1,2561)	1:209:A:SER:H	1:206:A:LYS:HG3	1	0.48
(1,2561)	1:209:A:SER:H	1:206:A:LYS:HG3	5	0.48
(1,2543)	1:185:A:LEU:H	1:185:B:LEU:HD23	6	0.48
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD12	3	0.48
(1,2405)	1:179:A:TRP:HA	1:182:A:ILE:HG12	1	0.48
(1,2404)	1:183:B:GLU:HA	1:201:B:MET:HB2	4	0.48
(1,2403)	1:183:A:GLU:HA	1:201:A:MET:HB2	4	0.48
(1,2395)	1:207:A:GLY:HA3	1:206:A:LYS:HG2	9	0.48
(1,2228)	1:208:B:TRP:HA	1:179:B:TRP:HH2	3	0.48
(1,2166)	1:189:B:ASN:HB3	1:185:B:LEU:HG	6	0.48
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD21	9	0.48
(1,2128)	1:185:B:LEU:HD11	1:178:A:PRO:HB2	1	0.48
(1,2128)	1:185:B:LEU:HD13	1:178:A:PRO:HB2	2	0.48
(1,2128)	1:185:B:LEU:HD12	1:189:B:ASN:HB2	6	0.48
(1,2127)	1:185:A:LEU:HD11	1:178:B:PRO:HB2	1	0.48
(1,2082)	1:175:B:LEU:HD21	1:190:A:PHE:HZ	1	0.48
(1,2081)	1:175:A:LEU:HD21	1:190:B:PHE:HZ	1	0.48
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD11	8	0.48
(1,1737)	1:195:A:ALA:H	1:194:A:GLN:HB3	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD11	7	0.48
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD11	7	0.48
(1,1200)	1:203:B:ARG:HD3	1:212:A:LYS:HA	5	0.48
(1,1199)	1:203:A:ARG:HD3	1:212:B:LYS:HA	5	0.48
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG12	6	0.48
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG12	1	0.48
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG12	9	0.48
(1,522)	1:190:B:PHE:H	1:191:B:GLU:HA	7	0.48
(1,398)	1:175:B:LEU:HB2	1:190:A:PHE:HZ	6	0.48
(1,394)	1:176:B:THR:H	1:175:B:LEU:HB2	8	0.48
(1,296)	1:185:B:LEU:HD22	1:182:A:ILE:HD11	8	0.48
(1,295)	1:185:A:LEU:HD22	1:182:B:ILE:HD12	5	0.48
(1,262)	1:175:B:LEU:HD13	1:199:A:GLN:HG3	1	0.48
(1,261)	1:175:A:LEU:HD13	1:199:B:GLN:HG3	1	0.48
(1,194)	1:201:B:MET:HE2	1:182:B:ILE:HD11	5	0.48
(1,193)	1:201:A:MET:HE2	1:182:A:ILE:HD11	5	0.48
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG22	7	0.48
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG22	7	0.48
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD12	6	0.48
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD12	6	0.48
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG22	5	0.48
(1,52)	1:195:B:ALA:HB3	1:194:B:GLN:H	1	0.48
(1,52)	1:195:B:ALA:HB1	1:194:B:GLN:H	9	0.48
(1,51)	1:195:A:ALA:HB1	1:194:A:GLN:H	9	0.48
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG13	7	0.48
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG13	7	0.48
(1,2874)	1:204:B:LEU:H	1:182:B:ILE:HD12	1	0.47
(1,2874)	1:204:B:LEU:H	1:182:A:ILE:HD13	2	0.47
(1,2873)	1:204:A:LEU:H	1:182:A:ILE:HD12	1	0.47
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD21	5	0.47
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD22	3	0.47
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD21	5	0.47
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD23	10	0.47
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB2	4	0.47
(1,2740)	1:196:B:ALA:H	1:197:B:VAL:HB	7	0.47
(1,2739)	1:196:A:ALA:H	1:197:A:VAL:HB	9	0.47
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD11	8	0.47
(1,2669)	1:202:A:GLU:H	1:179:A:TRP:HZ3	5	0.47
(1,2577)	1:208:A:TRP:HE1	1:204:B:LEU:HD21	3	0.47
(1,2573)	1:208:A:TRP:HE1	1:203:B:ARG:HD2	3	0.47
(1,2562)	1:209:B:SER:H	1:206:B:LYS:HG3	5	0.47
(1,2544)	1:185:B:LEU:H	1:185:A:LEU:HD23	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2543)	1:185:A:LEU:H	1:185:B:LEU:HD23	9	0.47
(1,2541)	1:185:A:LEU:H	1:186:A:LEU:HD22	2	0.47
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD12	3	0.47
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG13	3	0.47
(1,2396)	1:207:B:GLY:HA3	1:206:B:LYS:HG2	9	0.47
(1,2381)	1:182:A:ILE:HD11	1:186:B:LEU:H	10	0.47
(1,2371)	1:186:A:LEU:HD12	1:177:B:VAL:H	6	0.47
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD11	10	0.47
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD11	10	0.47
(1,2332)	1:212:B:LYS:HB3	1:211:B:ALA:H	2	0.47
(1,2332)	1:212:B:LYS:HB3	1:211:B:ALA:H	3	0.47
(1,2331)	1:212:A:LYS:HB3	1:211:A:ALA:H	2	0.47
(1,2331)	1:212:A:LYS:HB3	1:211:A:ALA:H	3	0.47
(1,2231)	1:187:A:LYS:H	1:197:A:VAL:HA	1	0.47
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD21	9	0.47
(1,2093)	1:185:A:LEU:HD21	1:181:B:ASP:H	9	0.47
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD11	8	0.47
(1,2019)	1:205:A:GLN:HE22	1:179:A:TRP:HD1	10	0.47
(1,1781)	1:175:A:LEU:H	1:177:A:VAL:HG23	10	0.47
(1,1678)	1:199:B:GLN:HE22	1:198:B:ARG:HD3	4	0.47
(1,1572)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	2	0.47
(1,1572)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	5	0.47
(1,1572)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	6	0.47
(1,1571)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	5	0.47
(1,1571)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	6	0.47
(1,1571)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	10	0.47
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG12	1	0.47
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG12	6	0.47
(1,1074)	1:192:B:ASN:H	1:187:B:LYS:HG3	4	0.47
(1,1073)	1:192:A:ASN:H	1:187:A:LYS:HG3	4	0.47
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD12	9	0.47
(1,915)	1:199:A:GLN:HG2	1:175:B:LEU:HD12	6	0.47
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG12	9	0.47
(1,521)	1:190:A:PHE:H	1:191:A:GLU:HA	7	0.47
(1,352)	1:203:B:ARG:H	1:202:B:GLU:HG2	9	0.47
(1,351)	1:203:A:ARG:H	1:202:A:GLU:HG2	9	0.47
(1,312)	1:173:B:GLN:HB2	1:173:B:GLN:H	7	0.47
(1,311)	1:173:A:GLN:HB2	1:173:A:GLN:H	7	0.47
(1,296)	1:185:B:LEU:HD22	1:182:A:ILE:HD12	5	0.47
(1,296)	1:185:B:LEU:HD22	1:182:A:ILE:HD11	6	0.47
(1,295)	1:185:A:LEU:HD22	1:182:B:ILE:HD12	2	0.47
(1,225)	1:177:A:VAL:HG21	1:200:B:VAL:HG12	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG21	1	0.47
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG22	8	0.47
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG21	1	0.47
(1,113)	1:173:A:GLN:HE21	1:175:A:LEU:HD11	4	0.47
(1,110)	1:210:B:LEU:HD12	1:212:A:LYS:H	2	0.47
(1,110)	1:210:B:LEU:HD12	1:212:A:LYS:H	10	0.47
(1,109)	1:210:A:LEU:HD12	1:212:B:LYS:H	2	0.47
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD13	5	0.47
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG21	1	0.47
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG21	1	0.47
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG22	5	0.47
(1,52)	1:195:B:ALA:HB2	1:194:B:GLN:H	6	0.47
(1,51)	1:195:A:ALA:HB1	1:194:A:GLN:H	3	0.47
(1,51)	1:195:A:ALA:HB2	1:194:A:GLN:H	6	0.47
(1,2863)	1:173:B:GLN:H	1:203:A:ARG:HG3	1	0.46
(1,2856)	1:174:B:GLU:H	1:196:A:ALA:HB3	3	0.46
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD22	3	0.46
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD22	8	0.46
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD23	10	0.46
(1,2740)	1:196:B:ALA:H	1:197:B:VAL:HB	3	0.46
(1,2739)	1:196:A:ALA:H	1:197:A:VAL:HB	3	0.46
(1,2739)	1:196:A:ALA:H	1:197:A:VAL:HB	7	0.46
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD12	2	0.46
(1,2670)	1:202:B:GLU:H	1:179:B:TRP:HZ3	2	0.46
(1,2669)	1:202:A:GLU:H	1:179:A:TRP:HZ3	2	0.46
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD13	4	0.46
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD13	4	0.46
(1,2582)	1:179:B:TRP:HE1	1:204:A:LEU:HG	1	0.46
(1,2581)	1:179:A:TRP:HE1	1:204:B:LEU:HG	1	0.46
(1,2573)	1:208:A:TRP:HE1	1:203:B:ARG:HD2	9	0.46
(1,2542)	1:185:B:LEU:H	1:186:B:LEU:HD22	2	0.46
(1,2474)	1:190:B:PHE:H	1:193:B:ASP:H	5	0.46
(1,2473)	1:190:A:PHE:H	1:193:A:ASP:H	5	0.46
(1,2416)	1:189:B:ASN:HA	1:186:B:LEU:HA	2	0.46
(1,2415)	1:189:A:ASN:HA	1:186:A:LEU:HA	2	0.46
(1,2407)	1:197:A:VAL:HA	1:196:A:ALA:HA	2	0.46
(1,2381)	1:182:A:ILE:HD13	1:186:B:LEU:H	9	0.46
(1,2298)	1:200:B:VAL:HG12	1:197:B:VAL:HA	2	0.46
(1,2297)	1:200:A:VAL:HG12	1:197:A:VAL:HA	2	0.46
(1,2232)	1:187:B:LYS:H	1:197:B:VAL:HA	1	0.46
(1,2228)	1:208:B:TRP:HA	1:179:B:TRP:HH2	4	0.46
(1,2227)	1:208:A:TRP:HA	1:179:A:TRP:HH2	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2173)	1:203:A:ARG:HD2	1:208:B:TRP:HZ3	8	0.46
(1,2128)	1:185:B:LEU:HD13	1:189:B:ASN:HB2	5	0.46
(1,2127)	1:185:A:LEU:HD13	1:189:A:ASN:HB2	5	0.46
(1,2076)	1:210:B:LEU:HD12	1:211:A:ALA:H	4	0.46
(1,1814)	1:192:B:ASN:H	1:191:B:GLU:HB3	7	0.46
(1,1813)	1:192:A:ASN:H	1:191:A:GLU:HB3	7	0.46
(1,1782)	1:175:B:LEU:H	1:177:B:VAL:HG23	10	0.46
(1,1572)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	3	0.46
(1,1572)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	4	0.46
(1,1572)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	8	0.46
(1,1572)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	9	0.46
(1,1572)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	10	0.46
(1,1571)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	2	0.46
(1,1571)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	3	0.46
(1,1571)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	4	0.46
(1,1571)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	8	0.46
(1,1571)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	9	0.46
(1,1466)	1:208:B:TRP:HE1	1:173:B:GLN:H	9	0.46
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB1	2	0.46
(1,1183)	1:199:A:GLN:HA	1:175:B:LEU:HD11	6	0.46
(1,1172)	1:209:B:SER:HB3	1:210:B:LEU:HD22	6	0.46
(1,1145)	1:211:A:ALA:HA	1:206:B:LYS:HE3	2	0.46
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG11	5	0.46
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG11	5	0.46
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG21	8	0.46
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG22	3	0.46
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG12	10	0.46
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG12	10	0.46
(1,716)	1:175:B:LEU:HA	1:200:A:VAL:HG11	10	0.46
(1,715)	1:175:A:LEU:HA	1:200:B:VAL:HG11	10	0.46
(1,296)	1:185:B:LEU:HD21	1:182:A:ILE:HD11	10	0.46
(1,226)	1:177:B:VAL:HG21	1:200:A:VAL:HG12	10	0.46
(1,180)	1:196:B:ALA:HB1	1:197:B:VAL:HA	2	0.46
(1,179)	1:196:A:ALA:HB1	1:197:A:VAL:HA	2	0.46
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG21	5	0.46
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG22	8	0.46
(1,136)	1:189:B:ASN:HD21	1:185:B:LEU:HD21	6	0.46
(1,135)	1:189:A:ASN:HD21	1:185:A:LEU:HD21	6	0.46
(1,114)	1:173:B:GLN:HE21	1:175:B:LEU:HD11	4	0.46
(1,109)	1:210:A:LEU:HD11	1:212:B:LYS:H	6	0.46
(1,109)	1:210:A:LEU:HD12	1:212:B:LYS:H	10	0.46
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD13	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:195:B:ALA:HB1	1:194:B:GLN:H	3	0.46
(1,2864)	1:173:A:GLN:H	1:203:B:ARG:HG3	1	0.45
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD22	8	0.45
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB1	2	0.45
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB3	8	0.45
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB1	2	0.45
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB3	8	0.45
(1,2772)	1:175:B:LEU:H	1:190:A:PHE:HZ	3	0.45
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD11	8	0.45
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD13	7	0.45
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD13	7	0.45
(1,2574)	1:208:B:TRP:HE1	1:203:A:ARG:HD2	4	0.45
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG13	3	0.45
(1,2416)	1:189:B:ASN:HA	1:186:B:LEU:HA	5	0.45
(1,2408)	1:197:B:VAL:HA	1:196:B:ALA:HA	2	0.45
(1,2408)	1:197:B:VAL:HA	1:196:B:ALA:HA	5	0.45
(1,2408)	1:197:B:VAL:HA	1:194:B:GLN:HA	9	0.45
(1,2407)	1:197:A:VAL:HA	1:196:A:ALA:HA	5	0.45
(1,2407)	1:197:A:VAL:HA	1:194:A:GLN:HA	9	0.45
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG13	3	0.45
(1,2382)	1:182:B:ILE:HD11	1:186:A:LEU:H	10	0.45
(1,2298)	1:197:B:VAL:HA	1:186:B:LEU:HB2	9	0.45
(1,2297)	1:197:A:VAL:HA	1:186:A:LEU:HB2	9	0.45
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD22	7	0.45
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD22	7	0.45
(1,2232)	1:187:B:LYS:H	1:197:B:VAL:HA	5	0.45
(1,2231)	1:187:A:LYS:H	1:197:A:VAL:HA	5	0.45
(1,2165)	1:189:A:ASN:HB3	1:185:A:LEU:HG	10	0.45
(1,2128)	1:185:B:LEU:HD13	1:178:A:PRO:HB2	9	0.45
(1,2125)	1:186:A:LEU:HD13	1:178:B:PRO:HG2	6	0.45
(1,2125)	1:186:A:LEU:HD13	1:178:B:PRO:HG2	10	0.45
(1,2094)	1:185:B:LEU:HD21	1:181:A:ASP:H	6	0.45
(1,2093)	1:185:A:LEU:HD21	1:181:B:ASP:H	3	0.45
(1,2093)	1:185:A:LEU:HD21	1:181:B:ASP:H	6	0.45
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD13	6	0.45
(1,2075)	1:210:A:LEU:HD11	1:211:B:ALA:H	6	0.45
(1,1677)	1:199:A:GLN:HE22	1:198:A:ARG:HD3	4	0.45
(1,1465)	1:208:A:TRP:HE1	1:173:A:GLN:H	9	0.45
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD11	2	0.45
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD11	2	0.45
(1,1336)	1:188:B:ASN:H	1:187:B:LYS:HG3	1	0.45
(1,1335)	1:188:A:ASN:H	1:187:A:LYS:HG3	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1171)	1:209:A:SER:HB3	1:210:A:LEU:HD22	6	0.45
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG21	1	0.45
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG22	2	0.45
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG21	4	0.45
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG21	5	0.45
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG22	6	0.45
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG21	8	0.45
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG21	10	0.45
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG21	1	0.45
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG22	2	0.45
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG21	4	0.45
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG21	5	0.45
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG22	6	0.45
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG21	10	0.45
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG22	3	0.45
(1,832)	1:182:B:ILE:HG21	1:179:B:TRP:HA	3	0.45
(1,234)	1:200:B:VAL:HG12	1:177:A:VAL:HG21	10	0.45
(1,194)	1:201:B:MET:HE3	1:182:B:ILE:HD11	2	0.45
(1,193)	1:201:A:MET:HE3	1:182:A:ILE:HD11	2	0.45
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG23	3	0.45
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG22	4	0.45
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG21	5	0.45
(1,122)	1:199:B:GLN:H	1:198:B:ARG:HG2	2	0.45
(1,122)	1:199:B:GLN:H	1:198:B:ARG:HG2	8	0.45
(1,121)	1:199:A:GLN:H	1:198:A:ARG:HG2	2	0.45
(1,121)	1:199:A:GLN:H	1:198:A:ARG:HG2	8	0.45
(1,110)	1:210:B:LEU:HD11	1:212:A:LYS:H	6	0.45
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG22	7	0.45
(1,2874)	1:204:B:LEU:H	1:182:A:ILE:HD12	6	0.44
(1,2873)	1:204:A:LEU:H	1:182:B:ILE:HD13	2	0.44
(1,2855)	1:174:A:GLU:H	1:196:B:ALA:HB3	3	0.44
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD23	1	0.44
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD23	1	0.44
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB2	9	0.44
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD21	8	0.44
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD12	2	0.44
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD11	6	0.44
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD11	6	0.44
(1,2573)	1:208:A:TRP:HE1	1:203:B:ARG:HD2	4	0.44
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD13	7	0.44
(1,2488)	1:180:B:ASP:H	1:178:B:PRO:HG2	7	0.44
(1,2487)	1:180:A:ASP:H	1:178:A:PRO:HG2	7	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2473)	1:190:A:PHE:H	1:193:A:ASP:H	4	0.44
(1,2415)	1:189:A:ASN:HA	1:186:A:LEU:HA	5	0.44
(1,2410)	1:197:B:VAL:HA	1:201:B:MET:HB2	2	0.44
(1,2409)	1:197:A:VAL:HA	1:201:A:MET:HB2	2	0.44
(1,2408)	1:197:B:VAL:HA	1:194:B:GLN:HA	7	0.44
(1,2408)	1:197:B:VAL:HA	1:196:B:ALA:HA	8	0.44
(1,2407)	1:197:A:VAL:HA	1:194:A:GLN:HA	7	0.44
(1,2407)	1:197:A:VAL:HA	1:196:A:ALA:HA	8	0.44
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG13	3	0.44
(1,2382)	1:182:B:ILE:HD12	1:186:A:LEU:H	7	0.44
(1,2382)	1:182:B:ILE:HD13	1:186:A:LEU:H	9	0.44
(1,2381)	1:182:A:ILE:HD12	1:186:B:LEU:H	7	0.44
(1,2371)	1:186:A:LEU:HD11	1:177:B:VAL:H	9	0.44
(1,2298)	1:200:B:VAL:HG11	1:197:B:VAL:HA	3	0.44
(1,2297)	1:200:A:VAL:HG11	1:197:A:VAL:HA	3	0.44
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD22	1	0.44
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD21	2	0.44
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD23	3	0.44
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD21	5	0.44
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD22	6	0.44
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD23	8	0.44
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD22	9	0.44
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD23	10	0.44
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD22	1	0.44
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD21	2	0.44
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD23	3	0.44
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD21	5	0.44
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD22	6	0.44
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD23	8	0.44
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD22	9	0.44
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD23	10	0.44
(1,2232)	1:187:B:LYS:H	1:197:B:VAL:HA	3	0.44
(1,2231)	1:187:A:LYS:H	1:197:A:VAL:HA	3	0.44
(1,2228)	1:208:B:TRP:HA	1:179:B:TRP:HH2	7	0.44
(1,2227)	1:208:A:TRP:HA	1:179:A:TRP:HH2	7	0.44
(1,2166)	1:189:B:ASN:HB3	1:185:B:LEU:HG	2	0.44
(1,2166)	1:189:B:ASN:HB3	1:185:B:LEU:HG	10	0.44
(1,2126)	1:186:B:LEU:HD13	1:178:A:PRO:HG2	10	0.44
(1,2094)	1:185:B:LEU:HD21	1:181:A:ASP:H	3	0.44
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD13	6	0.44
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD12	10	0.44
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD12	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB1	2	0.44
(1,1146)	1:211:B:ALA:HA	1:206:A:LYS:HE3	2	0.44
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG12	3	0.44
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG12	3	0.44
(1,1028)	1:178:B:PRO:HB2	1:186:A:LEU:HD13	7	0.44
(1,1027)	1:178:A:PRO:HB2	1:186:B:LEU:HD13	7	0.44
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG21	3	0.44
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG22	7	0.44
(1,936)	1:200:B:VAL:HA	1:200:B:VAL:HG22	9	0.44
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG21	3	0.44
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG22	7	0.44
(1,935)	1:200:A:VAL:HA	1:200:A:VAL:HG22	9	0.44
(1,859)	1:200:A:VAL:HA	1:175:B:LEU:HB3	6	0.44
(1,831)	1:182:A:ILE:HG21	1:179:A:TRP:HA	3	0.44
(1,352)	1:203:B:ARG:H	1:202:B:GLU:HG2	8	0.44
(1,351)	1:203:A:ARG:H	1:202:A:GLU:HG2	2	0.44
(1,351)	1:203:A:ARG:H	1:202:A:GLU:HG2	8	0.44
(1,348)	1:202:B:GLU:H	1:202:B:GLU:HG2	6	0.44
(1,347)	1:202:A:GLU:H	1:202:A:GLU:HG2	6	0.44
(1,296)	1:185:B:LEU:HD22	1:182:A:ILE:HD12	2	0.44
(1,254)	1:175:B:LEU:HD12	1:196:A:ALA:HA	4	0.44
(1,233)	1:200:A:VAL:HG12	1:177:B:VAL:HG21	10	0.44
(1,194)	1:201:B:MET:HE2	1:182:B:ILE:HD11	3	0.44
(1,193)	1:201:A:MET:HE2	1:182:A:ILE:HD11	3	0.44
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG23	3	0.44
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG22	4	0.44
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG22	6	0.44
(1,122)	1:199:B:GLN:H	1:198:B:ARG:HG2	1	0.44
(1,121)	1:199:A:GLN:H	1:198:A:ARG:HG2	1	0.44
(1,110)	1:210:B:LEU:HD11	1:212:A:LYS:H	9	0.44
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG22	7	0.44
(1,54)	1:195:B:ALA:HB1	1:199:B:GLN:H	2	0.44
(1,52)	1:195:B:ALA:HB2	1:194:B:GLN:H	2	0.44
(1,51)	1:195:A:ALA:HB2	1:194:A:GLN:H	2	0.44
(1,32)	1:201:B:MET:HE1	1:179:B:TRP:HZ3	9	0.44
(1,31)	1:201:A:MET:HE1	1:179:A:TRP:HZ3	9	0.44
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG21	5	0.44
(1,2864)	1:173:A:GLN:H	1:203:B:ARG:HG3	9	0.43
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB2	9	0.43
(1,2740)	1:196:B:ALA:H	1:197:B:VAL:HB	2	0.43
(1,2740)	1:196:B:ALA:H	1:197:B:VAL:HB	10	0.43
(1,2739)	1:196:A:ALA:H	1:197:A:VAL:HB	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2739)	1:196:A:ALA:H	1:197:A:VAL:HB	10	0.43
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD13	7	0.43
(1,2474)	1:190:B:PHE:H	1:193:B:ASP:H	4	0.43
(1,2450)	1:184:B:ALA:H	1:187:B:LYS:HE2	7	0.43
(1,2449)	1:184:A:ALA:H	1:187:A:LYS:HE2	7	0.43
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG12	5	0.43
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG12	5	0.43
(1,2396)	1:207:B:GLY:HA3	1:206:B:LYS:HG2	6	0.43
(1,2395)	1:207:A:GLY:HA3	1:206:A:LYS:HG2	6	0.43
(1,2394)	1:211:B:ALA:HA	1:207:A:GLY:HA2	3	0.43
(1,2372)	1:186:B:LEU:HD12	1:177:A:VAL:H	10	0.43
(1,2370)	1:175:B:LEU:HG	1:199:A:GLN:HE22	3	0.43
(1,2360)	1:200:B:VAL:HG12	1:175:A:LEU:H	4	0.43
(1,2298)	1:200:B:VAL:HG11	1:197:B:VAL:HA	4	0.43
(1,2297)	1:200:A:VAL:HG11	1:197:A:VAL:HA	4	0.43
(1,2282)	1:199:B:GLN:HA	1:199:B:GLN:HB2	5	0.43
(1,2282)	1:199:B:GLN:HA	1:199:B:GLN:HB2	7	0.43
(1,2281)	1:199:A:GLN:HA	1:199:A:GLN:HB2	5	0.43
(1,2281)	1:199:A:GLN:HA	1:199:A:GLN:HB2	7	0.43
(1,2246)	1:204:B:LEU:HB2	1:204:B:LEU:HD21	4	0.43
(1,2245)	1:204:A:LEU:HB2	1:204:A:LEU:HD21	4	0.43
(1,2232)	1:187:B:LYS:H	1:197:B:VAL:HA	6	0.43
(1,2231)	1:187:A:LYS:H	1:197:A:VAL:HA	6	0.43
(1,2166)	1:189:B:ASN:HB3	1:185:B:LEU:HG	1	0.43
(1,2166)	1:189:B:ASN:HB3	1:185:B:LEU:HG	4	0.43
(1,2165)	1:189:A:ASN:HB3	1:185:A:LEU:HG	1	0.43
(1,2165)	1:189:A:ASN:HB3	1:185:A:LEU:HG	2	0.43
(1,2126)	1:186:B:LEU:HD11	1:178:A:PRO:HG2	2	0.43
(1,2126)	1:186:B:LEU:HD13	1:178:A:PRO:HG2	6	0.43
(1,2096)	1:175:B:LEU:HD11	1:199:A:GLN:HE22	2	0.43
(1,2095)	1:175:A:LEU:HD11	1:199:B:GLN:HE22	2	0.43
(1,2094)	1:185:B:LEU:HD22	1:181:A:ASP:H	7	0.43
(1,2093)	1:185:A:LEU:HD22	1:181:B:ASP:H	7	0.43
(1,2093)	1:185:A:LEU:HD21	1:181:B:ASP:H	8	0.43
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD12	9	0.43
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD12	9	0.43
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD12	6	0.43
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD12	5	0.43
(1,1592)	1:205:B:GLN:H	1:205:B:GLN:HG3	9	0.43
(1,1591)	1:205:A:GLN:H	1:205:A:GLN:HG3	9	0.43
(1,1584)	1:173:B:GLN:HE21	1:200:A:VAL:HA	3	0.43
(1,1583)	1:173:A:GLN:HE21	1:200:B:VAL:HA	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD13	1	0.43
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD13	4	0.43
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD11	5	0.43
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD13	1	0.43
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD13	4	0.43
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD11	5	0.43
(1,1262)	1:176:B:THR:HG21	1:177:B:VAL:HB	3	0.43
(1,1261)	1:176:A:THR:HG21	1:177:A:VAL:HB	3	0.43
(1,1184)	1:199:B:GLN:HA	1:175:A:LEU:HD11	6	0.43
(1,1172)	1:209:B:SER:HB3	1:210:B:LEU:HD22	8	0.43
(1,1171)	1:209:A:SER:HB3	1:210:A:LEU:HD22	8	0.43
(1,916)	1:199:B:GLN:HG2	1:175:A:LEU:HD12	6	0.43
(1,786)	1:205:B:GLN:HA	1:205:B:GLN:HG2	9	0.43
(1,785)	1:205:A:GLN:HA	1:205:A:GLN:HG2	9	0.43
(1,421)	1:196:A:ALA:H	1:193:A:ASP:HB2	2	0.43
(1,397)	1:175:A:LEU:HB2	1:190:B:PHE:HZ	4	0.43
(1,352)	1:203:B:ARG:H	1:202:B:GLU:HG2	2	0.43
(1,352)	1:203:B:ARG:H	1:202:B:GLU:HG2	3	0.43
(1,352)	1:203:B:ARG:H	1:202:B:GLU:HG2	6	0.43
(1,351)	1:203:A:ARG:H	1:202:A:GLU:HG2	3	0.43
(1,348)	1:202:B:GLU:H	1:202:B:GLU:HG2	10	0.43
(1,347)	1:202:A:GLU:H	1:202:A:GLU:HG2	1	0.43
(1,347)	1:202:A:GLU:H	1:202:A:GLU:HG2	10	0.43
(1,295)	1:185:A:LEU:HD22	1:182:B:ILE:HD12	3	0.43
(1,295)	1:185:A:LEU:HD22	1:182:B:ILE:HD11	6	0.43
(1,295)	1:185:A:LEU:HD21	1:182:B:ILE:HD11	10	0.43
(1,180)	1:196:B:ALA:HB1	1:197:B:VAL:HA	3	0.43
(1,179)	1:196:A:ALA:HB1	1:197:A:VAL:HA	3	0.43
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG22	2	0.43
(1,148)	1:185:B:LEU:H	1:182:B:ILE:HG21	6	0.43
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG22	2	0.43
(1,147)	1:185:A:LEU:H	1:182:A:ILE:HG21	6	0.43
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG22	8	0.43
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG22	6	0.43
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG22	8	0.43
(1,53)	1:195:A:ALA:HB1	1:199:A:GLN:H	2	0.43
(1,51)	1:195:A:ALA:HB1	1:194:A:GLN:H	8	0.43
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG21	5	0.43
(1,2786)	1:190:B:PHE:H	1:186:B:LEU:HD22	4	0.42
(1,2785)	1:190:A:PHE:H	1:186:A:LEU:HD22	4	0.42
(1,2771)	1:175:A:LEU:H	1:190:B:PHE:HZ	3	0.42
(1,2670)	1:202:B:GLU:H	1:179:B:TRP:HZ3	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2670)	1:202:B:GLU:H	1:179:B:TRP:HZ3	8	0.42
(1,2669)	1:202:A:GLU:H	1:179:A:TRP:HZ3	3	0.42
(1,2669)	1:202:A:GLU:H	1:179:A:TRP:HZ3	8	0.42
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD11	3	0.42
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD11	3	0.42
(1,2574)	1:208:B:TRP:HE1	1:203:A:ARG:HD2	9	0.42
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD13	2	0.42
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD13	9	0.42
(1,2408)	1:197:B:VAL:HA	1:194:B:GLN:HA	1	0.42
(1,2407)	1:197:A:VAL:HA	1:194:A:GLN:HA	1	0.42
(1,2393)	1:211:A:ALA:HA	1:207:B:GLY:HA2	3	0.42
(1,2371)	1:186:A:LEU:HD13	1:177:B:VAL:H	8	0.42
(1,2334)	1:208:B:TRP:HB2	1:208:B:TRP:HD1	9	0.42
(1,2333)	1:208:A:TRP:HB2	1:208:A:TRP:HD1	9	0.42
(1,2297)	1:200:A:VAL:HG11	1:197:A:VAL:HA	8	0.42
(1,2282)	1:202:B:GLU:HB2	1:199:B:GLN:HA	4	0.42
(1,2232)	1:187:B:LYS:H	1:197:B:VAL:HA	2	0.42
(1,2232)	1:187:B:LYS:H	1:197:B:VAL:HA	4	0.42
(1,2231)	1:187:A:LYS:H	1:197:A:VAL:HA	2	0.42
(1,2231)	1:187:A:LYS:H	1:197:A:VAL:HA	4	0.42
(1,2165)	1:189:A:ASN:HB3	1:185:A:LEU:HG	4	0.42
(1,2127)	1:185:A:LEU:HD13	1:178:B:PRO:HB2	9	0.42
(1,2125)	1:186:A:LEU:HD11	1:178:B:PRO:HG2	2	0.42
(1,2094)	1:185:B:LEU:HD21	1:181:A:ASP:H	8	0.42
(1,2076)	1:210:B:LEU:HD11	1:211:A:ALA:H	6	0.42
(1,2076)	1:210:B:LEU:HD11	1:211:A:ALA:H	9	0.42
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD11	9	0.42
(1,1677)	1:199:A:GLN:HE22	1:198:A:ARG:HD3	2	0.42
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD23	1	0.42
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD23	1	0.42
(1,1190)	1:188:B:ASN:HA	1:191:B:GLU:HA	7	0.42
(1,1189)	1:188:A:ASN:HA	1:191:A:GLU:HA	7	0.42
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG11	8	0.42
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG11	8	0.42
(1,1074)	1:192:B:ASN:H	1:187:B:LYS:HG3	9	0.42
(1,1073)	1:192:A:ASN:H	1:187:A:LYS:HG3	8	0.42
(1,916)	1:199:B:GLN:HG2	1:175:A:LEU:HD13	9	0.42
(1,860)	1:200:B:VAL:HA	1:175:A:LEU:HB3	6	0.42
(1,842)	1:177:B:VAL:HG12	1:178:B:PRO:HD3	8	0.42
(1,841)	1:177:A:VAL:HG12	1:178:A:PRO:HD3	8	0.42
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG11	2	0.42
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG11	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,422)	1:196:B:ALA:H	1:193:B:ASP:HB2	2	0.42
(1,422)	1:196:B:ALA:H	1:193:B:ASP:HB2	3	0.42
(1,421)	1:196:A:ALA:H	1:193:A:ASP:HB2	3	0.42
(1,352)	1:203:B:ARG:H	1:202:B:GLU:HG2	1	0.42
(1,352)	1:203:B:ARG:H	1:202:B:GLU:HG2	7	0.42
(1,352)	1:203:B:ARG:H	1:202:B:GLU:HG2	10	0.42
(1,351)	1:203:A:ARG:H	1:202:A:GLU:HG2	1	0.42
(1,351)	1:203:A:ARG:H	1:202:A:GLU:HG2	6	0.42
(1,351)	1:203:A:ARG:H	1:202:A:GLU:HG2	7	0.42
(1,348)	1:202:B:GLU:H	1:202:B:GLU:HG2	1	0.42
(1,348)	1:202:B:GLU:H	1:202:B:GLU:HG2	4	0.42
(1,347)	1:202:A:GLU:H	1:202:A:GLU:HG2	5	0.42
(1,320)	1:173:B:GLN:HG3	1:173:B:GLN:H	4	0.42
(1,319)	1:173:A:GLN:HG3	1:173:A:GLN:H	4	0.42
(1,296)	1:185:B:LEU:HD22	1:182:A:ILE:HD11	1	0.42
(1,296)	1:185:B:LEU:HD22	1:182:A:ILE:HD12	3	0.42
(1,295)	1:185:A:LEU:HD22	1:182:B:ILE:HD11	1	0.42
(1,180)	1:196:B:ALA:HB1	1:197:B:VAL:HA	1	0.42
(1,180)	1:196:B:ALA:HB2	1:197:B:VAL:HA	4	0.42
(1,180)	1:196:B:ALA:HB2	1:197:B:VAL:HA	6	0.42
(1,180)	1:196:B:ALA:HB3	1:197:B:VAL:HA	8	0.42
(1,180)	1:196:B:ALA:HB1	1:197:B:VAL:HA	10	0.42
(1,179)	1:196:A:ALA:HB1	1:197:A:VAL:HA	1	0.42
(1,179)	1:196:A:ALA:HB2	1:197:A:VAL:HA	4	0.42
(1,179)	1:196:A:ALA:HB2	1:197:A:VAL:HA	6	0.42
(1,179)	1:196:A:ALA:HB3	1:197:A:VAL:HA	8	0.42
(1,179)	1:196:A:ALA:HB1	1:197:A:VAL:HA	10	0.42
(1,110)	1:210:B:LEU:HD11	1:212:A:LYS:H	1	0.42
(1,109)	1:210:A:LEU:HD11	1:212:B:LYS:H	1	0.42
(1,109)	1:210:A:LEU:HD11	1:212:B:LYS:H	9	0.42
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG23	2	0.42
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG22	2	0.42
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG22	10	0.42
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG22	2	0.42
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG22	10	0.42
(1,2874)	1:204:B:LEU:H	1:182:B:ILE:HD13	3	0.41
(1,2873)	1:204:A:LEU:H	1:182:A:ILE:HD13	3	0.41
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD21	8	0.41
(1,2709)	1:199:A:GLN:HE22	1:175:B:LEU:HA	6	0.41
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD11	6	0.41
(1,2694)	1:201:B:MET:H	1:179:B:TRP:HZ3	7	0.41
(1,2693)	1:201:A:MET:H	1:179:A:TRP:HZ3	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2686)	1:203:B:ARG:H	1:203:B:ARG:HG3	1	0.41
(1,2686)	1:203:B:ARG:H	1:203:B:ARG:HG3	6	0.41
(1,2686)	1:203:B:ARG:H	1:203:B:ARG:HG3	7	0.41
(1,2685)	1:203:A:ARG:H	1:203:A:ARG:HG3	1	0.41
(1,2685)	1:203:A:ARG:H	1:203:A:ARG:HG3	6	0.41
(1,2685)	1:203:A:ARG:H	1:203:A:ARG:HG3	7	0.41
(1,2650)	1:188:B:ASN:HD22	1:178:A:PRO:HG3	10	0.41
(1,2633)	1:173:A:GLN:HE21	1:203:B:ARG:HG3	8	0.41
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD11	1	0.41
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD11	1	0.41
(1,2562)	1:209:B:SER:H	1:206:B:LYS:HG3	3	0.41
(1,2561)	1:209:A:SER:H	1:206:A:LYS:HG3	3	0.41
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD13	2	0.41
(1,2507)	1:176:A:THR:H	1:200:B:VAL:HG12	10	0.41
(1,2446)	1:187:B:LYS:H	1:187:B:LYS:HG2	1	0.41
(1,2445)	1:187:A:LYS:H	1:187:A:LYS:HG2	1	0.41
(1,2416)	1:189:B:ASN:HA	1:186:B:LEU:HA	1	0.41
(1,2415)	1:189:A:ASN:HA	1:186:A:LEU:HA	1	0.41
(1,2408)	1:197:B:VAL:HA	1:194:B:GLN:HA	6	0.41
(1,2371)	1:186:A:LEU:HD12	1:177:B:VAL:H	10	0.41
(1,2334)	1:208:B:TRP:HB2	1:208:B:TRP:HD1	10	0.41
(1,2333)	1:208:A:TRP:HB2	1:208:A:TRP:HD1	10	0.41
(1,2321)	1:197:A:VAL:HG12	1:187:A:LYS:HG3	5	0.41
(1,2298)	1:200:B:VAL:HG11	1:197:B:VAL:HA	8	0.41
(1,2281)	1:202:A:GLU:HB2	1:199:A:GLN:HA	4	0.41
(1,2166)	1:189:B:ASN:HB3	1:185:B:LEU:HG	8	0.41
(1,2165)	1:189:A:ASN:HB3	1:185:A:LEU:HG	8	0.41
(1,2128)	1:185:B:LEU:HD13	1:178:A:PRO:HB2	7	0.41
(1,2127)	1:185:A:LEU:HD12	1:189:A:ASN:HB2	7	0.41
(1,2126)	1:186:B:LEU:HD13	1:178:A:PRO:HG2	5	0.41
(1,2082)	1:175:B:LEU:HD21	1:190:A:PHE:HZ	5	0.41
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD13	4	0.41
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD13	4	0.41
(1,2075)	1:210:A:LEU:HD11	1:211:B:ALA:H	9	0.41
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD12	5	0.41
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD12	6	0.41
(1,1794)	1:193:B:ASP:H	1:188:B:ASN:HA	9	0.41
(1,1793)	1:193:A:ASP:H	1:188:A:ASN:HA	9	0.41
(1,1694)	1:189:B:ASN:HD22	1:182:A:ILE:HD11	10	0.41
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD13	7	0.41
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD13	7	0.41
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG11	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	1:192:B:ASN:H	1:187:B:LYS:HG3	8	0.41
(1,1073)	1:192:A:ASN:H	1:187:A:LYS:HG3	9	0.41
(1,832)	1:182:B:ILE:HG23	1:179:B:TRP:HA	7	0.41
(1,831)	1:182:A:ILE:HG23	1:179:A:TRP:HA	7	0.41
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG11	6	0.41
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG11	6	0.41
(1,422)	1:196:B:ALA:H	1:193:B:ASP:HB2	6	0.41
(1,421)	1:196:A:ALA:H	1:193:A:ASP:HB2	6	0.41
(1,398)	1:175:B:LEU:HB2	1:190:A:PHE:HZ	1	0.41
(1,397)	1:175:A:LEU:HB2	1:190:B:PHE:HZ	1	0.41
(1,352)	1:203:B:ARG:H	1:202:B:GLU:HG2	4	0.41
(1,352)	1:203:B:ARG:H	1:202:B:GLU:HG2	5	0.41
(1,351)	1:203:A:ARG:H	1:202:A:GLU:HG2	4	0.41
(1,351)	1:203:A:ARG:H	1:202:A:GLU:HG2	5	0.41
(1,351)	1:203:A:ARG:H	1:202:A:GLU:HG2	10	0.41
(1,348)	1:202:B:GLU:H	1:202:B:GLU:HG2	5	0.41
(1,347)	1:202:A:GLU:H	1:202:A:GLU:HG2	4	0.41
(1,218)	1:210:B:LEU:HD12	1:211:A:ALA:HA	2	0.41
(1,217)	1:210:A:LEU:HD12	1:211:B:ALA:HA	2	0.41
(1,182)	1:196:B:ALA:HB3	1:193:B:ASP:HB2	4	0.41
(1,181)	1:196:A:ALA:HB3	1:193:A:ASP:HB2	4	0.41
(1,180)	1:196:B:ALA:HB2	1:197:B:VAL:HA	9	0.41
(1,179)	1:196:A:ALA:HB2	1:197:A:VAL:HA	9	0.41
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG22	5	0.41
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG23	2	0.41
(1,52)	1:195:B:ALA:HB3	1:194:B:GLN:H	5	0.41
(1,52)	1:195:B:ALA:HB1	1:194:B:GLN:H	8	0.41
(1,51)	1:195:A:ALA:HB3	1:194:A:GLN:H	5	0.41
(1,2870)	1:209:B:SER:H	1:206:B:LYS:HE3	2	0.4
(1,2869)	1:209:A:SER:H	1:206:A:LYS:HE3	2	0.4
(1,2863)	1:173:B:GLN:H	1:203:A:ARG:HG3	9	0.4
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD22	9	0.4
(1,2711)	1:199:A:GLN:HE22	1:195:A:ALA:HA	2	0.4
(1,2686)	1:203:B:ARG:H	1:203:B:ARG:HG3	2	0.4
(1,2686)	1:203:B:ARG:H	1:203:B:ARG:HG3	3	0.4
(1,2686)	1:203:B:ARG:H	1:203:B:ARG:HG3	4	0.4
(1,2686)	1:203:B:ARG:H	1:203:B:ARG:HG3	5	0.4
(1,2686)	1:203:B:ARG:H	1:203:B:ARG:HG3	8	0.4
(1,2686)	1:203:B:ARG:H	1:203:B:ARG:HG3	9	0.4
(1,2685)	1:203:A:ARG:H	1:203:A:ARG:HG3	2	0.4
(1,2685)	1:203:A:ARG:H	1:203:A:ARG:HG3	3	0.4
(1,2685)	1:203:A:ARG:H	1:203:A:ARG:HG3	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2685)	1:203:A:ARG:H	1:203:A:ARG:HG3	5	0.4
(1,2685)	1:203:A:ARG:H	1:203:A:ARG:HG3	8	0.4
(1,2685)	1:203:A:ARG:H	1:203:A:ARG:HG3	9	0.4
(1,2650)	1:188:B:ASN:HD22	1:178:A:PRO:HG3	9	0.4
(1,2634)	1:173:B:GLN:HE21	1:203:A:ARG:HG3	8	0.4
(1,2508)	1:176:B:THR:H	1:200:A:VAL:HG12	10	0.4
(1,2446)	1:187:B:LYS:H	1:187:B:LYS:HG2	10	0.4
(1,2445)	1:187:A:LYS:H	1:187:A:LYS:HG2	9	0.4
(1,2445)	1:187:A:LYS:H	1:187:A:LYS:HG2	10	0.4
(1,2407)	1:197:A:VAL:HA	1:194:A:GLN:HA	6	0.4
(1,2369)	1:175:A:LEU:HG	1:199:B:GLN:HE22	3	0.4
(1,2359)	1:200:A:VAL:HG12	1:175:B:LEU:H	4	0.4
(1,2334)	1:208:B:TRP:HB2	1:208:B:TRP:HD1	4	0.4
(1,2334)	1:208:B:TRP:HB2	1:208:B:TRP:HD1	5	0.4
(1,2334)	1:208:B:TRP:HB2	1:208:B:TRP:HD1	6	0.4
(1,2334)	1:208:B:TRP:HB2	1:208:B:TRP:HD1	7	0.4
(1,2334)	1:208:B:TRP:HB2	1:208:B:TRP:HD1	8	0.4
(1,2333)	1:208:A:TRP:HB2	1:208:A:TRP:HD1	4	0.4
(1,2333)	1:208:A:TRP:HB2	1:208:A:TRP:HD1	5	0.4
(1,2333)	1:208:A:TRP:HB2	1:208:A:TRP:HD1	6	0.4
(1,2333)	1:208:A:TRP:HB2	1:208:A:TRP:HD1	7	0.4
(1,2333)	1:208:A:TRP:HB2	1:208:A:TRP:HD1	8	0.4
(1,2322)	1:197:B:VAL:HG12	1:187:B:LYS:HG3	5	0.4
(1,2231)	1:187:A:LYS:H	1:197:A:VAL:HA	10	0.4
(1,2125)	1:186:A:LEU:HD13	1:178:B:PRO:HG2	5	0.4
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG21	3	0.4
(1,2076)	1:210:B:LEU:HD11	1:211:A:ALA:H	1	0.4
(1,2076)	1:210:B:LEU:HD12	1:211:A:ALA:H	5	0.4
(1,1978)	1:174:B:GLU:H	1:200:A:VAL:HG13	7	0.4
(1,1977)	1:174:A:GLU:H	1:200:B:VAL:HG13	7	0.4
(1,1678)	1:199:B:GLN:HE22	1:198:B:ARG:HD3	2	0.4
(1,1583)	1:173:A:GLN:HE21	1:200:B:VAL:HA	3	0.4
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD23	9	0.4
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD23	9	0.4
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG12	2	0.4
(1,1114)	1:200:B:VAL:H	1:197:B:VAL:HG11	4	0.4
(1,1113)	1:200:A:VAL:H	1:197:A:VAL:HG12	2	0.4
(1,942)	1:175:B:LEU:HD23	1:200:A:VAL:HG11	8	0.4
(1,941)	1:175:A:LEU:HD23	1:200:B:VAL:HG11	8	0.4
(1,918)	1:173:B:GLN:HG2	1:175:B:LEU:HD13	1	0.4
(1,831)	1:182:A:ILE:HG22	1:179:A:TRP:HA	5	0.4
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG13	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG13	5	0.4
(1,421)	1:196:A:ALA:H	1:193:A:ASP:HB2	10	0.4
(1,348)	1:202:B:GLU:H	1:202:B:GLU:HG2	3	0.4
(1,280)	1:187:B:LYS:HG3	1:187:B:LYS:HE2	9	0.4
(1,279)	1:187:A:LYS:HG3	1:187:A:LYS:HE2	7	0.4
(1,279)	1:187:A:LYS:HG3	1:187:A:LYS:HE2	9	0.4
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG22	5	0.4
(1,34)	1:205:B:GLN:HE22	1:201:B:MET:HE2	6	0.4
(1,33)	1:205:A:GLN:HE22	1:201:A:MET:HE2	6	0.4
(1,2762)	1:175:B:LEU:H	1:175:B:LEU:HD11	4	0.39
(1,2761)	1:175:A:LEU:H	1:175:A:LEU:HD11	4	0.39
(1,2712)	1:199:B:GLN:HE22	1:195:B:ALA:HA	2	0.39
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD13	9	0.39
(1,2581)	1:179:A:TRP:HE1	1:204:B:LEU:HG	9	0.39
(1,2556)	1:209:B:SER:H	1:204:B:LEU:HA	1	0.39
(1,2555)	1:209:A:SER:H	1:204:A:LEU:HA	1	0.39
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD13	9	0.39
(1,2446)	1:187:B:LYS:H	1:187:B:LYS:HG2	2	0.39
(1,2446)	1:187:B:LYS:H	1:187:B:LYS:HG2	3	0.39
(1,2446)	1:187:B:LYS:H	1:187:B:LYS:HG2	7	0.39
(1,2446)	1:187:B:LYS:H	1:187:B:LYS:HG2	9	0.39
(1,2445)	1:187:A:LYS:H	1:187:A:LYS:HG2	2	0.39
(1,2445)	1:187:A:LYS:H	1:187:A:LYS:HG2	7	0.39
(1,2416)	1:189:B:ASN:HA	1:186:B:LEU:HA	9	0.39
(1,2415)	1:189:A:ASN:HA	1:186:A:LEU:HA	9	0.39
(1,2410)	1:197:B:VAL:HA	1:201:B:MET:HB2	4	0.39
(1,2409)	1:197:A:VAL:HA	1:201:A:MET:HB2	4	0.39
(1,2408)	1:197:B:VAL:HA	1:194:B:GLN:HA	4	0.39
(1,2407)	1:197:A:VAL:HA	1:194:A:GLN:HA	4	0.39
(1,2372)	1:186:B:LEU:HD13	1:177:A:VAL:H	8	0.39
(1,2334)	1:208:B:TRP:HB2	1:208:B:TRP:HD1	1	0.39
(1,2334)	1:208:B:TRP:HB2	1:208:B:TRP:HD1	2	0.39
(1,2333)	1:208:A:TRP:HB2	1:208:A:TRP:HD1	1	0.39
(1,2333)	1:208:A:TRP:HB2	1:208:A:TRP:HD1	2	0.39
(1,2232)	1:187:B:LYS:H	1:197:B:VAL:HA	10	0.39
(1,2188)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	1	0.39
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG21	3	0.39
(1,2075)	1:210:A:LEU:HD11	1:211:B:ALA:H	1	0.39
(1,2075)	1:210:A:LEU:HD12	1:211:B:ALA:H	5	0.39
(1,2075)	1:210:A:LEU:HD12	1:211:B:ALA:H	10	0.39
(1,1998)	1:191:B:GLU:H	1:186:B:LEU:HD11	7	0.39
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD11	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD12	7	0.39
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD12	7	0.39
(1,1437)	1:211:A:ALA:H	1:203:B:ARG:HE	10	0.39
(1,1424)	1:181:B:ASP:H	1:182:B:ILE:HD13	8	0.39
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD22	4	0.39
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD22	4	0.39
(1,1171)	1:209:A:SER:HB3	1:210:A:LEU:HD22	4	0.39
(1,1116)	1:175:B:LEU:HD21	1:199:A:GLN:H	8	0.39
(1,1105)	1:176:A:THR:HG21	1:179:A:TRP:HD1	9	0.39
(1,1072)	1:175:B:LEU:HD13	1:201:A:MET:H	8	0.39
(1,917)	1:173:A:GLN:HG2	1:175:A:LEU:HD13	1	0.39
(1,841)	1:177:A:VAL:HG12	1:178:A:PRO:HD3	7	0.39
(1,832)	1:182:B:ILE:HG23	1:179:B:TRP:HA	2	0.39
(1,832)	1:182:B:ILE:HG22	1:179:B:TRP:HA	5	0.39
(1,831)	1:182:A:ILE:HG23	1:179:A:TRP:HA	2	0.39
(1,684)	1:211:B:ALA:HA	1:210:A:LEU:HD12	3	0.39
(1,683)	1:211:A:ALA:HA	1:210:B:LEU:HD12	3	0.39
(1,422)	1:196:B:ALA:H	1:193:B:ASP:HB2	10	0.39
(1,347)	1:202:A:GLU:H	1:202:A:GLU:HG2	3	0.39
(1,280)	1:187:B:LYS:HG3	1:187:B:LYS:HE2	7	0.39
(1,78)	1:200:B:VAL:HG12	1:208:A:TRP:HZ3	3	0.39
(1,77)	1:200:A:VAL:HG12	1:208:B:TRP:HZ3	3	0.39
(1,30)	1:201:B:MET:HE1	1:179:B:TRP:HE3	10	0.39
(1,29)	1:201:A:MET:HE1	1:179:A:TRP:HE3	10	0.39
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG13	8	0.39
(1,2698)	1:201:B:MET:H	1:182:A:ILE:HD11	6	0.38
(1,2697)	1:201:A:MET:H	1:182:B:ILE:HD13	9	0.38
(1,2623)	1:206:A:LYS:H	1:206:A:LYS:HG3	7	0.38
(1,2562)	1:209:B:SER:H	1:206:B:LYS:HG3	6	0.38
(1,2561)	1:209:A:SER:H	1:206:A:LYS:HG3	6	0.38
(1,2556)	1:209:B:SER:H	1:204:B:LEU:HA	3	0.38
(1,2555)	1:209:A:SER:H	1:204:A:LEU:HA	3	0.38
(1,2555)	1:209:A:SER:H	1:204:A:LEU:HA	7	0.38
(1,2446)	1:187:B:LYS:H	1:187:B:LYS:HG2	8	0.38
(1,2445)	1:187:A:LYS:H	1:187:A:LYS:HG2	3	0.38
(1,2445)	1:187:A:LYS:H	1:187:A:LYS:HG2	8	0.38
(1,2321)	1:197:A:VAL:HG13	1:187:A:LYS:HG3	6	0.38
(1,2187)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	1	0.38
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD23	2	0.38
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD23	2	0.38
(1,2094)	1:185:B:LEU:HD21	1:181:A:ASP:H	5	0.38
(1,2094)	1:185:B:LEU:HD23	1:181:A:ASP:H	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2093)	1:185:A:LEU:HD21	1:181:B:ASP:H	5	0.38
(1,2093)	1:185:A:LEU:HD23	1:181:B:ASP:H	10	0.38
(1,2081)	1:175:A:LEU:HD21	1:190:B:PHE:HZ	5	0.38
(1,2081)	1:175:A:LEU:HD23	1:190:B:PHE:HZ	10	0.38
(1,2076)	1:210:B:LEU:HD12	1:211:A:ALA:H	10	0.38
(1,2052)	1:192:B:ASN:HD22	1:192:B:ASN:H	1	0.38
(1,2051)	1:192:A:ASN:HD22	1:192:A:ASN:H	1	0.38
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD11	9	0.38
(1,1782)	1:175:B:LEU:H	1:177:B:VAL:HG21	9	0.38
(1,1781)	1:175:A:LEU:H	1:177:A:VAL:HG21	9	0.38
(1,1693)	1:189:A:ASN:HD22	1:182:B:ILE:HD11	10	0.38
(1,1630)	1:203:B:ARG:H	1:179:B:TRP:HZ3	7	0.38
(1,1584)	1:173:B:GLN:HE21	1:200:A:VAL:HA	4	0.38
(1,1438)	1:211:B:ALA:H	1:203:A:ARG:HE	10	0.38
(1,1423)	1:181:A:ASP:H	1:182:A:ILE:HD13	8	0.38
(1,1414)	1:212:B:LYS:H	1:210:A:LEU:HD13	8	0.38
(1,1413)	1:212:A:LYS:H	1:210:B:LEU:HD13	8	0.38
(1,1196)	1:188:B:ASN:HA	1:191:B:GLU:HB2	9	0.38
(1,1195)	1:188:A:ASN:HA	1:191:A:GLU:HB2	9	0.38
(1,1172)	1:209:B:SER:HB3	1:210:B:LEU:HD22	4	0.38
(1,1115)	1:175:A:LEU:HD21	1:199:B:GLN:H	8	0.38
(1,1106)	1:176:B:THR:HG21	1:179:B:TRP:HD1	9	0.38
(1,1073)	1:192:A:ASN:H	1:187:A:LYS:HG3	2	0.38
(1,1071)	1:175:A:LEU:HD13	1:201:B:MET:H	8	0.38
(1,882)	1:192:B:ASN:HB3	1:191:B:GLU:HA	7	0.38
(1,881)	1:192:A:ASN:HB3	1:191:A:GLU:HA	7	0.38
(1,874)	1:185:B:LEU:HD13	1:188:B:ASN:HB2	1	0.38
(1,873)	1:185:A:LEU:HD13	1:188:A:ASN:HB2	1	0.38
(1,842)	1:177:B:VAL:HG12	1:178:B:PRO:HD3	4	0.38
(1,842)	1:177:B:VAL:HG12	1:178:B:PRO:HD3	7	0.38
(1,841)	1:177:A:VAL:HG12	1:178:A:PRO:HD3	4	0.38
(1,407)	1:185:A:LEU:HB2	1:186:A:LEU:H	2	0.38
(1,407)	1:185:A:LEU:HB2	1:186:A:LEU:H	6	0.38
(1,398)	1:175:B:LEU:HB2	1:190:A:PHE:HZ	4	0.38
(1,180)	1:196:B:ALA:HB3	1:197:B:VAL:HA	5	0.38
(1,179)	1:196:A:ALA:HB3	1:197:A:VAL:HA	5	0.38
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG21	9	0.38
(1,110)	1:210:B:LEU:HD12	1:212:A:LYS:H	5	0.38
(1,109)	1:210:A:LEU:HD12	1:212:B:LYS:H	5	0.38
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG22	8	0.38
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG23	3	0.38
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG22	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG11	5	0.38
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG13	8	0.38
(1,2768)	1:175:B:LEU:H	1:173:B:GLN:HB3	2	0.37
(1,2740)	1:196:B:ALA:H	1:197:B:VAL:HB	4	0.37
(1,2722)	1:189:B:ASN:HD22	1:178:A:PRO:HG2	4	0.37
(1,2710)	1:199:B:GLN:HE22	1:175:A:LEU:HA	6	0.37
(1,2649)	1:188:A:ASN:HD22	1:178:B:PRO:HG3	9	0.37
(1,2649)	1:188:A:ASN:HD22	1:178:B:PRO:HG3	10	0.37
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD12	5	0.37
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD12	5	0.37
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD13	8	0.37
(1,2624)	1:206:B:LYS:H	1:206:B:LYS:HG3	2	0.37
(1,2624)	1:206:B:LYS:H	1:206:B:LYS:HG3	7	0.37
(1,2624)	1:206:B:LYS:H	1:206:B:LYS:HG3	10	0.37
(1,2623)	1:206:A:LYS:H	1:206:A:LYS:HG3	2	0.37
(1,2623)	1:206:A:LYS:H	1:206:A:LYS:HG3	10	0.37
(1,2586)	1:179:B:TRP:HE1	1:205:B:GLN:HA	7	0.37
(1,2585)	1:179:A:TRP:HE1	1:205:A:GLN:HA	7	0.37
(1,2582)	1:179:B:TRP:HE1	1:204:A:LEU:HG	6	0.37
(1,2582)	1:179:B:TRP:HE1	1:204:A:LEU:HG	9	0.37
(1,2556)	1:209:B:SER:H	1:204:B:LEU:HA	7	0.37
(1,2555)	1:209:A:SER:H	1:204:A:LEU:HA	2	0.37
(1,2512)	1:176:B:THR:H	1:174:B:GLU:HB3	5	0.37
(1,2511)	1:176:A:THR:H	1:174:A:GLU:HB3	5	0.37
(1,2473)	1:190:A:PHE:H	1:193:A:ASP:H	2	0.37
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD21	7	0.37
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD21	7	0.37
(1,2416)	1:189:B:ASN:HA	1:186:B:LEU:HA	6	0.37
(1,2416)	1:189:B:ASN:HA	1:186:B:LEU:HA	8	0.37
(1,2416)	1:189:B:ASN:HA	1:186:B:LEU:HA	10	0.37
(1,2415)	1:189:A:ASN:HA	1:186:A:LEU:HA	6	0.37
(1,2415)	1:189:A:ASN:HA	1:186:A:LEU:HA	8	0.37
(1,2415)	1:189:A:ASN:HA	1:186:A:LEU:HA	10	0.37
(1,2396)	1:207:B:GLY:HA3	1:206:B:LYS:HG2	4	0.37
(1,2395)	1:207:A:GLY:HA3	1:206:A:LYS:HG2	4	0.37
(1,2334)	1:208:B:TRP:HB2	1:208:B:TRP:HD1	3	0.37
(1,2333)	1:208:A:TRP:HB2	1:208:A:TRP:HD1	3	0.37
(1,2322)	1:197:B:VAL:HG13	1:187:B:LYS:HG3	6	0.37
(1,2282)	1:202:B:GLU:HB2	1:199:B:GLN:HA	3	0.37
(1,2281)	1:202:A:GLU:HB2	1:199:A:GLN:HA	3	0.37
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD11	3	0.37
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD11	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD13	2	0.37
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD13	8	0.37
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD13	2	0.37
(1,1793)	1:193:A:ASP:H	1:188:A:ASN:HA	2	0.37
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG13	8	0.37
(1,1629)	1:203:A:ARG:H	1:179:A:TRP:HZ3	7	0.37
(1,1456)	1:209:B:SER:H	1:208:B:TRP:HB2	7	0.37
(1,1455)	1:209:A:SER:H	1:208:A:TRP:HB2	7	0.37
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD22	10	0.37
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD22	10	0.37
(1,1336)	1:188:B:ASN:H	1:187:B:LYS:HG3	8	0.37
(1,1262)	1:176:B:THR:HG22	1:177:B:VAL:HB	1	0.37
(1,1262)	1:176:B:THR:HG21	1:177:B:VAL:HB	8	0.37
(1,1261)	1:176:A:THR:HG22	1:177:A:VAL:HB	1	0.37
(1,1184)	1:199:B:GLN:HA	1:175:A:LEU:HD12	8	0.37
(1,1183)	1:199:A:GLN:HA	1:175:B:LEU:HD12	8	0.37
(1,1146)	1:211:B:ALA:HA	1:206:A:LYS:HE3	8	0.37
(1,1145)	1:211:A:ALA:HA	1:206:B:LYS:HE3	8	0.37
(1,1074)	1:192:B:ASN:H	1:187:B:LYS:HG3	2	0.37
(1,1074)	1:192:B:ASN:H	1:187:B:LYS:HG3	3	0.37
(1,1073)	1:192:A:ASN:H	1:187:A:LYS:HG3	3	0.37
(1,1072)	1:175:B:LEU:HD13	1:201:A:MET:H	6	0.37
(1,1071)	1:175:A:LEU:HD13	1:201:B:MET:H	6	0.37
(1,918)	1:173:B:GLN:HG2	1:175:B:LEU:HD13	5	0.37
(1,917)	1:173:A:GLN:HG2	1:175:A:LEU:HD13	5	0.37
(1,917)	1:173:A:GLN:HG2	1:175:A:LEU:HD12	9	0.37
(1,882)	1:192:B:ASN:HB3	1:191:B:GLU:HA	1	0.37
(1,881)	1:192:A:ASN:HB3	1:191:A:GLU:HA	5	0.37
(1,842)	1:177:B:VAL:HG13	1:178:B:PRO:HD3	1	0.37
(1,842)	1:177:B:VAL:HG12	1:178:B:PRO:HD3	2	0.37
(1,842)	1:177:B:VAL:HG13	1:178:B:PRO:HD3	5	0.37
(1,842)	1:177:B:VAL:HG13	1:178:B:PRO:HD3	10	0.37
(1,841)	1:177:A:VAL:HG12	1:178:A:PRO:HD3	2	0.37
(1,841)	1:177:A:VAL:HG13	1:178:A:PRO:HD3	5	0.37
(1,841)	1:177:A:VAL:HG13	1:178:A:PRO:HD3	10	0.37
(1,408)	1:185:B:LEU:HB2	1:186:B:LEU:H	2	0.37
(1,408)	1:185:B:LEU:HB2	1:186:B:LEU:H	5	0.37
(1,408)	1:185:B:LEU:HB2	1:186:B:LEU:H	6	0.37
(1,407)	1:185:A:LEU:HB2	1:186:A:LEU:H	5	0.37
(1,309)	1:201:A:MET:HB2	1:202:A:GLU:H	10	0.37
(1,261)	1:175:A:LEU:HD13	1:199:B:GLN:HG3	9	0.37
(1,218)	1:210:B:LEU:HD12	1:211:A:ALA:HA	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:210:A:LEU:HD12	1:211:B:ALA:HA	4	0.37
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG21	9	0.37
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG21	4	0.37
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG21	4	0.37
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG11	8	0.37
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG11	8	0.37
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG23	3	0.37
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG11	5	0.37
(1,2861)	1:173:B:GLN:H	1:212:B:LYS:HG2	3	0.36
(1,2772)	1:175:B:LEU:H	1:190:A:PHE:HZ	7	0.36
(1,2767)	1:175:A:LEU:H	1:173:A:GLN:HB3	2	0.36
(1,2739)	1:196:A:ALA:H	1:197:A:VAL:HB	4	0.36
(1,2721)	1:189:A:ASN:HD22	1:178:B:PRO:HG2	4	0.36
(1,2688)	1:202:B:GLU:H	1:197:B:VAL:HA	3	0.36
(1,2687)	1:202:A:GLU:H	1:197:A:VAL:HA	3	0.36
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD13	8	0.36
(1,2624)	1:206:B:LYS:H	1:206:B:LYS:HG3	3	0.36
(1,2624)	1:206:B:LYS:H	1:206:B:LYS:HG3	5	0.36
(1,2624)	1:206:B:LYS:H	1:206:B:LYS:HG3	8	0.36
(1,2623)	1:206:A:LYS:H	1:206:A:LYS:HG3	3	0.36
(1,2623)	1:206:A:LYS:H	1:206:A:LYS:HG3	4	0.36
(1,2623)	1:206:A:LYS:H	1:206:A:LYS:HG3	5	0.36
(1,2623)	1:206:A:LYS:H	1:206:A:LYS:HG3	8	0.36
(1,2582)	1:179:B:TRP:HE1	1:204:A:LEU:HG	10	0.36
(1,2581)	1:179:A:TRP:HE1	1:204:B:LEU:HG	10	0.36
(1,2566)	1:208:B:TRP:HE1	1:208:B:TRP:HA	3	0.36
(1,2565)	1:208:A:TRP:HE1	1:208:A:TRP:HA	3	0.36
(1,2556)	1:209:B:SER:H	1:204:B:LEU:HA	2	0.36
(1,2474)	1:190:B:PHE:H	1:193:B:ASP:H	2	0.36
(1,2474)	1:190:B:PHE:H	1:193:B:ASP:H	8	0.36
(1,2473)	1:190:A:PHE:H	1:193:A:ASP:H	8	0.36
(1,2473)	1:190:A:PHE:H	1:193:A:ASP:H	9	0.36
(1,2446)	1:187:B:LYS:H	1:187:B:LYS:HG2	6	0.36
(1,2445)	1:187:A:LYS:H	1:187:A:LYS:HG2	5	0.36
(1,2445)	1:187:A:LYS:H	1:187:A:LYS:HG2	6	0.36
(1,2409)	1:197:A:VAL:HA	1:201:A:MET:HB2	5	0.36
(1,2408)	1:197:B:VAL:HA	1:194:B:GLN:HA	3	0.36
(1,2407)	1:197:A:VAL:HA	1:194:A:GLN:HA	3	0.36
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG12	8	0.36
(1,2330)	1:199:B:GLN:HG3	1:196:B:ALA:H	6	0.36
(1,2280)	1:194:B:GLN:HA	1:197:B:VAL:HB	2	0.36
(1,2279)	1:194:A:GLN:HA	1:197:A:VAL:HB	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2232)	1:187:B:LYS:H	1:197:B:VAL:HA	7	0.36
(1,2231)	1:187:A:LYS:H	1:197:A:VAL:HA	7	0.36
(1,2166)	1:189:B:ASN:HB3	1:185:B:LEU:HG	7	0.36
(1,2095)	1:175:A:LEU:HD13	1:199:B:GLN:HE22	10	0.36
(1,2082)	1:175:B:LEU:HD23	1:190:A:PHE:HZ	10	0.36
(1,2078)	1:189:B:ASN:H	1:186:B:LEU:HD13	10	0.36
(1,2077)	1:189:A:ASN:H	1:186:A:LEU:HD13	10	0.36
(1,2076)	1:210:B:LEU:HD13	1:211:A:ALA:H	7	0.36
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG13	7	0.36
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG13	7	0.36
(1,2022)	1:179:B:TRP:HE1	1:205:B:GLN:HE22	1	0.36
(1,2020)	1:205:B:GLN:HE22	1:179:B:TRP:HD1	2	0.36
(1,2019)	1:205:A:GLN:HE22	1:179:A:TRP:HD1	2	0.36
(1,1986)	1:173:A:GLN:H	1:175:A:LEU:HD11	6	0.36
(1,1985)	1:173:B:GLN:H	1:175:B:LEU:HD11	6	0.36
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD13	3	0.36
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD13	8	0.36
(1,1794)	1:193:B:ASP:H	1:188:B:ASN:HA	2	0.36
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG13	8	0.36
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG12	3	0.36
(1,1335)	1:188:A:ASN:H	1:187:A:LYS:HG3	8	0.36
(1,1261)	1:176:A:THR:HG21	1:177:A:VAL:HB	8	0.36
(1,1136)	1:188:B:ASN:HD22	1:188:B:ASN:HA	10	0.36
(1,1135)	1:188:A:ASN:HD22	1:188:A:ASN:HA	10	0.36
(1,1106)	1:176:B:THR:HG21	1:179:B:TRP:HD1	10	0.36
(1,1105)	1:176:A:THR:HG21	1:179:A:TRP:HD1	10	0.36
(1,1074)	1:192:B:ASN:H	1:187:B:LYS:HG3	6	0.36
(1,1053)	1:199:A:GLN:HG3	1:175:B:LEU:HD13	3	0.36
(1,976)	1:212:B:LYS:HB3	1:212:B:LYS:HA	9	0.36
(1,975)	1:212:A:LYS:HB3	1:212:A:LYS:HA	6	0.36
(1,975)	1:212:A:LYS:HB3	1:212:A:LYS:HA	9	0.36
(1,918)	1:173:B:GLN:HG2	1:175:B:LEU:HD12	9	0.36
(1,882)	1:192:B:ASN:HB3	1:191:B:GLU:HA	5	0.36
(1,881)	1:192:A:ASN:HB3	1:191:A:GLU:HA	1	0.36
(1,841)	1:177:A:VAL:HG13	1:178:A:PRO:HD3	1	0.36
(1,778)	1:206:B:LYS:HA	1:206:B:LYS:HB3	1	0.36
(1,778)	1:206:B:LYS:HA	1:206:B:LYS:HB3	2	0.36
(1,778)	1:206:B:LYS:HA	1:206:B:LYS:HB3	3	0.36
(1,778)	1:206:B:LYS:HA	1:206:B:LYS:HB3	4	0.36
(1,778)	1:206:B:LYS:HA	1:206:B:LYS:HB3	5	0.36
(1,778)	1:206:B:LYS:HA	1:206:B:LYS:HB3	6	0.36
(1,778)	1:206:B:LYS:HA	1:206:B:LYS:HB3	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:206:B:LYS:HA	1:206:B:LYS:HB3	8	0.36
(1,778)	1:206:B:LYS:HA	1:206:B:LYS:HB3	9	0.36
(1,778)	1:206:B:LYS:HA	1:206:B:LYS:HB3	10	0.36
(1,777)	1:206:A:LYS:HA	1:206:A:LYS:HB3	1	0.36
(1,777)	1:206:A:LYS:HA	1:206:A:LYS:HB3	2	0.36
(1,777)	1:206:A:LYS:HA	1:206:A:LYS:HB3	3	0.36
(1,777)	1:206:A:LYS:HA	1:206:A:LYS:HB3	4	0.36
(1,777)	1:206:A:LYS:HA	1:206:A:LYS:HB3	5	0.36
(1,777)	1:206:A:LYS:HA	1:206:A:LYS:HB3	6	0.36
(1,777)	1:206:A:LYS:HA	1:206:A:LYS:HB3	7	0.36
(1,777)	1:206:A:LYS:HA	1:206:A:LYS:HB3	8	0.36
(1,777)	1:206:A:LYS:HA	1:206:A:LYS:HB3	9	0.36
(1,777)	1:206:A:LYS:HA	1:206:A:LYS:HB3	10	0.36
(1,648)	1:195:B:ALA:HB2	1:198:B:ARG:HD3	1	0.36
(1,422)	1:196:B:ALA:H	1:193:B:ASP:HB2	8	0.36
(1,421)	1:196:A:ALA:H	1:193:A:ASP:HB2	8	0.36
(1,347)	1:202:A:GLU:H	1:202:A:GLU:HG2	7	0.36
(1,310)	1:201:B:MET:HB2	1:202:B:GLU:H	3	0.36
(1,310)	1:201:B:MET:HB2	1:202:B:GLU:H	10	0.36
(1,309)	1:201:A:MET:HB2	1:202:A:GLU:H	3	0.36
(1,262)	1:175:B:LEU:HD12	1:199:A:GLN:HG3	8	0.36
(1,261)	1:175:A:LEU:HD13	1:199:B:GLN:HG3	5	0.36
(1,261)	1:175:A:LEU:HD12	1:199:B:GLN:HG3	8	0.36
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG21	1	0.36
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG22	8	0.36
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG21	1	0.36
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG22	8	0.36
(1,26)	1:201:B:MET:HE3	1:179:B:TRP:HB3	6	0.36
(1,25)	1:201:A:MET:HE3	1:179:A:TRP:HB3	6	0.36
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG21	1	0.36
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG22	4	0.36
(1,18)	1:186:B:LEU:H	1:182:B:ILE:HG21	6	0.36
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG21	1	0.36
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG22	4	0.36
(1,17)	1:186:A:LEU:H	1:182:A:ILE:HG21	6	0.36
(1,2771)	1:175:A:LEU:H	1:190:B:PHE:HZ	6	0.35
(1,2771)	1:175:A:LEU:H	1:190:B:PHE:HZ	7	0.35
(1,2746)	1:195:B:ALA:H	1:196:B:ALA:HB2	4	0.35
(1,2745)	1:195:A:ALA:H	1:196:A:ALA:HB2	4	0.35
(1,2712)	1:199:B:GLN:HE22	1:195:B:ALA:HA	8	0.35
(1,2711)	1:199:A:GLN:HE22	1:195:A:ALA:HA	8	0.35
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD12	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD12	10	0.35
(1,2624)	1:206:B:LYS:H	1:206:B:LYS:HG3	1	0.35
(1,2624)	1:206:B:LYS:H	1:206:B:LYS:HG3	4	0.35
(1,2624)	1:206:B:LYS:H	1:206:B:LYS:HG3	9	0.35
(1,2623)	1:206:A:LYS:H	1:206:A:LYS:HG3	1	0.35
(1,2623)	1:206:A:LYS:H	1:206:A:LYS:HG3	9	0.35
(1,2581)	1:179:A:TRP:HE1	1:204:B:LEU:HG	6	0.35
(1,2562)	1:209:B:SER:H	1:206:B:LYS:HG3	4	0.35
(1,2561)	1:209:A:SER:H	1:206:A:LYS:HG3	4	0.35
(1,2474)	1:190:B:PHE:H	1:193:B:ASP:H	1	0.35
(1,2474)	1:190:B:PHE:H	1:193:B:ASP:H	9	0.35
(1,2473)	1:190:A:PHE:H	1:193:A:ASP:H	1	0.35
(1,2470)	1:204:B:LEU:H	1:179:B:TRP:HZ3	7	0.35
(1,2469)	1:204:A:LEU:H	1:179:A:TRP:HZ3	7	0.35
(1,2446)	1:187:B:LYS:H	1:187:B:LYS:HG2	5	0.35
(1,2416)	1:189:B:ASN:HA	1:186:B:LEU:HA	4	0.35
(1,2415)	1:189:A:ASN:HA	1:186:A:LEU:HA	4	0.35
(1,2410)	1:197:B:VAL:HA	1:201:B:MET:HB2	5	0.35
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG12	8	0.35
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG12	4	0.35
(1,2371)	1:186:A:LEU:HD13	1:177:B:VAL:H	2	0.35
(1,2369)	1:175:A:LEU:HG	1:199:B:GLN:HE22	10	0.35
(1,2359)	1:200:A:VAL:HG13	1:175:B:LEU:H	2	0.35
(1,2329)	1:199:A:GLN:HG3	1:196:A:ALA:H	6	0.35
(1,2322)	1:197:B:VAL:HG12	1:187:B:LYS:HG3	8	0.35
(1,2321)	1:197:A:VAL:HG12	1:187:A:LYS:HG3	8	0.35
(1,2180)	1:186:B:LEU:HB2	1:190:B:PHE:HD2	2	0.35
(1,2179)	1:186:A:LEU:HB2	1:190:A:PHE:HD2	6	0.35
(1,2165)	1:189:A:ASN:HB3	1:185:A:LEU:HG	7	0.35
(1,2128)	1:185:B:LEU:HD12	1:178:A:PRO:HB2	10	0.35
(1,2126)	1:186:B:LEU:HD12	1:178:A:PRO:HG2	9	0.35
(1,2096)	1:175:B:LEU:HD13	1:199:A:GLN:HE22	10	0.35
(1,2094)	1:185:B:LEU:HD22	1:181:A:ASP:H	4	0.35
(1,2075)	1:210:A:LEU:HD13	1:211:B:ALA:H	7	0.35
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG11	10	0.35
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG11	10	0.35
(1,1456)	1:209:B:SER:H	1:208:B:TRP:HB2	8	0.35
(1,1455)	1:209:A:SER:H	1:208:A:TRP:HB2	8	0.35
(1,1336)	1:188:B:ASN:H	1:187:B:LYS:HG3	7	0.35
(1,1336)	1:188:B:ASN:H	1:187:B:LYS:HG3	9	0.35
(1,1335)	1:188:A:ASN:H	1:187:A:LYS:HG3	7	0.35
(1,1335)	1:188:A:ASN:H	1:187:A:LYS:HG3	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1103)	1:179:A:TRP:HE1	1:176:A:THR:HG21	10	0.35
(1,1091)	1:199:A:GLN:HG2	1:173:B:GLN:HE21	7	0.35
(1,1073)	1:192:A:ASN:H	1:187:A:LYS:HG3	6	0.35
(1,976)	1:212:B:LYS:HB3	1:212:B:LYS:HA	6	0.35
(1,915)	1:199:A:GLN:HG2	1:175:B:LEU:HD13	9	0.35
(1,842)	1:177:B:VAL:HG12	1:178:B:PRO:HD3	6	0.35
(1,841)	1:177:A:VAL:HG12	1:178:A:PRO:HD3	6	0.35
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG11	1	0.35
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG11	1	0.35
(1,647)	1:195:A:ALA:HB2	1:198:A:ARG:HD3	1	0.35
(1,522)	1:190:B:PHE:H	1:191:B:GLU:HA	2	0.35
(1,521)	1:190:A:PHE:H	1:191:A:GLU:HA	2	0.35
(1,422)	1:196:B:ALA:H	1:193:B:ASP:HB2	1	0.35
(1,421)	1:196:A:ALA:H	1:193:A:ASP:HB2	1	0.35
(1,408)	1:185:B:LEU:HB2	1:186:B:LEU:H	4	0.35
(1,408)	1:185:B:LEU:HB2	1:186:B:LEU:H	7	0.35
(1,407)	1:185:A:LEU:HB2	1:186:A:LEU:H	4	0.35
(1,407)	1:185:A:LEU:HB2	1:186:A:LEU:H	7	0.35
(1,348)	1:202:B:GLU:H	1:202:B:GLU:HG2	7	0.35
(1,253)	1:175:A:LEU:HD13	1:196:B:ALA:HA	10	0.35
(1,229)	1:204:A:LEU:HD11	1:177:B:VAL:HG23	8	0.35
(1,93)	1:175:A:LEU:HD23	1:200:B:VAL:H	8	0.35
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG12	1	0.35
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG12	1	0.35
(1,54)	1:195:B:ALA:HB1	1:199:B:GLN:H	4	0.35
(1,53)	1:195:A:ALA:HB1	1:199:A:GLN:H	4	0.35
(1,34)	1:205:B:GLN:HE22	1:201:B:MET:HE3	5	0.35
(1,33)	1:205:A:GLN:HE22	1:201:A:MET:HE3	5	0.35
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG13	2	0.35
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG13	2	0.35
(1,2876)	1:205:B:GLN:H	1:177:B:VAL:HG21	8	0.34
(1,2875)	1:205:A:GLN:H	1:177:A:VAL:HG21	8	0.34
(1,2869)	1:209:A:SER:H	1:206:A:LYS:HE3	8	0.34
(1,2862)	1:173:A:GLN:H	1:212:A:LYS:HG2	3	0.34
(1,2711)	1:199:A:GLN:HE22	1:195:A:ALA:HA	5	0.34
(1,2710)	1:199:B:GLN:HE22	1:175:A:LEU:HA	9	0.34
(1,2688)	1:202:B:GLU:H	1:197:B:VAL:HA	2	0.34
(1,2687)	1:202:A:GLU:H	1:197:A:VAL:HA	2	0.34
(1,2628)	1:206:B:LYS:H	1:210:B:LEU:HD11	9	0.34
(1,2627)	1:206:A:LYS:H	1:210:A:LEU:HD11	9	0.34
(1,2624)	1:206:B:LYS:H	1:206:B:LYS:HG3	6	0.34
(1,2623)	1:206:A:LYS:H	1:206:A:LYS:HG3	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2562)	1:209:B:SER:H	1:206:B:LYS:HG3	9	0.34
(1,2561)	1:209:A:SER:H	1:206:A:LYS:HG3	9	0.34
(1,2556)	1:209:B:SER:H	1:204:B:LEU:HA	8	0.34
(1,2555)	1:209:A:SER:H	1:204:A:LEU:HA	8	0.34
(1,2474)	1:190:B:PHE:H	1:193:B:ASP:H	6	0.34
(1,2446)	1:187:B:LYS:H	1:187:B:LYS:HG2	4	0.34
(1,2445)	1:187:A:LYS:H	1:187:A:LYS:HG2	4	0.34
(1,2416)	1:189:B:ASN:HA	1:186:B:LEU:HA	3	0.34
(1,2415)	1:189:A:ASN:HA	1:186:A:LEU:HA	3	0.34
(1,2410)	1:197:B:VAL:HA	1:201:B:MET:HB2	8	0.34
(1,2408)	1:197:B:VAL:HA	1:194:B:GLN:HA	10	0.34
(1,2407)	1:197:A:VAL:HA	1:194:A:GLN:HA	10	0.34
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG12	4	0.34
(1,2394)	1:211:B:ALA:HA	1:207:A:GLY:HA2	2	0.34
(1,2372)	1:186:B:LEU:HD13	1:177:A:VAL:H	2	0.34
(1,2370)	1:175:B:LEU:HG	1:199:A:GLN:HE22	10	0.34
(1,2360)	1:200:B:VAL:HG11	1:175:A:LEU:H	9	0.34
(1,2359)	1:200:A:VAL:HG12	1:175:B:LEU:H	8	0.34
(1,2330)	1:199:B:GLN:HG3	1:196:B:ALA:H	1	0.34
(1,2330)	1:194:B:GLN:HG3	1:193:B:ASP:H	7	0.34
(1,2329)	1:199:A:GLN:HG3	1:196:A:ALA:H	1	0.34
(1,2329)	1:194:A:GLN:HG3	1:193:A:ASP:H	7	0.34
(1,2322)	1:197:B:VAL:HG11	1:187:B:LYS:HG3	10	0.34
(1,2321)	1:197:A:VAL:HG11	1:187:A:LYS:HG3	10	0.34
(1,2180)	1:186:B:LEU:HB2	1:190:B:PHE:HD2	6	0.34
(1,2180)	1:186:B:LEU:HB2	1:190:B:PHE:HD2	7	0.34
(1,2180)	1:186:B:LEU:HB2	1:190:B:PHE:HD2	10	0.34
(1,2179)	1:186:A:LEU:HB2	1:190:A:PHE:HD2	2	0.34
(1,2179)	1:186:A:LEU:HB2	1:190:A:PHE:HD2	7	0.34
(1,2179)	1:186:A:LEU:HB2	1:190:A:PHE:HD2	10	0.34
(1,2173)	1:203:A:ARG:HD2	1:208:B:TRP:HZ3	9	0.34
(1,2093)	1:185:A:LEU:HD21	1:181:B:ASP:H	2	0.34
(1,2093)	1:185:A:LEU:HD22	1:181:B:ASP:H	4	0.34
(1,2082)	1:175:B:LEU:HD21	1:190:A:PHE:HZ	9	0.34
(1,2021)	1:179:A:TRP:HE1	1:205:A:GLN:HE22	1	0.34
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD13	1	0.34
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD13	1	0.34
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD13	3	0.34
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG11	1	0.34
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG13	4	0.34
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG13	7	0.34
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG11	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG13	7	0.34
(1,1736)	1:195:B:ALA:H	1:194:B:GLN:HG3	4	0.34
(1,1735)	1:195:A:ALA:H	1:194:A:GLN:HG3	4	0.34
(1,1694)	1:189:B:ASN:HD22	1:182:A:ILE:HD13	9	0.34
(1,1677)	1:199:A:GLN:HE22	1:198:A:ARG:HD3	5	0.34
(1,1455)	1:209:A:SER:H	1:208:A:TRP:HB2	9	0.34
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD21	3	0.34
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD21	3	0.34
(1,1196)	1:188:B:ASN:HA	1:191:B:GLU:HB2	2	0.34
(1,1195)	1:188:A:ASN:HA	1:191:A:GLU:HB2	2	0.34
(1,1185)	1:175:A:LEU:HA	1:196:B:ALA:HB2	5	0.34
(1,1174)	1:203:B:ARG:HA	1:203:B:ARG:HD3	3	0.34
(1,1174)	1:203:B:ARG:HA	1:203:B:ARG:HD3	4	0.34
(1,1173)	1:203:A:ARG:HA	1:203:A:ARG:HD3	3	0.34
(1,1173)	1:203:A:ARG:HA	1:203:A:ARG:HD3	4	0.34
(1,1136)	1:188:B:ASN:HD22	1:188:B:ASN:HA	9	0.34
(1,1135)	1:188:A:ASN:HD22	1:188:A:ASN:HA	9	0.34
(1,1104)	1:179:B:TRP:HE1	1:176:B:THR:HG23	9	0.34
(1,1104)	1:179:B:TRP:HE1	1:176:B:THR:HG21	10	0.34
(1,1103)	1:179:A:TRP:HE1	1:176:A:THR:HG23	9	0.34
(1,960)	1:200:B:VAL:HG12	1:200:B:VAL:HG23	10	0.34
(1,959)	1:200:A:VAL:HG12	1:200:A:VAL:HG23	10	0.34
(1,906)	1:186:B:LEU:HD21	1:186:B:LEU:HB3	3	0.34
(1,905)	1:186:A:LEU:HD21	1:186:A:LEU:HB3	3	0.34
(1,842)	1:177:B:VAL:HG12	1:178:B:PRO:HD3	3	0.34
(1,841)	1:177:A:VAL:HG12	1:178:A:PRO:HD3	3	0.34
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD22	4	0.34
(1,408)	1:185:B:LEU:HB2	1:186:B:LEU:H	3	0.34
(1,408)	1:185:B:LEU:HB2	1:186:B:LEU:H	8	0.34
(1,407)	1:185:A:LEU:HB2	1:186:A:LEU:H	3	0.34
(1,407)	1:185:A:LEU:HB2	1:186:A:LEU:H	8	0.34
(1,296)	1:185:B:LEU:HD23	1:182:A:ILE:HD11	4	0.34
(1,230)	1:204:B:LEU:HD11	1:177:A:VAL:HG23	8	0.34
(1,224)	1:177:B:VAL:HG23	1:204:A:LEU:HD11	8	0.34
(1,223)	1:177:A:VAL:HG23	1:204:B:LEU:HD11	8	0.34
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG21	7	0.34
(1,94)	1:175:B:LEU:HD23	1:200:A:VAL:H	8	0.34
(1,78)	1:200:B:VAL:HG11	1:208:A:TRP:HZ3	10	0.34
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG11	5	0.34
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG11	5	0.34
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB1	10	0.33
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD22	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2712)	1:199:B:GLN:HE22	1:195:B:ALA:HA	5	0.33
(1,2688)	1:202:B:GLU:H	1:197:B:VAL:HA	4	0.33
(1,2688)	1:202:B:GLU:H	1:197:B:VAL:HA	5	0.33
(1,2687)	1:202:A:GLU:H	1:197:A:VAL:HA	4	0.33
(1,2687)	1:202:A:GLU:H	1:197:A:VAL:HA	5	0.33
(1,2670)	1:202:B:GLU:H	1:179:B:TRP:HZ3	6	0.33
(1,2669)	1:202:A:GLU:H	1:179:A:TRP:HZ3	6	0.33
(1,2474)	1:190:B:PHE:H	1:193:B:ASP:H	10	0.33
(1,2473)	1:190:A:PHE:H	1:193:A:ASP:H	6	0.33
(1,2473)	1:190:A:PHE:H	1:193:A:ASP:H	10	0.33
(1,2409)	1:197:A:VAL:HA	1:201:A:MET:HB2	8	0.33
(1,2382)	1:182:B:ILE:HD11	1:186:A:LEU:H	1	0.33
(1,2381)	1:182:A:ILE:HD11	1:186:B:LEU:H	1	0.33
(1,2370)	1:175:B:LEU:HG	1:199:A:GLN:HE22	1	0.33
(1,2360)	1:200:B:VAL:HG13	1:175:A:LEU:H	2	0.33
(1,2360)	1:200:B:VAL:HG11	1:175:A:LEU:H	10	0.33
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD12	3	0.33
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD12	3	0.33
(1,2179)	1:186:A:LEU:HB2	1:190:A:PHE:HD2	5	0.33
(1,2174)	1:203:B:ARG:HD2	1:208:A:TRP:HZ3	9	0.33
(1,2125)	1:186:A:LEU:HD12	1:178:B:PRO:HG2	9	0.33
(1,2094)	1:185:B:LEU:HD21	1:181:A:ASP:H	1	0.33
(1,2094)	1:185:B:LEU:HD21	1:181:A:ASP:H	2	0.33
(1,2093)	1:185:A:LEU:HD21	1:181:B:ASP:H	1	0.33
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG21	5	0.33
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG21	5	0.33
(1,2076)	1:210:B:LEU:HD12	1:211:A:ALA:H	2	0.33
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG13	4	0.33
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG13	1	0.33
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG13	1	0.33
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG12	3	0.33
(1,1738)	1:195:B:ALA:H	1:194:B:GLN:HB3	5	0.33
(1,1737)	1:195:A:ALA:H	1:194:A:GLN:HB3	5	0.33
(1,1693)	1:189:A:ASN:HD22	1:182:B:ILE:HD13	9	0.33
(1,1678)	1:199:B:GLN:HE22	1:198:B:ARG:HD3	5	0.33
(1,1554)	1:173:B:GLN:HE21	1:175:B:LEU:HB3	9	0.33
(1,1553)	1:173:A:GLN:HE21	1:175:A:LEU:HB3	9	0.33
(1,1456)	1:209:B:SER:H	1:208:B:TRP:HB2	9	0.33
(1,1429)	1:211:A:ALA:H	1:206:B:LYS:HE3	7	0.33
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD22	6	0.33
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD22	6	0.33
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB2	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1335)	1:188:A:ASN:H	1:187:A:LYS:HG3	6	0.33
(1,1186)	1:175:B:LEU:HA	1:196:A:ALA:HB1	7	0.33
(1,1185)	1:175:A:LEU:HA	1:196:B:ALA:HB1	7	0.33
(1,1184)	1:199:B:GLN:HA	1:175:A:LEU:HD13	9	0.33
(1,1092)	1:199:B:GLN:HG2	1:173:A:GLN:HE21	7	0.33
(1,1054)	1:199:B:GLN:HG3	1:175:A:LEU:HD13	3	0.33
(1,972)	1:204:B:LEU:HD22	1:182:A:ILE:HD13	7	0.33
(1,960)	1:200:B:VAL:HG13	1:200:B:VAL:HG23	3	0.33
(1,960)	1:200:B:VAL:HG13	1:200:B:VAL:HG23	4	0.33
(1,960)	1:200:B:VAL:HG11	1:200:B:VAL:HG23	6	0.33
(1,960)	1:200:B:VAL:HG11	1:200:B:VAL:HG21	7	0.33
(1,960)	1:200:B:VAL:HG12	1:200:B:VAL:HG21	9	0.33
(1,959)	1:200:A:VAL:HG13	1:200:A:VAL:HG23	3	0.33
(1,959)	1:200:A:VAL:HG13	1:200:A:VAL:HG23	4	0.33
(1,959)	1:200:A:VAL:HG11	1:200:A:VAL:HG23	6	0.33
(1,959)	1:200:A:VAL:HG11	1:200:A:VAL:HG21	7	0.33
(1,959)	1:200:A:VAL:HG12	1:200:A:VAL:HG21	9	0.33
(1,917)	1:173:A:GLN:HG2	1:175:A:LEU:HD13	3	0.33
(1,916)	1:199:B:GLN:HG2	1:175:A:LEU:HD12	8	0.33
(1,906)	1:186:B:LEU:HD22	1:186:B:LEU:HB3	1	0.33
(1,906)	1:186:B:LEU:HD21	1:186:B:LEU:HB3	8	0.33
(1,905)	1:186:A:LEU:HD22	1:186:A:LEU:HB3	1	0.33
(1,905)	1:186:A:LEU:HD21	1:186:A:LEU:HB3	4	0.33
(1,905)	1:186:A:LEU:HD21	1:186:A:LEU:HB3	8	0.33
(1,842)	1:177:B:VAL:HG13	1:178:B:PRO:HD3	9	0.33
(1,841)	1:177:A:VAL:HG13	1:178:A:PRO:HD3	9	0.33
(1,832)	1:182:B:ILE:HG22	1:179:B:TRP:HA	9	0.33
(1,831)	1:182:A:ILE:HG22	1:179:A:TRP:HA	9	0.33
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG11	3	0.33
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD22	4	0.33
(1,522)	1:190:B:PHE:H	1:191:B:GLU:HA	5	0.33
(1,521)	1:190:A:PHE:H	1:191:A:GLU:HA	1	0.33
(1,521)	1:190:A:PHE:H	1:191:A:GLU:HA	5	0.33
(1,432)	1:189:B:ASN:H	1:188:B:ASN:HB3	8	0.33
(1,408)	1:185:B:LEU:HB2	1:186:B:LEU:H	1	0.33
(1,408)	1:185:B:LEU:HB2	1:186:B:LEU:H	9	0.33
(1,407)	1:185:A:LEU:HB2	1:186:A:LEU:H	9	0.33
(1,262)	1:175:B:LEU:HD13	1:199:A:GLN:HG3	5	0.33
(1,254)	1:175:B:LEU:HD13	1:196:A:ALA:HA	10	0.33
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG21	7	0.33
(1,77)	1:200:A:VAL:HG11	1:208:B:TRP:HZ3	10	0.33
(1,28)	1:183:B:GLU:H	1:201:B:MET:HE1	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:183:A:GLU:H	1:201:A:MET:HE1	10	0.33
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG13	6	0.33
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG12	10	0.33
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG12	10	0.33
(1,2870)	1:209:B:SER:H	1:206:B:LYS:HE3	8	0.32
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB1	10	0.32
(1,2589)	1:208:A:TRP:H	1:203:B:ARG:HG2	5	0.32
(1,2474)	1:190:B:PHE:H	1:193:B:ASP:H	3	0.32
(1,2393)	1:211:A:ALA:HA	1:207:B:GLY:HA2	2	0.32
(1,2369)	1:175:A:LEU:HG	1:199:B:GLN:HE22	1	0.32
(1,2366)	1:189:B:ASN:H	1:185:B:LEU:HG	5	0.32
(1,2366)	1:189:B:ASN:H	1:185:B:LEU:HG	9	0.32
(1,2365)	1:189:A:ASN:H	1:185:A:LEU:HG	5	0.32
(1,2180)	1:186:B:LEU:HB2	1:190:B:PHE:HD2	5	0.32
(1,2180)	1:186:B:LEU:HB2	1:190:B:PHE:HD2	8	0.32
(1,2179)	1:186:A:LEU:HB2	1:190:A:PHE:HD2	8	0.32
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD23	1	0.32
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD22	6	0.32
(1,2139)	1:206:A:LYS:HD3	1:203:A:ARG:HA	3	0.32
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG21	4	0.32
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG22	7	0.32
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG21	4	0.32
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG22	7	0.32
(1,2082)	1:175:B:LEU:HD23	1:190:A:PHE:HE1	2	0.32
(1,2075)	1:210:A:LEU:HD12	1:211:B:ALA:H	2	0.32
(1,2022)	1:179:B:TRP:HE1	1:205:B:GLN:HE22	4	0.32
(1,1945)	1:179:A:TRP:H	1:186:B:LEU:HD12	4	0.32
(1,1794)	1:193:B:ASP:H	1:188:B:ASN:HA	6	0.32
(1,1794)	1:193:B:ASP:H	1:188:B:ASN:HA	10	0.32
(1,1793)	1:193:A:ASP:H	1:188:A:ASN:HA	6	0.32
(1,1793)	1:193:A:ASP:H	1:188:A:ASN:HA	10	0.32
(1,1456)	1:209:B:SER:H	1:208:B:TRP:HB2	5	0.32
(1,1455)	1:209:A:SER:H	1:208:A:TRP:HB2	5	0.32
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD22	7	0.32
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD22	7	0.32
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB2	2	0.32
(1,1336)	1:188:B:ASN:H	1:187:B:LYS:HG3	3	0.32
(1,1336)	1:188:B:ASN:H	1:187:B:LYS:HG3	5	0.32
(1,1336)	1:188:B:ASN:H	1:187:B:LYS:HG3	6	0.32
(1,1335)	1:188:A:ASN:H	1:187:A:LYS:HG3	5	0.32
(1,1186)	1:175:B:LEU:HA	1:196:A:ALA:HB2	8	0.32
(1,1174)	1:203:B:ARG:HA	1:203:B:ARG:HD3	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1174)	1:203:B:ARG:HA	1:203:B:ARG:HD3	5	0.32
(1,1174)	1:203:B:ARG:HA	1:203:B:ARG:HD3	6	0.32
(1,1173)	1:203:A:ARG:HA	1:203:A:ARG:HD3	2	0.32
(1,1173)	1:203:A:ARG:HA	1:203:A:ARG:HD3	5	0.32
(1,1173)	1:203:A:ARG:HA	1:203:A:ARG:HD3	6	0.32
(1,971)	1:204:A:LEU:HD22	1:182:B:ILE:HD13	7	0.32
(1,918)	1:173:B:GLN:HG2	1:175:B:LEU:HD13	3	0.32
(1,915)	1:199:A:GLN:HG2	1:175:B:LEU:HD12	8	0.32
(1,906)	1:186:B:LEU:HD22	1:186:B:LEU:HB3	2	0.32
(1,906)	1:186:B:LEU:HD21	1:186:B:LEU:HB3	4	0.32
(1,906)	1:186:B:LEU:HD23	1:186:B:LEU:HB3	5	0.32
(1,906)	1:186:B:LEU:HD21	1:186:B:LEU:HB3	6	0.32
(1,906)	1:186:B:LEU:HD23	1:186:B:LEU:HB3	7	0.32
(1,906)	1:186:B:LEU:HD23	1:186:B:LEU:HB3	9	0.32
(1,906)	1:186:B:LEU:HD22	1:186:B:LEU:HB3	10	0.32
(1,905)	1:186:A:LEU:HD22	1:186:A:LEU:HB3	2	0.32
(1,905)	1:186:A:LEU:HD23	1:186:A:LEU:HB3	5	0.32
(1,905)	1:186:A:LEU:HD21	1:186:A:LEU:HB3	6	0.32
(1,905)	1:186:A:LEU:HD23	1:186:A:LEU:HB3	7	0.32
(1,905)	1:186:A:LEU:HD23	1:186:A:LEU:HB3	9	0.32
(1,905)	1:186:A:LEU:HD22	1:186:A:LEU:HB3	10	0.32
(1,873)	1:185:A:LEU:HD12	1:188:A:ASN:HB2	7	0.32
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG22	8	0.32
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG22	8	0.32
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG13	4	0.32
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG11	3	0.32
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG13	4	0.32
(1,698)	1:184:B:ALA:HA	1:183:B:GLU:HB3	4	0.32
(1,697)	1:184:A:ALA:HA	1:183:A:GLU:HB3	4	0.32
(1,522)	1:190:B:PHE:H	1:191:B:GLU:HA	1	0.32
(1,522)	1:190:B:PHE:H	1:191:B:GLU:HA	4	0.32
(1,521)	1:190:A:PHE:H	1:191:A:GLU:HA	4	0.32
(1,431)	1:189:A:ASN:H	1:188:A:ASN:HB3	8	0.32
(1,407)	1:185:A:LEU:HB2	1:186:A:LEU:H	1	0.32
(1,310)	1:201:B:MET:HB2	1:202:B:GLU:H	7	0.32
(1,309)	1:201:A:MET:HB2	1:202:A:GLU:H	7	0.32
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG23	3	0.32
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG22	6	0.32
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG22	6	0.32
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG12	2	0.32
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG12	2	0.32
(1,4)	1:177:B:VAL:HG11	1:179:B:TRP:HE3	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:177:A:VAL:HG11	1:179:A:TRP:HE3	10	0.32
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG13	6	0.32
(1,2870)	1:209:B:SER:H	1:206:B:LYS:HE3	7	0.31
(1,2869)	1:209:A:SER:H	1:206:A:LYS:HE3	7	0.31
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB2	1	0.31
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB2	1	0.31
(1,2772)	1:175:B:LEU:H	1:190:A:PHE:HZ	6	0.31
(1,2712)	1:199:B:GLN:HE22	1:195:B:ALA:HA	9	0.31
(1,2711)	1:199:A:GLN:HE22	1:195:A:ALA:HA	9	0.31
(1,2670)	1:202:B:GLU:H	1:179:B:TRP:HZ3	9	0.31
(1,2669)	1:202:A:GLU:H	1:179:A:TRP:HZ3	9	0.31
(1,2590)	1:208:B:TRP:H	1:203:A:ARG:HG2	5	0.31
(1,2512)	1:176:B:THR:H	1:174:B:GLU:HB3	3	0.31
(1,2511)	1:176:A:THR:H	1:174:A:GLU:HB3	3	0.31
(1,2473)	1:190:A:PHE:H	1:193:A:ASP:H	3	0.31
(1,2410)	1:197:B:VAL:HA	1:201:B:MET:HB2	1	0.31
(1,2365)	1:189:A:ASN:H	1:185:A:LEU:HG	9	0.31
(1,2360)	1:200:B:VAL:HG12	1:175:A:LEU:H	8	0.31
(1,2359)	1:200:A:VAL:HG11	1:175:B:LEU:H	10	0.31
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD11	1	0.31
(1,2330)	1:199:B:GLN:HG3	1:196:B:ALA:H	10	0.31
(1,2329)	1:199:A:GLN:HG3	1:196:A:ALA:H	10	0.31
(1,2282)	1:202:B:GLU:HB2	1:199:B:GLN:HA	1	0.31
(1,2281)	1:202:A:GLU:HB2	1:199:A:GLN:HA	1	0.31
(1,2281)	1:202:A:GLU:HB2	1:199:A:GLN:HA	8	0.31
(1,2281)	1:202:A:GLU:HB2	1:199:A:GLN:HA	10	0.31
(1,2180)	1:186:B:LEU:HB2	1:190:B:PHE:HD2	3	0.31
(1,2174)	1:203:B:ARG:HD2	1:208:A:TRP:HZ3	1	0.31
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD23	1	0.31
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD22	6	0.31
(1,2140)	1:206:B:LYS:HD3	1:203:B:ARG:HA	3	0.31
(1,2127)	1:185:A:LEU:HD12	1:178:B:PRO:HB2	10	0.31
(1,2110)	1:177:B:VAL:HG23	1:179:B:TRP:HH2	9	0.31
(1,2109)	1:177:A:VAL:HG23	1:179:A:TRP:HH2	9	0.31
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG22	2	0.31
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG22	2	0.31
(1,2076)	1:210:B:LEU:HD11	1:211:A:ALA:H	3	0.31
(1,2075)	1:210:A:LEU:HD11	1:211:B:ALA:H	3	0.31
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG11	10	0.31
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG11	10	0.31
(1,1946)	1:179:B:TRP:H	1:186:A:LEU:HD12	4	0.31
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG13	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG11	5	0.31
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG13	6	0.31
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG11	9	0.31
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG13	2	0.31
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG13	6	0.31
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG11	9	0.31
(1,1464)	1:208:B:TRP:HE1	1:203:A:ARG:HE	10	0.31
(1,1456)	1:209:B:SER:H	1:208:B:TRP:HB2	2	0.31
(1,1456)	1:209:B:SER:H	1:208:B:TRP:HB2	6	0.31
(1,1455)	1:209:A:SER:H	1:208:A:TRP:HB2	2	0.31
(1,1455)	1:209:A:SER:H	1:208:A:TRP:HB2	6	0.31
(1,1430)	1:211:B:ALA:H	1:206:A:LYS:HE3	7	0.31
(1,1335)	1:188:A:ASN:H	1:187:A:LYS:HG3	3	0.31
(1,1186)	1:175:B:LEU:HA	1:196:A:ALA:HB2	5	0.31
(1,1173)	1:203:A:ARG:HA	1:203:A:ARG:HD3	1	0.31
(1,960)	1:200:B:VAL:HG11	1:200:B:VAL:HG21	2	0.31
(1,960)	1:200:B:VAL:HG13	1:200:B:VAL:HG23	8	0.31
(1,959)	1:200:A:VAL:HG11	1:200:A:VAL:HG21	2	0.31
(1,959)	1:200:A:VAL:HG13	1:200:A:VAL:HG23	8	0.31
(1,874)	1:185:B:LEU:HD12	1:188:B:ASN:HB2	7	0.31
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG23	2	0.31
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG23	2	0.31
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG21	5	0.31
(1,826)	1:183:B:GLU:HA	1:197:B:VAL:HG13	8	0.31
(1,825)	1:183:A:GLU:HA	1:197:A:VAL:HG13	8	0.31
(1,698)	1:184:B:ALA:HA	1:183:B:GLU:HB3	8	0.31
(1,698)	1:184:B:ALA:HA	1:183:B:GLU:HB3	10	0.31
(1,697)	1:184:A:ALA:HA	1:183:A:GLU:HB3	8	0.31
(1,697)	1:184:A:ALA:HA	1:183:A:GLU:HB3	10	0.31
(1,619)	1:200:A:VAL:HA	1:199:A:GLN:H	10	0.31
(1,524)	1:191:B:GLU:H	1:191:B:GLU:HA	7	0.31
(1,523)	1:191:A:GLU:H	1:191:A:GLU:HA	7	0.31
(1,522)	1:190:B:PHE:H	1:191:B:GLU:HA	10	0.31
(1,521)	1:190:A:PHE:H	1:191:A:GLU:HA	10	0.31
(1,408)	1:185:B:LEU:HB2	1:186:B:LEU:H	10	0.31
(1,407)	1:185:A:LEU:HB2	1:186:A:LEU:H	10	0.31
(1,278)	1:187:B:LYS:HG2	1:187:B:LYS:HE3	1	0.31
(1,277)	1:187:A:LYS:HG2	1:187:A:LYS:HE3	1	0.31
(1,225)	1:177:A:VAL:HG22	1:200:B:VAL:HG11	7	0.31
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG23	3	0.31
(1,78)	1:200:B:VAL:HG13	1:208:A:TRP:HZ3	1	0.31
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB3	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB3	9	0.31
(1,24)	1:201:B:MET:HE1	1:183:B:GLU:HA	7	0.31
(1,4)	1:177:B:VAL:HG11	1:179:B:TRP:HE3	9	0.31
(1,3)	1:177:A:VAL:HG11	1:179:A:TRP:HE3	9	0.31
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB2	4	0.3
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB2	7	0.3
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB2	9	0.3
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB2	4	0.3
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB2	9	0.3
(1,2688)	1:202:B:GLU:H	1:197:B:VAL:HA	10	0.3
(1,2687)	1:202:A:GLU:H	1:197:A:VAL:HA	10	0.3
(1,2674)	1:202:B:GLU:H	1:179:B:TRP:HE3	2	0.3
(1,2661)	1:173:A:GLN:HE21	1:196:B:ALA:HA	6	0.3
(1,2590)	1:208:B:TRP:H	1:206:B:LYS:HG2	10	0.3
(1,2589)	1:208:A:TRP:H	1:206:A:LYS:HG2	10	0.3
(1,2566)	1:208:B:TRP:HE1	1:209:B:SER:HA	1	0.3
(1,2565)	1:208:A:TRP:HE1	1:209:A:SER:HA	1	0.3
(1,2556)	1:209:B:SER:H	1:204:B:LEU:HA	10	0.3
(1,2555)	1:209:A:SER:H	1:204:A:LEU:HA	4	0.3
(1,2555)	1:209:A:SER:H	1:204:A:LEU:HA	10	0.3
(1,2488)	1:180:B:ASP:H	1:178:B:PRO:HG2	9	0.3
(1,2487)	1:180:A:ASP:H	1:178:A:PRO:HG2	9	0.3
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG21	1	0.3
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG21	1	0.3
(1,2436)	1:197:B:VAL:HG13	1:187:B:LYS:HD3	2	0.3
(1,2435)	1:197:A:VAL:HG13	1:187:A:LYS:HD3	2	0.3
(1,2409)	1:197:A:VAL:HA	1:201:A:MET:HB2	1	0.3
(1,2400)	1:184:B:ALA:HA	1:197:B:VAL:HG11	9	0.3
(1,2399)	1:184:A:ALA:HA	1:197:A:VAL:HG11	9	0.3
(1,2372)	1:186:B:LEU:HD13	1:177:A:VAL:H	1	0.3
(1,2372)	1:186:B:LEU:HD12	1:177:A:VAL:H	4	0.3
(1,2371)	1:186:A:LEU:HD13	1:177:B:VAL:H	1	0.3
(1,2371)	1:186:A:LEU:HD13	1:177:B:VAL:H	3	0.3
(1,2359)	1:200:A:VAL:HG11	1:175:B:LEU:H	9	0.3
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD11	1	0.3
(1,2322)	1:197:B:VAL:HG13	1:187:B:LYS:HG3	3	0.3
(1,2321)	1:197:A:VAL:HG13	1:187:A:LYS:HG3	3	0.3
(1,2288)	1:182:B:ILE:HG21	1:183:B:GLU:HA	1	0.3
(1,2288)	1:182:B:ILE:HG22	1:183:B:GLU:HA	4	0.3
(1,2288)	1:182:B:ILE:HG22	1:183:B:GLU:HA	8	0.3
(1,2287)	1:182:A:ILE:HG21	1:183:A:GLU:HA	1	0.3
(1,2287)	1:182:A:ILE:HG22	1:183:A:GLU:HA	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2287)	1:182:A:ILE:HG22	1:183:A:GLU:HA	8	0.3
(1,2282)	1:202:B:GLU:HB2	1:199:B:GLN:HA	6	0.3
(1,2282)	1:202:B:GLU:HB2	1:199:B:GLN:HA	8	0.3
(1,2282)	1:202:B:GLU:HB2	1:199:B:GLN:HA	10	0.3
(1,2179)	1:186:A:LEU:HB2	1:190:A:PHE:HD2	3	0.3
(1,2179)	1:186:A:LEU:HB2	1:190:A:PHE:HD2	4	0.3
(1,2173)	1:203:A:ARG:HD2	1:208:B:TRP:HZ3	1	0.3
(1,2166)	1:189:B:ASN:HB3	1:185:B:LEU:HG	5	0.3
(1,2165)	1:189:A:ASN:HB3	1:185:A:LEU:HG	5	0.3
(1,2021)	1:179:A:TRP:HE1	1:205:A:GLN:HE22	4	0.3
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG11	5	0.3
(1,1737)	1:195:A:ALA:H	1:194:A:GLN:HB3	6	0.3
(1,1456)	1:209:B:SER:H	1:208:B:TRP:HB2	1	0.3
(1,1455)	1:209:A:SER:H	1:208:A:TRP:HB2	1	0.3
(1,1174)	1:203:B:ARG:HA	1:203:B:ARG:HD3	1	0.3
(1,1174)	1:203:B:ARG:HA	1:203:B:ARG:HD3	9	0.3
(1,1173)	1:203:A:ARG:HA	1:203:A:ARG:HD3	9	0.3
(1,1104)	1:179:B:TRP:HE1	1:176:B:THR:HG21	5	0.3
(1,1103)	1:179:A:TRP:HE1	1:176:A:THR:HG21	5	0.3
(1,882)	1:192:B:ASN:HB3	1:191:B:GLU:HA	4	0.3
(1,881)	1:192:A:ASN:HB3	1:191:A:GLU:HA	4	0.3
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG23	1	0.3
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG21	5	0.3
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG23	1	0.3
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD21	9	0.3
(1,620)	1:200:B:VAL:HA	1:199:B:GLN:H	1	0.3
(1,620)	1:200:B:VAL:HA	1:199:B:GLN:H	2	0.3
(1,620)	1:200:B:VAL:HA	1:199:B:GLN:H	5	0.3
(1,620)	1:200:B:VAL:HA	1:199:B:GLN:H	10	0.3
(1,619)	1:200:A:VAL:HA	1:199:A:GLN:H	1	0.3
(1,619)	1:200:A:VAL:HA	1:199:A:GLN:H	2	0.3
(1,619)	1:200:A:VAL:HA	1:199:A:GLN:H	5	0.3
(1,522)	1:190:B:PHE:H	1:191:B:GLU:HA	6	0.3
(1,521)	1:190:A:PHE:H	1:191:A:GLU:HA	6	0.3
(1,295)	1:185:A:LEU:HD23	1:182:B:ILE:HD11	4	0.3
(1,262)	1:175:B:LEU:HD13	1:199:A:GLN:HG3	9	0.3
(1,226)	1:177:B:VAL:HG22	1:200:A:VAL:HG11	7	0.3
(1,225)	1:177:A:VAL:HG21	1:200:B:VAL:HG13	4	0.3
(1,225)	1:177:A:VAL:HG22	1:200:B:VAL:HG12	5	0.3
(1,225)	1:177:A:VAL:HG23	1:200:B:VAL:HG13	6	0.3
(1,225)	1:177:A:VAL:HG22	1:200:B:VAL:HG12	9	0.3
(1,180)	1:196:B:ALA:HB2	1:197:B:VAL:HA	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:196:A:ALA:HB2	1:197:A:VAL:HA	7	0.3
(1,110)	1:210:B:LEU:HD13	1:212:A:LYS:H	7	0.3
(1,109)	1:210:A:LEU:HD13	1:212:B:LYS:H	7	0.3
(1,77)	1:200:A:VAL:HG13	1:208:B:TRP:HZ3	1	0.3
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG12	3	0.3
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG12	6	0.3
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG13	9	0.3
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG12	3	0.3
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG12	6	0.3
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG13	9	0.3
(1,23)	1:201:A:MET:HE1	1:183:A:GLU:HA	7	0.3
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG11	1	0.3
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB1	3	0.29
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB3	6	0.29
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB1	3	0.29
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB2	7	0.29
(1,2778)	1:193:B:ASP:H	1:196:B:ALA:HB3	5	0.29
(1,2777)	1:193:A:ASP:H	1:196:A:ALA:HB3	5	0.29
(1,2674)	1:202:B:GLU:H	1:179:B:TRP:HE3	1	0.29
(1,2674)	1:202:B:GLU:H	1:179:B:TRP:HE3	9	0.29
(1,2673)	1:202:A:GLU:H	1:179:A:TRP:HE3	1	0.29
(1,2673)	1:202:A:GLU:H	1:179:A:TRP:HE3	2	0.29
(1,2673)	1:202:A:GLU:H	1:179:A:TRP:HE3	9	0.29
(1,2566)	1:208:B:TRP:HE1	1:209:B:SER:HA	2	0.29
(1,2565)	1:208:A:TRP:HE1	1:209:A:SER:HA	2	0.29
(1,2556)	1:209:B:SER:H	1:204:B:LEU:HA	4	0.29
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD21	4	0.29
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD21	4	0.29
(1,2396)	1:207:B:GLY:HA3	1:206:B:LYS:HG2	1	0.29
(1,2395)	1:207:A:GLY:HA3	1:206:A:LYS:HG2	1	0.29
(1,2366)	1:189:B:ASN:H	1:185:B:LEU:HG	2	0.29
(1,2366)	1:189:B:ASN:H	1:185:B:LEU:HG	8	0.29
(1,2365)	1:189:A:ASN:H	1:185:A:LEU:HG	2	0.29
(1,2360)	1:200:B:VAL:HG12	1:175:A:LEU:H	6	0.29
(1,2354)	1:206:B:LYS:HG3	1:210:B:LEU:H	6	0.29
(1,2353)	1:206:A:LYS:HG3	1:210:A:LEU:H	6	0.29
(1,2330)	1:199:B:GLN:HG3	1:196:B:ALA:H	9	0.29
(1,2329)	1:199:A:GLN:HG3	1:196:A:ALA:H	9	0.29
(1,2282)	1:202:B:GLU:HB2	1:199:B:GLN:HA	2	0.29
(1,2281)	1:202:A:GLU:HB2	1:199:A:GLN:HA	2	0.29
(1,2281)	1:202:A:GLU:HB2	1:199:A:GLN:HA	6	0.29
(1,2231)	1:187:A:LYS:H	1:197:A:VAL:HA	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2180)	1:186:B:LEU:HB2	1:190:B:PHE:HD2	1	0.29
(1,2180)	1:186:B:LEU:HB2	1:190:B:PHE:HD2	4	0.29
(1,2180)	1:186:B:LEU:HB2	1:190:B:PHE:HD2	9	0.29
(1,2179)	1:186:A:LEU:HB2	1:190:A:PHE:HD2	1	0.29
(1,2179)	1:186:A:LEU:HB2	1:190:A:PHE:HD2	9	0.29
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD23	10	0.29
(1,2101)	1:204:A:LEU:HD12	1:179:A:TRP:HZ3	8	0.29
(1,2095)	1:175:A:LEU:HD13	1:199:B:GLN:HE22	5	0.29
(1,2091)	1:175:A:LEU:H	1:175:A:LEU:HD12	5	0.29
(1,2081)	1:175:A:LEU:HD23	1:190:B:PHE:HE1	2	0.29
(1,2081)	1:175:A:LEU:HD21	1:190:B:PHE:HZ	9	0.29
(1,2020)	1:205:B:GLN:HE22	1:179:B:TRP:HD1	3	0.29
(1,1988)	1:173:A:GLN:H	1:173:A:GLN:HE22	7	0.29
(1,1987)	1:173:B:GLN:H	1:173:B:GLN:HE22	7	0.29
(1,1738)	1:195:B:ALA:H	1:194:B:GLN:HB3	6	0.29
(1,1738)	1:195:B:ALA:H	1:194:B:GLN:HB3	9	0.29
(1,1737)	1:195:A:ALA:H	1:194:A:GLN:HB3	8	0.29
(1,1737)	1:195:A:ALA:H	1:194:A:GLN:HB3	9	0.29
(1,1577)	1:192:A:ASN:HD21	1:193:A:ASP:HA	7	0.29
(1,1463)	1:208:A:TRP:HE1	1:203:B:ARG:HE	10	0.29
(1,1456)	1:209:B:SER:H	1:208:B:TRP:HB2	4	0.29
(1,1456)	1:209:B:SER:H	1:208:B:TRP:HB2	10	0.29
(1,1455)	1:209:A:SER:H	1:208:A:TRP:HB2	4	0.29
(1,1455)	1:209:A:SER:H	1:208:A:TRP:HB2	10	0.29
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD22	8	0.29
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD22	8	0.29
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB2	4	0.29
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB2	7	0.29
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB2	7	0.29
(1,1336)	1:188:B:ASN:H	1:187:B:LYS:HG3	10	0.29
(1,1335)	1:188:A:ASN:H	1:187:A:LYS:HG3	10	0.29
(1,1291)	1:191:A:GLU:H	1:193:A:ASP:HB3	4	0.29
(1,1262)	1:176:B:THR:HG22	1:177:B:VAL:HB	2	0.29
(1,1261)	1:176:A:THR:HG22	1:177:A:VAL:HB	2	0.29
(1,1255)	1:173:A:GLN:HB2	1:175:A:LEU:HD11	7	0.29
(1,1185)	1:175:A:LEU:HA	1:196:B:ALA:HB2	8	0.29
(1,1174)	1:203:B:ARG:HA	1:203:B:ARG:HD3	7	0.29
(1,1173)	1:203:A:ARG:HA	1:203:A:ARG:HD3	7	0.29
(1,1136)	1:188:B:ASN:HD22	1:188:B:ASN:HA	1	0.29
(1,1135)	1:188:A:ASN:HD22	1:188:A:ASN:HA	1	0.29
(1,960)	1:200:B:VAL:HG11	1:200:B:VAL:HG23	1	0.29
(1,960)	1:200:B:VAL:HG12	1:200:B:VAL:HG23	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:200:A:VAL:HG11	1:200:A:VAL:HG23	1	0.29
(1,959)	1:200:A:VAL:HG12	1:200:A:VAL:HG23	5	0.29
(1,860)	1:200:B:VAL:HA	1:175:A:LEU:HB3	9	0.29
(1,822)	1:208:B:TRP:HA	1:203:A:ARG:HG3	5	0.29
(1,821)	1:208:A:TRP:HA	1:203:B:ARG:HG3	5	0.29
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD22	7	0.29
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD21	9	0.29
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD22	7	0.29
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG22	2	0.29
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG22	2	0.29
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG21	5	0.29
(1,698)	1:184:B:ALA:HA	1:183:B:GLU:HB3	6	0.29
(1,697)	1:184:A:ALA:HA	1:183:A:GLU:HB3	6	0.29
(1,620)	1:200:B:VAL:HA	1:199:B:GLN:H	8	0.29
(1,522)	1:190:B:PHE:H	1:191:B:GLU:HA	8	0.29
(1,521)	1:190:A:PHE:H	1:191:A:GLU:HA	8	0.29
(1,422)	1:196:B:ALA:H	1:193:B:ASP:HB2	9	0.29
(1,421)	1:196:A:ALA:H	1:193:A:ASP:HB2	9	0.29
(1,393)	1:176:A:THR:H	1:175:A:LEU:HB2	7	0.29
(1,234)	1:200:B:VAL:HG13	1:177:A:VAL:HG21	4	0.29
(1,234)	1:200:B:VAL:HG12	1:177:A:VAL:HG22	5	0.29
(1,234)	1:200:B:VAL:HG11	1:177:A:VAL:HG22	7	0.29
(1,233)	1:200:A:VAL:HG11	1:177:B:VAL:HG22	7	0.29
(1,226)	1:177:B:VAL:HG21	1:200:A:VAL:HG13	4	0.29
(1,226)	1:177:B:VAL:HG22	1:200:A:VAL:HG12	5	0.29
(1,226)	1:177:B:VAL:HG23	1:200:A:VAL:HG13	6	0.29
(1,193)	1:201:A:MET:HE3	1:182:A:ILE:HD13	1	0.29
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD21	7	0.29
(1,42)	1:196:B:ALA:H	1:195:B:ALA:HB2	4	0.29
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG11	1	0.29
(1,2869)	1:209:A:SER:H	1:206:A:LYS:HE3	5	0.28
(1,2863)	1:173:B:GLN:H	1:203:A:ARG:HG3	3	0.28
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD13	10	0.28
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD13	10	0.28
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB3	6	0.28
(1,2710)	1:199:B:GLN:HE22	1:175:A:LEU:HA	8	0.28
(1,2688)	1:202:B:GLU:H	1:197:B:VAL:HA	6	0.28
(1,2687)	1:202:A:GLU:H	1:197:A:VAL:HA	6	0.28
(1,2574)	1:208:B:TRP:HE1	1:212:B:LYS:HB3	1	0.28
(1,2566)	1:208:B:TRP:HE1	1:209:B:SER:HA	10	0.28
(1,2565)	1:208:A:TRP:HE1	1:209:A:SER:HA	10	0.28
(1,2556)	1:209:B:SER:H	1:204:B:LEU:HA	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2556)	1:209:B:SER:H	1:204:B:LEU:HA	6	0.28
(1,2556)	1:209:B:SER:H	1:204:B:LEU:HA	9	0.28
(1,2555)	1:209:A:SER:H	1:204:A:LEU:HA	9	0.28
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD11	1	0.28
(1,2488)	1:180:B:ASP:H	1:178:B:PRO:HG2	2	0.28
(1,2484)	1:180:B:ASP:H	1:182:B:ILE:HA	7	0.28
(1,2483)	1:180:A:ASP:H	1:182:A:ILE:HA	7	0.28
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD23	3	0.28
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD23	3	0.28
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD22	10	0.28
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG22	8	0.28
(1,2450)	1:184:B:ALA:H	1:187:B:LYS:HE2	9	0.28
(1,2449)	1:184:A:ALA:H	1:187:A:LYS:HE2	9	0.28
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD23	4	0.28
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD23	5	0.28
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD23	4	0.28
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD23	5	0.28
(1,2395)	1:207:A:GLY:HA3	1:206:A:LYS:HG2	8	0.28
(1,2382)	1:182:B:ILE:HD12	1:186:A:LEU:H	3	0.28
(1,2372)	1:186:B:LEU:HD13	1:177:A:VAL:H	3	0.28
(1,2366)	1:189:B:ASN:H	1:185:B:LEU:HG	1	0.28
(1,2366)	1:189:B:ASN:H	1:185:B:LEU:HG	6	0.28
(1,2365)	1:189:A:ASN:H	1:185:A:LEU:HG	1	0.28
(1,2365)	1:189:A:ASN:H	1:185:A:LEU:HG	8	0.28
(1,2359)	1:200:A:VAL:HG12	1:175:B:LEU:H	6	0.28
(1,2232)	1:187:B:LYS:H	1:197:B:VAL:HA	9	0.28
(1,2173)	1:203:A:ARG:HD2	1:208:B:TRP:HZ3	6	0.28
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD23	10	0.28
(1,2150)	1:175:B:LEU:H	1:173:B:GLN:HB3	2	0.28
(1,2126)	1:186:B:LEU:HD13	1:178:A:PRO:HG2	7	0.28
(1,2125)	1:186:A:LEU:HD13	1:178:B:PRO:HG2	7	0.28
(1,2107)	1:177:A:VAL:HG21	1:190:B:PHE:HE2	10	0.28
(1,2102)	1:204:B:LEU:HD12	1:179:B:TRP:HZ3	8	0.28
(1,2096)	1:175:B:LEU:HD12	1:199:A:GLN:HE22	4	0.28
(1,2092)	1:175:B:LEU:H	1:175:B:LEU:HD12	5	0.28
(1,2019)	1:205:A:GLN:HE22	1:179:A:TRP:HD1	3	0.28
(1,1793)	1:193:A:ASP:H	1:188:A:ASN:HA	4	0.28
(1,1792)	1:177:B:VAL:H	1:177:B:VAL:HG13	3	0.28
(1,1791)	1:177:A:VAL:H	1:177:A:VAL:HG13	3	0.28
(1,1738)	1:195:B:ALA:H	1:194:B:GLN:HB3	8	0.28
(1,1629)	1:203:A:ARG:H	1:179:A:TRP:HZ3	1	0.28
(1,1578)	1:192:B:ASN:HD21	1:193:B:ASP:HA	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:209:A:SER:H	1:208:A:TRP:HB2	3	0.28
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB2	4	0.28
(1,1292)	1:191:B:GLU:H	1:193:B:ASP:HB3	4	0.28
(1,1256)	1:173:B:GLN:HB2	1:175:B:LEU:HD11	7	0.28
(1,1196)	1:188:B:ASN:HA	1:191:B:GLU:HB2	5	0.28
(1,1195)	1:188:A:ASN:HA	1:191:A:GLU:HB2	5	0.28
(1,1071)	1:175:A:LEU:HD13	1:201:B:MET:H	4	0.28
(1,882)	1:192:B:ASN:HB3	1:191:B:GLU:HA	2	0.28
(1,881)	1:192:A:ASN:HB3	1:191:A:GLU:HA	2	0.28
(1,756)	1:185:B:LEU:HB3	1:185:B:LEU:HA	1	0.28
(1,756)	1:185:B:LEU:HB3	1:185:B:LEU:HA	2	0.28
(1,756)	1:185:B:LEU:HB3	1:185:B:LEU:HA	3	0.28
(1,756)	1:185:B:LEU:HB3	1:185:B:LEU:HA	4	0.28
(1,756)	1:185:B:LEU:HB3	1:185:B:LEU:HA	5	0.28
(1,756)	1:185:B:LEU:HB3	1:185:B:LEU:HA	6	0.28
(1,756)	1:185:B:LEU:HB3	1:185:B:LEU:HA	7	0.28
(1,756)	1:185:B:LEU:HB3	1:185:B:LEU:HA	8	0.28
(1,756)	1:185:B:LEU:HB3	1:185:B:LEU:HA	9	0.28
(1,756)	1:185:B:LEU:HB3	1:185:B:LEU:HA	10	0.28
(1,755)	1:185:A:LEU:HB3	1:185:A:LEU:HA	1	0.28
(1,755)	1:185:A:LEU:HB3	1:185:A:LEU:HA	2	0.28
(1,755)	1:185:A:LEU:HB3	1:185:A:LEU:HA	3	0.28
(1,755)	1:185:A:LEU:HB3	1:185:A:LEU:HA	4	0.28
(1,755)	1:185:A:LEU:HB3	1:185:A:LEU:HA	5	0.28
(1,755)	1:185:A:LEU:HB3	1:185:A:LEU:HA	6	0.28
(1,755)	1:185:A:LEU:HB3	1:185:A:LEU:HA	7	0.28
(1,755)	1:185:A:LEU:HB3	1:185:A:LEU:HA	8	0.28
(1,755)	1:185:A:LEU:HB3	1:185:A:LEU:HA	9	0.28
(1,755)	1:185:A:LEU:HB3	1:185:A:LEU:HA	10	0.28
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG21	5	0.28
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG21	8	0.28
(1,698)	1:184:B:ALA:HA	1:183:B:GLU:HB3	9	0.28
(1,697)	1:184:A:ALA:HA	1:183:A:GLU:HB3	9	0.28
(1,620)	1:200:B:VAL:HA	1:199:B:GLN:H	4	0.28
(1,619)	1:200:A:VAL:HA	1:199:A:GLN:H	3	0.28
(1,619)	1:200:A:VAL:HA	1:199:A:GLN:H	4	0.28
(1,619)	1:200:A:VAL:HA	1:199:A:GLN:H	8	0.28
(1,522)	1:190:B:PHE:H	1:191:B:GLU:HA	9	0.28
(1,521)	1:190:A:PHE:H	1:191:A:GLU:HA	9	0.28
(1,394)	1:176:B:THR:H	1:175:B:LEU:HB2	7	0.28
(1,308)	1:199:B:GLN:HB3	1:200:B:VAL:HG11	6	0.28
(1,307)	1:199:A:GLN:HB3	1:200:A:VAL:HG11	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:200:B:VAL:HG13	1:177:A:VAL:HG23	6	0.28
(1,234)	1:200:B:VAL:HG12	1:177:A:VAL:HG22	9	0.28
(1,233)	1:200:A:VAL:HG12	1:177:B:VAL:HG22	5	0.28
(1,233)	1:200:A:VAL:HG13	1:177:B:VAL:HG23	6	0.28
(1,196)	1:201:B:MET:HE2	1:205:B:GLN:HG3	10	0.28
(1,195)	1:201:A:MET:HE2	1:205:A:GLN:HG3	10	0.28
(1,194)	1:201:B:MET:HE3	1:182:B:ILE:HD13	1	0.28
(1,194)	1:201:B:MET:HE1	1:182:B:ILE:HD13	6	0.28
(1,193)	1:201:A:MET:HE1	1:182:A:ILE:HD13	6	0.28
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD21	7	0.28
(1,41)	1:196:A:ALA:H	1:195:A:ALA:HB2	4	0.28
(1,2870)	1:209:B:SER:H	1:206:B:LYS:HE3	5	0.27
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB3	8	0.27
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB3	8	0.27
(1,2790)	1:189:B:ASN:H	1:191:B:GLU:HA	2	0.27
(1,2789)	1:189:A:ASN:H	1:191:A:GLU:HA	2	0.27
(1,2762)	1:175:B:LEU:H	1:175:B:LEU:HD13	2	0.27
(1,2721)	1:189:A:ASN:HD22	1:178:B:PRO:HG2	2	0.27
(1,2712)	1:199:B:GLN:HE22	1:195:B:ALA:HA	3	0.27
(1,2709)	1:199:A:GLN:HE22	1:175:B:LEU:HA	8	0.27
(1,2709)	1:199:A:GLN:HE22	1:175:B:LEU:HA	9	0.27
(1,2688)	1:202:B:GLU:H	1:197:B:VAL:HA	1	0.27
(1,2687)	1:202:A:GLU:H	1:197:A:VAL:HA	1	0.27
(1,2573)	1:208:A:TRP:HE1	1:212:A:LYS:HB3	1	0.27
(1,2555)	1:209:A:SER:H	1:204:A:LEU:HA	5	0.27
(1,2555)	1:209:A:SER:H	1:204:A:LEU:HA	6	0.27
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD11	1	0.27
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD13	5	0.27
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD13	5	0.27
(1,2487)	1:180:A:ASP:H	1:178:A:PRO:HG2	2	0.27
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD22	10	0.27
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG22	8	0.27
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD21	1	0.27
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD22	3	0.27
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD21	1	0.27
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD22	3	0.27
(1,2410)	1:197:B:VAL:HA	1:201:B:MET:HB2	6	0.27
(1,2409)	1:197:A:VAL:HA	1:201:A:MET:HB2	6	0.27
(1,2396)	1:207:B:GLY:HA3	1:206:B:LYS:HG2	3	0.27
(1,2396)	1:207:B:GLY:HA3	1:206:B:LYS:HG2	5	0.27
(1,2396)	1:207:B:GLY:HA3	1:206:B:LYS:HG2	8	0.27
(1,2395)	1:207:A:GLY:HA3	1:206:A:LYS:HG2	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2395)	1:207:A:GLY:HA3	1:206:A:LYS:HG2	5	0.27
(1,2371)	1:186:A:LEU:HD12	1:177:B:VAL:H	4	0.27
(1,2365)	1:189:A:ASN:H	1:185:A:LEU:HG	6	0.27
(1,2330)	1:199:B:GLN:HG3	1:196:B:ALA:H	3	0.27
(1,2329)	1:199:A:GLN:HG3	1:196:A:ALA:H	3	0.27
(1,2288)	1:182:B:ILE:HG21	1:183:B:GLU:HA	6	0.27
(1,2096)	1:175:B:LEU:HD13	1:199:A:GLN:HE22	5	0.27
(1,2095)	1:175:A:LEU:HD12	1:199:B:GLN:HE22	4	0.27
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG21	1	0.27
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG22	6	0.27
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG21	10	0.27
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG21	1	0.27
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG22	6	0.27
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG21	10	0.27
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG13	8	0.27
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG13	8	0.27
(1,2040)	1:203:B:ARG:H	1:205:B:GLN:HE22	1	0.27
(1,2039)	1:203:A:ARG:H	1:205:A:GLN:HE22	1	0.27
(1,1986)	1:173:A:GLN:H	1:175:A:LEU:HD12	10	0.27
(1,1794)	1:193:B:ASP:H	1:188:B:ASN:HA	4	0.27
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG12	4	0.27
(1,1738)	1:195:B:ALA:H	1:194:B:GLN:HB3	1	0.27
(1,1738)	1:195:B:ALA:H	1:194:B:GLN:HB3	3	0.27
(1,1737)	1:195:A:ALA:H	1:194:A:GLN:HB3	1	0.27
(1,1737)	1:195:A:ALA:H	1:194:A:GLN:HB3	3	0.27
(1,1630)	1:203:B:ARG:H	1:179:B:TRP:HZ3	1	0.27
(1,1456)	1:209:B:SER:H	1:208:B:TRP:HB2	3	0.27
(1,1411)	1:212:A:LYS:H	1:212:A:LYS:HG2	5	0.27
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB1	8	0.27
(1,1336)	1:188:B:ASN:H	1:187:B:LYS:HG3	2	0.27
(1,1335)	1:188:A:ASN:H	1:187:A:LYS:HG3	2	0.27
(1,1183)	1:199:A:GLN:HA	1:175:B:LEU:HD13	9	0.27
(1,1174)	1:203:B:ARG:HA	1:203:B:ARG:HD3	8	0.27
(1,1173)	1:203:A:ARG:HA	1:203:A:ARG:HD3	8	0.27
(1,1071)	1:175:A:LEU:HD11	1:201:B:MET:H	10	0.27
(1,863)	1:200:A:VAL:HA	1:175:B:LEU:HD11	7	0.27
(1,852)	1:182:B:ILE:HA	1:185:B:LEU:HB2	2	0.27
(1,851)	1:182:A:ILE:HA	1:185:A:LEU:HB2	2	0.27
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG21	1	0.27
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG21	3	0.27
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG21	4	0.27
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG21	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG21	10	0.27
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG21	1	0.27
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG21	3	0.27
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG21	4	0.27
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG21	10	0.27
(1,698)	1:184:B:ALA:HA	1:183:B:GLU:HB3	3	0.27
(1,697)	1:184:A:ALA:HA	1:183:A:GLU:HB3	3	0.27
(1,684)	1:211:B:ALA:HA	1:210:A:LEU:HD12	2	0.27
(1,683)	1:211:A:ALA:HA	1:210:B:LEU:HD12	2	0.27
(1,648)	1:195:B:ALA:HB2	1:198:B:ARG:HD3	3	0.27
(1,620)	1:200:B:VAL:HA	1:199:B:GLN:H	3	0.27
(1,620)	1:200:B:VAL:HA	1:199:B:GLN:H	7	0.27
(1,619)	1:200:A:VAL:HA	1:199:A:GLN:H	6	0.27
(1,619)	1:200:A:VAL:HA	1:199:A:GLN:H	7	0.27
(1,544)	1:199:B:GLN:HA	1:202:B:GLU:H	7	0.27
(1,543)	1:199:A:GLN:HA	1:202:A:GLU:H	7	0.27
(1,522)	1:190:B:PHE:H	1:191:B:GLU:HA	3	0.27
(1,521)	1:190:A:PHE:H	1:191:A:GLU:HA	3	0.27
(1,320)	1:173:B:GLN:HG3	1:173:B:GLN:H	8	0.27
(1,319)	1:173:A:GLN:HG3	1:173:A:GLN:H	8	0.27
(1,233)	1:200:A:VAL:HG13	1:177:B:VAL:HG21	4	0.27
(1,230)	1:204:B:LEU:HD13	1:177:A:VAL:HG22	7	0.27
(1,230)	1:204:B:LEU:HD12	1:177:A:VAL:HG22	9	0.27
(1,229)	1:204:A:LEU:HD13	1:177:B:VAL:HG22	7	0.27
(1,226)	1:177:B:VAL:HG22	1:200:A:VAL:HG12	9	0.27
(1,224)	1:177:B:VAL:HG22	1:204:A:LEU:HD13	7	0.27
(1,223)	1:177:A:VAL:HG22	1:204:B:LEU:HD13	7	0.27
(1,223)	1:177:A:VAL:HG22	1:204:B:LEU:HD12	9	0.27
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG21	9	0.27
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG21	9	0.27
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG11	4	0.27
(1,2864)	1:173:A:GLN:H	1:203:B:ARG:HG3	3	0.26
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB2	5	0.26
(1,2789)	1:189:A:ASN:H	1:191:A:GLU:HA	9	0.26
(1,2780)	1:190:B:PHE:H	1:187:B:LYS:HG3	1	0.26
(1,2761)	1:175:A:LEU:H	1:175:A:LEU:HD13	2	0.26
(1,2722)	1:189:B:ASN:HD22	1:178:A:PRO:HG2	10	0.26
(1,2711)	1:199:A:GLN:HE22	1:195:A:ALA:HA	3	0.26
(1,2674)	1:202:B:GLU:H	1:179:B:TRP:HE3	5	0.26
(1,2673)	1:202:A:GLU:H	1:179:A:TRP:HE3	5	0.26
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD13	8	0.26
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD13	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2486)	1:180:B:ASP:H	1:201:B:MET:HE1	10	0.26
(1,2381)	1:182:A:ILE:HD12	1:186:B:LEU:H	3	0.26
(1,2366)	1:189:B:ASN:H	1:185:B:LEU:HG	7	0.26
(1,2366)	1:189:B:ASN:H	1:185:B:LEU:HG	10	0.26
(1,2365)	1:189:A:ASN:H	1:185:A:LEU:HG	7	0.26
(1,2365)	1:189:A:ASN:H	1:185:A:LEU:HG	10	0.26
(1,2287)	1:182:A:ILE:HG21	1:183:A:GLU:HA	6	0.26
(1,2253)	1:211:A:ALA:HA	1:206:B:LYS:HG2	4	0.26
(1,2226)	1:208:B:TRP:HA	1:208:B:TRP:HE3	9	0.26
(1,2225)	1:208:A:TRP:HA	1:208:A:TRP:HE3	9	0.26
(1,2174)	1:203:B:ARG:HD2	1:208:A:TRP:HZ3	2	0.26
(1,2173)	1:203:A:ARG:HD2	1:208:B:TRP:HZ3	4	0.26
(1,2172)	1:210:B:LEU:H	1:210:B:LEU:HB3	2	0.26
(1,2172)	1:210:B:LEU:H	1:210:B:LEU:HB3	4	0.26
(1,2171)	1:210:A:LEU:H	1:210:A:LEU:HB3	4	0.26
(1,2149)	1:175:A:LEU:H	1:173:A:GLN:HB3	2	0.26
(1,2108)	1:177:B:VAL:HG21	1:190:A:PHE:HE2	10	0.26
(1,2107)	1:177:A:VAL:HG23	1:190:B:PHE:HE2	6	0.26
(1,2081)	1:175:A:LEU:HD23	1:190:B:PHE:HZ	4	0.26
(1,1985)	1:173:B:GLN:H	1:175:B:LEU:HD12	10	0.26
(1,1433)	1:210:A:LEU:H	1:208:A:TRP:HB2	7	0.26
(1,1433)	1:210:A:LEU:H	1:208:A:TRP:HB2	9	0.26
(1,1412)	1:212:B:LYS:H	1:212:B:LYS:HG2	5	0.26
(1,1391)	1:176:A:THR:H	1:175:A:LEU:HD23	5	0.26
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB1	8	0.26
(1,1072)	1:175:B:LEU:HD13	1:201:A:MET:H	4	0.26
(1,1072)	1:175:B:LEU:HD11	1:201:A:MET:H	10	0.26
(1,1054)	1:199:B:GLN:HG3	1:175:A:LEU:HD12	7	0.26
(1,882)	1:192:B:ASN:HB3	1:191:B:GLU:HA	6	0.26
(1,882)	1:192:B:ASN:HB3	1:191:B:GLU:HA	8	0.26
(1,882)	1:192:B:ASN:HB3	1:191:B:GLU:HA	9	0.26
(1,881)	1:192:A:ASN:HB3	1:191:A:GLU:HA	6	0.26
(1,881)	1:192:A:ASN:HB3	1:191:A:GLU:HA	8	0.26
(1,864)	1:200:B:VAL:HA	1:175:A:LEU:HD11	7	0.26
(1,859)	1:200:A:VAL:HA	1:175:B:LEU:HB3	9	0.26
(1,852)	1:182:B:ILE:HA	1:185:B:LEU:HB2	7	0.26
(1,851)	1:182:A:ILE:HA	1:185:A:LEU:HB2	7	0.26
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD23	10	0.26
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD21	3	0.26
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD21	5	0.26
(1,648)	1:195:B:ALA:HB1	1:198:B:ARG:HD3	6	0.26
(1,647)	1:195:A:ALA:HB2	1:198:A:ARG:HD3	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:195:A:ALA:HB1	1:198:A:ARG:HD3	6	0.26
(1,646)	1:198:B:ARG:HD3	1:198:B:ARG:HB2	8	0.26
(1,645)	1:198:A:ARG:HD3	1:198:A:ARG:HB2	8	0.26
(1,642)	1:198:B:ARG:H	1:198:B:ARG:HD3	1	0.26
(1,641)	1:198:A:ARG:H	1:198:A:ARG:HD3	1	0.26
(1,620)	1:200:B:VAL:HA	1:199:B:GLN:H	6	0.26
(1,619)	1:200:A:VAL:HA	1:199:A:GLN:H	9	0.26
(1,320)	1:173:B:GLN:HG3	1:173:B:GLN:H	3	0.26
(1,319)	1:173:A:GLN:HG3	1:173:A:GLN:H	3	0.26
(1,229)	1:204:A:LEU:HD12	1:177:B:VAL:HG23	9	0.26
(1,226)	1:177:B:VAL:HG23	1:200:A:VAL:HG13	3	0.26
(1,110)	1:210:B:LEU:HD13	1:212:A:LYS:H	8	0.26
(1,109)	1:210:A:LEU:HD13	1:212:B:LYS:H	8	0.26
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG22	7	0.26
(1,78)	1:200:B:VAL:HG12	1:208:A:TRP:HZ3	6	0.26
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG13	5	0.26
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG11	8	0.26
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG11	8	0.26
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG11	4	0.26
(1,62)	1:212:B:LYS:H	1:211:B:ALA:HB1	10	0.26
(1,61)	1:212:A:LYS:H	1:211:A:ALA:HB1	10	0.26
(1,41)	1:196:A:ALA:H	1:195:A:ALA:HB2	2	0.26
(1,26)	1:201:B:MET:HE2	1:179:B:TRP:HB3	5	0.26
(1,25)	1:201:A:MET:HE1	1:179:A:TRP:HB3	5	0.26
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG13	3	0.26
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG13	3	0.26
(1,2862)	1:173:A:GLN:H	1:175:A:LEU:HB2	2	0.25
(1,2861)	1:173:B:GLN:H	1:175:B:LEU:HB2	2	0.25
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB2	5	0.25
(1,2790)	1:189:B:ASN:H	1:191:B:GLU:HA	9	0.25
(1,2779)	1:190:A:PHE:H	1:187:A:LYS:HG3	1	0.25
(1,2722)	1:189:B:ASN:HD22	1:178:A:PRO:HG2	2	0.25
(1,2721)	1:189:A:ASN:HD22	1:178:B:PRO:HG2	7	0.25
(1,2662)	1:173:B:GLN:HE21	1:196:A:ALA:HA	6	0.25
(1,2590)	1:208:B:TRP:H	1:203:A:ARG:HG2	1	0.25
(1,2589)	1:208:A:TRP:H	1:203:B:ARG:HG2	1	0.25
(1,2586)	1:179:B:TRP:HE1	1:205:B:GLN:HA	9	0.25
(1,2565)	1:208:A:TRP:HE1	1:209:A:SER:HA	8	0.25
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD13	3	0.25
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD11	4	0.25
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD13	3	0.25
(1,2485)	1:180:A:ASP:H	1:201:A:MET:HE1	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG22	4	0.25
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG21	6	0.25
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG22	4	0.25
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG21	6	0.25
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD21	6	0.25
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD22	8	0.25
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD21	6	0.25
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD22	8	0.25
(1,2280)	1:194:B:GLN:HA	1:197:B:VAL:HB	8	0.25
(1,2279)	1:194:A:GLN:HA	1:197:A:VAL:HB	8	0.25
(1,2173)	1:203:A:ARG:HD2	1:208:B:TRP:HZ3	7	0.25
(1,2172)	1:210:B:LEU:H	1:210:B:LEU:HB3	1	0.25
(1,2172)	1:210:B:LEU:H	1:210:B:LEU:HB3	3	0.25
(1,2172)	1:210:B:LEU:H	1:210:B:LEU:HB3	5	0.25
(1,2172)	1:210:B:LEU:H	1:210:B:LEU:HB3	6	0.25
(1,2172)	1:210:B:LEU:H	1:210:B:LEU:HB3	7	0.25
(1,2172)	1:210:B:LEU:H	1:210:B:LEU:HB3	8	0.25
(1,2172)	1:210:B:LEU:H	1:210:B:LEU:HB3	9	0.25
(1,2172)	1:210:B:LEU:H	1:210:B:LEU:HB3	10	0.25
(1,2171)	1:210:A:LEU:H	1:210:A:LEU:HB3	1	0.25
(1,2171)	1:210:A:LEU:H	1:210:A:LEU:HB3	2	0.25
(1,2171)	1:210:A:LEU:H	1:210:A:LEU:HB3	3	0.25
(1,2171)	1:210:A:LEU:H	1:210:A:LEU:HB3	5	0.25
(1,2171)	1:210:A:LEU:H	1:210:A:LEU:HB3	6	0.25
(1,2171)	1:210:A:LEU:H	1:210:A:LEU:HB3	7	0.25
(1,2171)	1:210:A:LEU:H	1:210:A:LEU:HB3	8	0.25
(1,2171)	1:210:A:LEU:H	1:210:A:LEU:HB3	10	0.25
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD21	5	0.25
(1,2140)	1:206:B:LYS:HD3	1:203:B:ARG:HA	5	0.25
(1,2139)	1:206:A:LYS:HD3	1:203:A:ARG:HA	5	0.25
(1,2092)	1:175:B:LEU:H	1:175:B:LEU:HD12	3	0.25
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG21	8	0.25
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG21	8	0.25
(1,1998)	1:191:B:GLU:H	1:186:B:LEU:HD12	2	0.25
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD12	2	0.25
(1,1793)	1:193:A:ASP:H	1:188:A:ASN:HA	3	0.25
(1,1554)	1:173:B:GLN:HE21	1:175:B:LEU:HB3	10	0.25
(1,1434)	1:210:B:LEU:H	1:208:B:TRP:HB2	7	0.25
(1,1434)	1:210:B:LEU:H	1:208:B:TRP:HB2	9	0.25
(1,1392)	1:176:B:THR:H	1:175:B:LEU:HD23	5	0.25
(1,1390)	1:198:B:ARG:H	1:195:B:ALA:HB1	4	0.25
(1,1389)	1:198:A:ARG:H	1:195:A:ALA:HB1	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1262)	1:176:B:THR:HG23	1:177:B:VAL:HB	4	0.25
(1,1261)	1:176:A:THR:HG23	1:177:A:VAL:HB	4	0.25
(1,1174)	1:203:B:ARG:HA	1:203:B:ARG:HD3	10	0.25
(1,1173)	1:203:A:ARG:HA	1:203:A:ARG:HD3	10	0.25
(1,1071)	1:175:A:LEU:HD11	1:201:B:MET:H	9	0.25
(1,1054)	1:199:B:GLN:HG3	1:175:A:LEU:HD13	10	0.25
(1,1053)	1:199:A:GLN:HG3	1:175:B:LEU:HD12	7	0.25
(1,918)	1:173:B:GLN:HG3	1:175:B:LEU:HD11	6	0.25
(1,915)	1:199:A:GLN:HG2	1:175:B:LEU:HD13	3	0.25
(1,881)	1:192:A:ASN:HB3	1:191:A:GLU:HA	9	0.25
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD21	3	0.25
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD21	5	0.25
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD23	10	0.25
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG22	6	0.25
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG22	9	0.25
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG22	6	0.25
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG22	9	0.25
(1,620)	1:200:B:VAL:HA	1:199:B:GLN:H	9	0.25
(1,398)	1:175:B:LEU:HB2	1:190:A:PHE:HZ	2	0.25
(1,310)	1:201:B:MET:HB2	1:202:B:GLU:H	9	0.25
(1,309)	1:201:A:MET:HB2	1:202:A:GLU:H	9	0.25
(1,308)	1:199:B:GLN:HB3	1:200:B:VAL:HG13	9	0.25
(1,233)	1:200:A:VAL:HG12	1:177:B:VAL:HG22	9	0.25
(1,225)	1:177:A:VAL:HG23	1:200:B:VAL:HG13	3	0.25
(1,224)	1:177:B:VAL:HG23	1:204:A:LEU:HD12	9	0.25
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG22	7	0.25
(1,82)	1:192:B:ASN:H	1:197:B:VAL:HG22	10	0.25
(1,81)	1:192:A:ASN:H	1:197:A:VAL:HG22	10	0.25
(1,78)	1:200:B:VAL:HG11	1:208:A:TRP:HZ3	5	0.25
(1,78)	1:200:B:VAL:HG11	1:208:A:TRP:HZ3	9	0.25
(1,77)	1:200:A:VAL:HG11	1:208:B:TRP:HZ3	5	0.25
(1,77)	1:200:A:VAL:HG11	1:208:B:TRP:HZ3	9	0.25
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG12	2	0.25
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG13	10	0.25
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG13	5	0.25
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG11	6	0.25
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG13	10	0.25
(1,42)	1:196:B:ALA:H	1:195:B:ALA:HB2	2	0.25
(1,26)	1:201:B:MET:HE2	1:179:B:TRP:HB3	8	0.25
(1,25)	1:201:A:MET:HE2	1:179:A:TRP:HB3	8	0.25
(1,4)	1:177:B:VAL:HG13	1:179:B:TRP:HE3	7	0.25
(1,3)	1:177:A:VAL:HG13	1:179:A:TRP:HE3	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD11	3	0.24
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD11	3	0.24
(1,2798)	1:186:B:LEU:H	1:184:B:ALA:HB3	2	0.24
(1,2797)	1:186:A:LEU:H	1:184:A:ALA:HB3	2	0.24
(1,2722)	1:189:B:ASN:HD22	1:178:A:PRO:HG2	7	0.24
(1,2721)	1:189:A:ASN:HD22	1:178:B:PRO:HG2	5	0.24
(1,2721)	1:189:A:ASN:HD22	1:178:B:PRO:HG2	10	0.24
(1,2688)	1:202:B:GLU:H	1:197:B:VAL:HA	8	0.24
(1,2687)	1:202:A:GLU:H	1:197:A:VAL:HA	8	0.24
(1,2585)	1:179:A:TRP:HE1	1:205:A:GLN:HA	9	0.24
(1,2566)	1:208:B:TRP:HE1	1:209:B:SER:HA	8	0.24
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD11	4	0.24
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG23	3	0.24
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG23	3	0.24
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD21	9	0.24
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD22	10	0.24
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD21	9	0.24
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD22	10	0.24
(1,2382)	1:182:B:ILE:HD11	1:186:A:LEU:H	8	0.24
(1,2366)	1:189:B:ASN:H	1:185:B:LEU:HG	3	0.24
(1,2365)	1:189:A:ASN:H	1:185:A:LEU:HG	3	0.24
(1,2354)	1:211:B:ALA:H	1:212:B:LYS:HG2	5	0.24
(1,2353)	1:211:A:ALA:H	1:212:A:LYS:HG2	5	0.24
(1,2322)	1:197:B:VAL:HG13	1:187:B:LYS:HG3	2	0.24
(1,2321)	1:197:A:VAL:HG13	1:187:A:LYS:HG3	2	0.24
(1,2280)	1:194:B:GLN:HA	1:197:B:VAL:HB	7	0.24
(1,2279)	1:194:A:GLN:HA	1:197:A:VAL:HB	7	0.24
(1,2254)	1:211:B:ALA:HA	1:206:A:LYS:HG2	4	0.24
(1,2222)	1:208:B:TRP:HA	1:207:A:GLY:H	3	0.24
(1,2221)	1:208:A:TRP:HA	1:207:B:GLY:H	3	0.24
(1,2174)	1:203:B:ARG:HD2	1:208:A:TRP:HZ3	6	0.24
(1,2174)	1:203:B:ARG:HD2	1:208:A:TRP:HZ3	7	0.24
(1,2173)	1:203:A:ARG:HD2	1:208:B:TRP:HZ3	2	0.24
(1,2171)	1:210:A:LEU:H	1:210:A:LEU:HB3	9	0.24
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD22	3	0.24
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD22	3	0.24
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD21	5	0.24
(1,2138)	1:187:B:LYS:HD3	1:184:B:ALA:HA	5	0.24
(1,2137)	1:187:A:LYS:HD3	1:184:A:ALA:HA	5	0.24
(1,2108)	1:177:B:VAL:HG23	1:190:A:PHE:HE2	6	0.24
(1,2102)	1:204:B:LEU:HD13	1:179:B:TRP:HZ3	2	0.24
(1,2101)	1:204:A:LEU:HD13	1:179:A:TRP:HZ3	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2091)	1:175:A:LEU:H	1:175:A:LEU:HD12	3	0.24
(1,2076)	1:210:B:LEU:HD13	1:211:A:ALA:H	8	0.24
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG11	1	0.24
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG13	2	0.24
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG11	9	0.24
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG11	1	0.24
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG13	2	0.24
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG11	9	0.24
(1,2040)	1:203:B:ARG:H	1:205:B:GLN:HE22	4	0.24
(1,2039)	1:203:A:ARG:H	1:205:A:GLN:HE22	4	0.24
(1,1982)	1:173:A:GLN:H	1:173:A:GLN:HG3	7	0.24
(1,1981)	1:173:B:GLN:H	1:173:B:GLN:HG3	7	0.24
(1,1942)	1:179:B:TRP:H	1:201:B:MET:HE2	7	0.24
(1,1941)	1:179:A:TRP:H	1:201:A:MET:HE2	7	0.24
(1,1794)	1:193:B:ASP:H	1:188:B:ASN:HA	3	0.24
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG12	4	0.24
(1,1735)	1:195:A:ALA:H	1:194:A:GLN:HG3	7	0.24
(1,1553)	1:173:A:GLN:HE21	1:175:A:LEU:HB3	10	0.24
(1,1433)	1:210:A:LEU:H	1:208:A:TRP:HB2	8	0.24
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB3	1	0.24
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB2	6	0.24
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB3	1	0.24
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB3	10	0.24
(1,1196)	1:188:B:ASN:HA	1:191:B:GLU:HB2	7	0.24
(1,1136)	1:188:B:ASN:HD22	1:188:B:ASN:HA	2	0.24
(1,1135)	1:188:A:ASN:HD22	1:188:A:ASN:HA	2	0.24
(1,1135)	1:188:A:ASN:HD22	1:188:A:ASN:HA	7	0.24
(1,1054)	1:199:B:GLN:HG3	1:175:A:LEU:HD11	2	0.24
(1,1053)	1:199:A:GLN:HG3	1:175:B:LEU:HD11	2	0.24
(1,1053)	1:199:A:GLN:HG3	1:175:B:LEU:HD13	10	0.24
(1,1002)	1:199:B:GLN:H	1:197:B:VAL:HB	1	0.24
(1,1001)	1:199:A:GLN:H	1:197:A:VAL:HB	1	0.24
(1,917)	1:173:A:GLN:HG3	1:175:A:LEU:HD11	6	0.24
(1,852)	1:182:B:ILE:HA	1:185:B:LEU:HB2	5	0.24
(1,851)	1:182:A:ILE:HA	1:185:A:LEU:HB2	5	0.24
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD21	2	0.24
(1,480)	1:192:B:ASN:H	1:192:B:ASN:HA	5	0.24
(1,479)	1:192:A:ASN:H	1:192:A:ASN:HA	5	0.24
(1,307)	1:199:A:GLN:HB3	1:200:A:VAL:HG13	9	0.24
(1,233)	1:200:A:VAL:HG13	1:177:B:VAL:HG23	3	0.24
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG12	1	0.24
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG11	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG12	1	0.24
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG12	2	0.24
(1,3)	1:177:A:VAL:HG11	1:179:A:TRP:HE3	1	0.24
(1,2)	1:179:B:TRP:HE1	1:177:B:VAL:HG11	9	0.24
(1,1)	1:179:A:TRP:HE1	1:177:A:VAL:HG11	9	0.24
(1,2790)	1:189:B:ASN:H	1:191:B:GLU:HA	3	0.23
(1,2789)	1:189:A:ASN:H	1:191:A:GLU:HA	3	0.23
(1,2722)	1:189:B:ASN:HD22	1:178:A:PRO:HG2	5	0.23
(1,2721)	1:189:A:ASN:HD22	1:178:B:PRO:HG2	8	0.23
(1,2710)	1:199:B:GLN:HE22	1:175:A:LEU:HA	10	0.23
(1,2709)	1:199:A:GLN:HE22	1:175:B:LEU:HA	10	0.23
(1,2590)	1:208:B:TRP:H	1:203:A:ARG:HG2	8	0.23
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD12	1	0.23
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD13	6	0.23
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD12	1	0.23
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD13	6	0.23
(1,2511)	1:176:A:THR:H	1:174:A:GLU:HB3	1	0.23
(1,2511)	1:176:A:THR:H	1:174:A:GLU:HB3	4	0.23
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD23	5	0.23
(1,2384)	1:202:B:GLU:HG3	1:203:B:ARG:H	9	0.23
(1,2383)	1:202:A:GLU:HG3	1:203:A:ARG:H	9	0.23
(1,2382)	1:182:B:ILE:HD12	1:186:A:LEU:H	2	0.23
(1,2288)	1:182:B:ILE:HG23	1:183:B:GLU:HA	3	0.23
(1,2287)	1:182:A:ILE:HG23	1:183:A:GLU:HA	3	0.23
(1,2280)	1:194:B:GLN:HA	1:197:B:VAL:HB	5	0.23
(1,2279)	1:194:A:GLN:HA	1:197:A:VAL:HB	5	0.23
(1,2174)	1:203:B:ARG:HD2	1:208:A:TRP:HZ3	4	0.23
(1,2082)	1:175:B:LEU:HD23	1:190:A:PHE:HZ	4	0.23
(1,2052)	1:192:B:ASN:HD22	1:192:B:ASN:H	7	0.23
(1,2051)	1:192:A:ASN:HD22	1:192:A:ASN:H	7	0.23
(1,1998)	1:191:B:GLU:H	1:186:B:LEU:HD13	9	0.23
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD13	9	0.23
(1,1840)	1:188:B:ASN:HD22	1:186:B:LEU:HA	8	0.23
(1,1839)	1:188:A:ASN:HD22	1:186:A:LEU:HA	8	0.23
(1,1736)	1:195:B:ALA:H	1:194:B:GLN:HG3	7	0.23
(1,1434)	1:210:B:LEU:H	1:208:B:TRP:HB2	8	0.23
(1,1378)	1:180:B:ASP:H	1:183:B:GLU:HA	7	0.23
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB1	9	0.23
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB3	10	0.23
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB2	6	0.23
(1,1262)	1:176:B:THR:HG22	1:177:B:VAL:HB	5	0.23
(1,1261)	1:176:A:THR:HG22	1:177:A:VAL:HB	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1195)	1:188:A:ASN:HA	1:191:A:GLU:HB2	7	0.23
(1,1136)	1:188:B:ASN:HD22	1:188:B:ASN:HA	5	0.23
(1,1136)	1:188:B:ASN:HD22	1:188:B:ASN:HA	6	0.23
(1,1136)	1:188:B:ASN:HD22	1:188:B:ASN:HA	7	0.23
(1,1135)	1:188:A:ASN:HD22	1:188:A:ASN:HA	4	0.23
(1,1135)	1:188:A:ASN:HD22	1:188:A:ASN:HA	5	0.23
(1,1135)	1:188:A:ASN:HD22	1:188:A:ASN:HA	6	0.23
(1,1054)	1:199:B:GLN:HG3	1:175:A:LEU:HD12	4	0.23
(1,916)	1:199:B:GLN:HG2	1:175:A:LEU:HD13	3	0.23
(1,882)	1:192:B:ASN:HB3	1:191:B:GLU:HA	10	0.23
(1,881)	1:192:A:ASN:HB3	1:191:A:GLU:HA	10	0.23
(1,860)	1:200:B:VAL:HA	1:175:A:LEU:HB3	5	0.23
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG21	9	0.23
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD21	1	0.23
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD21	1	0.23
(1,698)	1:184:B:ALA:HA	1:183:B:GLU:HB3	5	0.23
(1,684)	1:211:B:ALA:HA	1:210:A:LEU:HD12	4	0.23
(1,683)	1:211:A:ALA:HA	1:210:B:LEU:HD12	4	0.23
(1,648)	1:195:B:ALA:HB2	1:198:B:ARG:HD3	9	0.23
(1,647)	1:195:A:ALA:HB2	1:198:A:ARG:HD3	9	0.23
(1,360)	1:188:B:ASN:H	1:189:B:ASN:HB2	9	0.23
(1,276)	1:198:B:ARG:HG2	1:198:B:ARG:HD3	1	0.23
(1,276)	1:198:B:ARG:HG2	1:198:B:ARG:HD3	2	0.23
(1,276)	1:198:B:ARG:HG2	1:198:B:ARG:HD3	3	0.23
(1,276)	1:198:B:ARG:HG2	1:198:B:ARG:HD3	4	0.23
(1,276)	1:198:B:ARG:HG2	1:198:B:ARG:HD3	5	0.23
(1,276)	1:198:B:ARG:HG2	1:198:B:ARG:HD3	6	0.23
(1,276)	1:198:B:ARG:HG2	1:198:B:ARG:HD3	7	0.23
(1,276)	1:198:B:ARG:HG2	1:198:B:ARG:HD3	9	0.23
(1,275)	1:198:A:ARG:HG2	1:198:A:ARG:HD3	1	0.23
(1,275)	1:198:A:ARG:HG2	1:198:A:ARG:HD3	2	0.23
(1,275)	1:198:A:ARG:HG2	1:198:A:ARG:HD3	3	0.23
(1,275)	1:198:A:ARG:HG2	1:198:A:ARG:HD3	4	0.23
(1,275)	1:198:A:ARG:HG2	1:198:A:ARG:HD3	5	0.23
(1,275)	1:198:A:ARG:HG2	1:198:A:ARG:HD3	6	0.23
(1,275)	1:198:A:ARG:HG2	1:198:A:ARG:HD3	7	0.23
(1,275)	1:198:A:ARG:HG2	1:198:A:ARG:HD3	9	0.23
(1,262)	1:175:B:LEU:HD12	1:199:A:GLN:HG3	6	0.23
(1,246)	1:200:B:VAL:HG12	1:197:B:VAL:HA	7	0.23
(1,245)	1:200:A:VAL:HG12	1:197:A:VAL:HA	7	0.23
(1,234)	1:200:B:VAL:HG13	1:177:A:VAL:HG23	3	0.23
(1,140)	1:179:B:TRP:HE1	1:177:B:VAL:HG23	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:179:A:TRP:HE1	1:177:A:VAL:HG23	10	0.23
(1,77)	1:200:A:VAL:HG13	1:208:B:TRP:HZ3	2	0.23
(1,77)	1:200:A:VAL:HG12	1:208:B:TRP:HZ3	6	0.23
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG13	10	0.23
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG13	10	0.23
(1,26)	1:201:B:MET:HE3	1:179:B:TRP:HB3	1	0.23
(1,4)	1:177:B:VAL:HG11	1:179:B:TRP:HE3	1	0.23
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD21	6	0.22
(1,2722)	1:189:B:ASN:HD22	1:178:A:PRO:HG2	8	0.22
(1,2688)	1:202:B:GLU:H	1:197:B:VAL:HA	7	0.22
(1,2687)	1:202:A:GLU:H	1:197:A:VAL:HA	7	0.22
(1,2589)	1:208:A:TRP:H	1:203:B:ARG:HG2	8	0.22
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD11	2	0.22
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD11	2	0.22
(1,2512)	1:176:B:THR:H	1:174:B:GLU:HB3	1	0.22
(1,2512)	1:176:B:THR:H	1:174:B:GLU:HB3	4	0.22
(1,2488)	1:180:B:ASP:H	1:178:B:PRO:HG2	5	0.22
(1,2487)	1:180:A:ASP:H	1:178:A:PRO:HG2	8	0.22
(1,2470)	1:204:B:LEU:H	1:179:B:TRP:HZ3	1	0.22
(1,2469)	1:204:A:LEU:H	1:179:A:TRP:HZ3	1	0.22
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD23	5	0.22
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD21	9	0.22
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG21	5	0.22
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG21	5	0.22
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD21	7	0.22
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD21	7	0.22
(1,2382)	1:182:B:ILE:HD12	1:186:A:LEU:H	5	0.22
(1,2381)	1:182:A:ILE:HD12	1:186:B:LEU:H	5	0.22
(1,2381)	1:182:A:ILE:HD11	1:186:B:LEU:H	6	0.22
(1,2366)	1:189:B:ASN:H	1:185:B:LEU:HG	4	0.22
(1,2365)	1:189:A:ASN:H	1:185:A:LEU:HG	4	0.22
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD12	2	0.22
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD12	2	0.22
(1,2341)	1:204:A:LEU:HG	1:182:B:ILE:HD12	4	0.22
(1,2326)	1:197:B:VAL:HG11	1:198:B:ARG:HA	8	0.22
(1,2325)	1:197:A:VAL:HG11	1:198:A:ARG:HA	8	0.22
(1,2319)	1:210:A:LEU:HD13	1:210:A:LEU:HB2	7	0.22
(1,2194)	1:173:B:GLN:HA	1:174:B:GLU:H	10	0.22
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD22	4	0.22
(1,2102)	1:204:B:LEU:HD11	1:179:B:TRP:HZ3	1	0.22
(1,2101)	1:204:A:LEU:HD11	1:179:A:TRP:HZ3	1	0.22
(1,2092)	1:175:B:LEU:H	1:175:B:LEU:HD12	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2091)	1:175:A:LEU:H	1:175:A:LEU:HD12	1	0.22
(1,2075)	1:210:A:LEU:HD13	1:211:B:ALA:H	8	0.22
(1,1988)	1:173:A:GLN:H	1:173:A:GLN:HE22	4	0.22
(1,1678)	1:199:B:GLN:HE22	1:198:B:ARG:HD3	3	0.22
(1,1529)	1:207:A:GLY:H	1:206:A:LYS:HB2	7	0.22
(1,1434)	1:210:B:LEU:H	1:208:B:TRP:HB2	5	0.22
(1,1433)	1:210:A:LEU:H	1:208:A:TRP:HB2	2	0.22
(1,1377)	1:180:A:ASP:H	1:183:A:GLU:HA	7	0.22
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB1	3	0.22
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB1	3	0.22
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB1	9	0.22
(1,1336)	1:188:B:ASN:H	1:187:B:LYS:HG3	4	0.22
(1,1195)	1:188:A:ASN:HA	1:191:A:GLU:HB2	1	0.22
(1,1136)	1:188:B:ASN:HD22	1:188:B:ASN:HA	3	0.22
(1,1136)	1:188:B:ASN:HD22	1:188:B:ASN:HA	4	0.22
(1,1135)	1:188:A:ASN:HD22	1:188:A:ASN:HA	3	0.22
(1,1103)	1:179:A:TRP:HE1	1:176:A:THR:HG22	4	0.22
(1,1062)	1:189:B:ASN:HB2	1:191:B:GLU:H	7	0.22
(1,1061)	1:189:A:ASN:HB2	1:191:A:GLU:H	7	0.22
(1,882)	1:192:B:ASN:HB3	1:191:B:GLU:HA	3	0.22
(1,881)	1:192:A:ASN:HB3	1:191:A:GLU:HA	3	0.22
(1,852)	1:182:B:ILE:HA	1:185:B:LEU:HB2	6	0.22
(1,852)	1:182:B:ILE:HA	1:185:B:LEU:HB2	9	0.22
(1,851)	1:182:A:ILE:HA	1:185:A:LEU:HB2	6	0.22
(1,851)	1:182:A:ILE:HA	1:185:A:LEU:HB2	9	0.22
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG23	4	0.22
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG23	4	0.22
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG21	7	0.22
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG21	9	0.22
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD21	2	0.22
(1,722)	1:190:B:PHE:HA	1:189:B:ASN:HB3	8	0.22
(1,721)	1:190:A:PHE:HA	1:189:A:ASN:HB3	8	0.22
(1,698)	1:184:B:ALA:HA	1:183:B:GLU:HB3	2	0.22
(1,697)	1:184:A:ALA:HA	1:183:A:GLU:HB3	2	0.22
(1,697)	1:184:A:ALA:HA	1:183:A:GLU:HB3	5	0.22
(1,648)	1:195:B:ALA:HB1	1:198:B:ARG:HD3	5	0.22
(1,647)	1:195:A:ALA:HB1	1:198:A:ARG:HD3	5	0.22
(1,544)	1:199:B:GLN:HA	1:202:B:GLU:H	5	0.22
(1,543)	1:199:A:GLN:HA	1:202:A:GLU:H	5	0.22
(1,480)	1:192:B:ASN:H	1:192:B:ASN:HA	7	0.22
(1,78)	1:200:B:VAL:HG13	1:208:A:TRP:HZ3	2	0.22
(1,78)	1:200:B:VAL:HG12	1:208:A:TRP:HZ3	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG11	4	0.22
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB2	7	0.22
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB2	7	0.22
(1,32)	1:201:B:MET:HE3	1:179:B:TRP:HZ3	7	0.22
(1,31)	1:201:A:MET:HE3	1:179:A:TRP:HZ3	7	0.22
(1,25)	1:201:A:MET:HE3	1:179:A:TRP:HB3	1	0.22
(1,2870)	1:209:B:SER:H	1:206:B:LYS:HE3	10	0.21
(1,2869)	1:209:A:SER:H	1:206:A:LYS:HE3	10	0.21
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD13	6	0.21
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD21	6	0.21
(1,2737)	1:197:A:VAL:H	1:187:A:LYS:H	7	0.21
(1,2688)	1:202:B:GLU:H	1:197:B:VAL:HA	9	0.21
(1,2687)	1:202:A:GLU:H	1:197:A:VAL:HA	9	0.21
(1,2673)	1:202:A:GLU:H	1:179:A:TRP:HE3	3	0.21
(1,2606)	1:207:B:GLY:H	1:205:B:GLN:HA	9	0.21
(1,2605)	1:207:A:GLY:H	1:205:A:GLN:HA	9	0.21
(1,2590)	1:208:B:TRP:H	1:203:A:ARG:HG2	7	0.21
(1,2566)	1:208:B:TRP:HE1	1:209:B:SER:HA	5	0.21
(1,2565)	1:208:A:TRP:HE1	1:209:A:SER:HA	5	0.21
(1,2488)	1:180:B:ASP:H	1:178:B:PRO:HG2	8	0.21
(1,2487)	1:180:A:ASP:H	1:178:A:PRO:HG2	5	0.21
(1,2442)	1:204:B:LEU:H	1:204:B:LEU:HD23	2	0.21
(1,2441)	1:204:A:LEU:H	1:204:A:LEU:HD23	2	0.21
(1,2396)	1:207:B:GLY:HA3	1:206:B:LYS:HG2	2	0.21
(1,2395)	1:207:A:GLY:HA3	1:206:A:LYS:HG2	2	0.21
(1,2381)	1:182:A:ILE:HD12	1:186:B:LEU:H	2	0.21
(1,2381)	1:182:A:ILE:HD11	1:186:B:LEU:H	8	0.21
(1,2320)	1:210:B:LEU:HD13	1:210:B:LEU:HB2	7	0.21
(1,2288)	1:182:B:ILE:HG21	1:183:B:GLU:HA	5	0.21
(1,2287)	1:182:A:ILE:HG21	1:183:A:GLU:HA	5	0.21
(1,2276)	1:202:B:GLU:HA	1:202:B:GLU:HB2	1	0.21
(1,2221)	1:208:A:TRP:HA	1:207:B:GLY:H	2	0.21
(1,2193)	1:173:A:GLN:HA	1:174:A:GLU:H	10	0.21
(1,2174)	1:203:B:ARG:HD2	1:208:A:TRP:HZ3	3	0.21
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD22	4	0.21
(1,2106)	1:177:B:VAL:HG21	1:208:B:TRP:HE3	8	0.21
(1,2105)	1:177:A:VAL:HG21	1:208:A:TRP:HE3	8	0.21
(1,2102)	1:204:B:LEU:HD13	1:179:B:TRP:HZ3	4	0.21
(1,2101)	1:204:A:LEU:HD13	1:179:A:TRP:HZ3	4	0.21
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG13	6	0.21
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG13	6	0.21
(1,1987)	1:173:B:GLN:H	1:173:B:GLN:HE22	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1677)	1:199:A:GLN:HE22	1:198:A:ARG:HD3	3	0.21
(1,1630)	1:203:B:ARG:H	1:179:B:TRP:HZ3	4	0.21
(1,1629)	1:203:A:ARG:H	1:179:A:TRP:HZ3	4	0.21
(1,1542)	1:206:B:LYS:H	1:206:B:LYS:HE3	2	0.21
(1,1530)	1:207:B:GLY:H	1:206:B:LYS:HB2	7	0.21
(1,1530)	1:207:B:GLY:H	1:206:B:LYS:HB2	9	0.21
(1,1529)	1:207:A:GLY:H	1:206:A:LYS:HB2	9	0.21
(1,1434)	1:210:B:LEU:H	1:208:B:TRP:HB2	2	0.21
(1,1433)	1:210:A:LEU:H	1:208:A:TRP:HB2	5	0.21
(1,1433)	1:210:A:LEU:H	1:208:A:TRP:HB2	6	0.21
(1,1412)	1:212:B:LYS:H	1:212:B:LYS:HG2	8	0.21
(1,1411)	1:212:A:LYS:H	1:212:A:LYS:HG2	8	0.21
(1,1354)	1:197:B:VAL:H	1:195:B:ALA:HB3	5	0.21
(1,1335)	1:188:A:ASN:H	1:187:A:LYS:HG3	4	0.21
(1,1262)	1:176:B:THR:HG21	1:177:B:VAL:HB	9	0.21
(1,1261)	1:176:A:THR:HG21	1:177:A:VAL:HB	9	0.21
(1,1196)	1:188:B:ASN:HA	1:191:B:GLU:HB2	1	0.21
(1,1196)	1:188:B:ASN:HA	1:191:B:GLU:HB2	6	0.21
(1,1195)	1:188:A:ASN:HA	1:191:A:GLU:HB2	6	0.21
(1,1186)	1:175:B:LEU:HA	1:196:A:ALA:HB3	3	0.21
(1,1104)	1:179:B:TRP:HE1	1:176:B:THR:HG22	4	0.21
(1,1072)	1:175:B:LEU:HD12	1:201:A:MET:H	2	0.21
(1,1072)	1:175:B:LEU:HD11	1:201:A:MET:H	9	0.21
(1,1053)	1:199:A:GLN:HG3	1:175:B:LEU:HD12	4	0.21
(1,1030)	1:182:B:ILE:HD12	1:178:B:PRO:HB2	9	0.21
(1,1029)	1:182:A:ILE:HD12	1:178:A:PRO:HB2	9	0.21
(1,860)	1:200:B:VAL:HA	1:175:A:LEU:HB3	1	0.21
(1,859)	1:200:A:VAL:HA	1:175:B:LEU:HB3	1	0.21
(1,852)	1:182:B:ILE:HA	1:185:B:LEU:HB2	3	0.21
(1,852)	1:182:B:ILE:HA	1:185:B:LEU:HB2	8	0.21
(1,851)	1:182:A:ILE:HA	1:185:A:LEU:HB2	3	0.21
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG21	7	0.21
(1,832)	1:182:B:ILE:HG23	1:179:B:TRP:HA	10	0.21
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD21	6	0.21
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB3	3	0.21
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB3	4	0.21
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB1	7	0.21
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB2	9	0.21
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB1	10	0.21
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB3	3	0.21
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB1	4	0.21
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB2	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB1	10	0.21
(1,697)	1:184:A:ALA:HA	1:183:A:GLU:HB3	7	0.21
(1,686)	1:192:B:ASN:HA	1:192:B:ASN:HB3	5	0.21
(1,686)	1:192:B:ASN:HA	1:192:B:ASN:HB3	7	0.21
(1,685)	1:192:A:ASN:HA	1:192:A:ASN:HB3	5	0.21
(1,685)	1:192:A:ASN:HA	1:192:A:ASN:HB3	6	0.21
(1,685)	1:192:A:ASN:HA	1:192:A:ASN:HB3	10	0.21
(1,646)	1:198:B:ARG:HD3	1:198:B:ARG:HB2	10	0.21
(1,645)	1:198:A:ARG:HD3	1:198:A:ARG:HB2	10	0.21
(1,544)	1:199:B:GLN:HA	1:202:B:GLU:H	4	0.21
(1,543)	1:199:A:GLN:HA	1:202:A:GLU:H	4	0.21
(1,524)	1:191:B:GLU:H	1:191:B:GLU:HA	5	0.21
(1,523)	1:191:A:GLU:H	1:191:A:GLU:HA	5	0.21
(1,480)	1:192:B:ASN:H	1:192:B:ASN:HA	4	0.21
(1,479)	1:192:A:ASN:H	1:192:A:ASN:HA	4	0.21
(1,479)	1:192:A:ASN:H	1:192:A:ASN:HA	7	0.21
(1,397)	1:175:A:LEU:HB2	1:190:B:PHE:HZ	2	0.21
(1,360)	1:188:B:ASN:H	1:189:B:ASN:HB2	2	0.21
(1,359)	1:188:A:ASN:H	1:189:A:ASN:HB2	2	0.21
(1,359)	1:188:A:ASN:H	1:189:A:ASN:HB2	9	0.21
(1,300)	1:186:B:LEU:HD22	1:183:B:GLU:HA	10	0.21
(1,299)	1:186:A:LEU:HD22	1:183:A:GLU:HA	10	0.21
(1,229)	1:204:A:LEU:HD12	1:177:B:VAL:HG21	2	0.21
(1,224)	1:177:B:VAL:HG21	1:204:A:LEU:HD12	2	0.21
(1,193)	1:201:A:MET:HE2	1:182:A:ILE:HD13	4	0.21
(1,182)	1:196:B:ALA:HB2	1:193:B:ASP:HB2	7	0.21
(1,181)	1:196:A:ALA:HB2	1:193:A:ASP:HB2	7	0.21
(1,90)	1:195:B:ALA:H	1:197:B:VAL:HG22	10	0.21
(1,89)	1:195:A:ALA:H	1:197:A:VAL:HG22	10	0.21
(1,77)	1:200:A:VAL:HG12	1:208:B:TRP:HZ3	8	0.21
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG11	4	0.21
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG13	9	0.21
(1,42)	1:196:B:ALA:H	1:195:B:ALA:HB2	7	0.21
(1,41)	1:196:A:ALA:H	1:195:A:ALA:HB2	7	0.21
(1,4)	1:177:B:VAL:HG13	1:179:B:TRP:HE3	6	0.21
(1,3)	1:177:A:VAL:HG13	1:179:A:TRP:HE3	6	0.21
(1,2876)	1:205:B:GLN:H	1:177:A:VAL:HG23	7	0.2
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD11	5	0.2
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD13	6	0.2
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD11	5	0.2
(1,2790)	1:189:B:ASN:H	1:191:B:GLU:HA	5	0.2
(1,2789)	1:189:A:ASN:H	1:191:A:GLU:HA	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2772)	1:175:B:LEU:H	1:190:A:PHE:HZ	1	0.2
(1,2771)	1:175:A:LEU:H	1:190:B:PHE:HZ	1	0.2
(1,2741)	1:196:A:ALA:H	1:175:B:LEU:HD13	7	0.2
(1,2738)	1:197:B:VAL:H	1:187:B:LYS:H	7	0.2
(1,2674)	1:202:B:GLU:H	1:179:B:TRP:HE3	3	0.2
(1,2590)	1:208:B:TRP:H	1:203:A:ARG:HG2	6	0.2
(1,2589)	1:208:A:TRP:H	1:203:B:ARG:HG2	6	0.2
(1,2589)	1:208:A:TRP:H	1:203:B:ARG:HG2	7	0.2
(1,2589)	1:208:A:TRP:H	1:203:B:ARG:HG2	9	0.2
(1,2572)	1:208:B:TRP:HE1	1:203:A:ARG:HB3	8	0.2
(1,2571)	1:208:A:TRP:HE1	1:203:B:ARG:HB3	8	0.2
(1,2564)	1:209:B:SER:H	1:210:B:LEU:HD23	1	0.2
(1,2533)	1:181:A:ASP:H	1:185:B:LEU:HD12	10	0.2
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD12	10	0.2
(1,2511)	1:176:A:THR:H	1:174:A:GLU:HB3	6	0.2
(1,2502)	1:198:B:ARG:H	1:197:B:VAL:HG11	8	0.2
(1,2501)	1:198:A:ARG:H	1:197:A:VAL:HG11	8	0.2
(1,2488)	1:180:B:ASP:H	1:178:B:PRO:HG2	3	0.2
(1,2488)	1:180:B:ASP:H	1:178:B:PRO:HG2	4	0.2
(1,2487)	1:180:A:ASP:H	1:178:A:PRO:HG2	3	0.2
(1,2487)	1:180:A:ASP:H	1:178:A:PRO:HG2	4	0.2
(1,2486)	1:180:B:ASP:H	1:201:B:MET:HE2	7	0.2
(1,2485)	1:180:A:ASP:H	1:201:A:MET:HE2	7	0.2
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD21	9	0.2
(1,2384)	1:202:B:GLU:HG3	1:203:B:ARG:H	2	0.2
(1,2384)	1:202:B:GLU:HG3	1:203:B:ARG:H	5	0.2
(1,2383)	1:202:A:GLU:HG3	1:203:A:ARG:H	2	0.2
(1,2383)	1:202:A:GLU:HG3	1:203:A:ARG:H	5	0.2
(1,2383)	1:202:A:GLU:HG3	1:203:A:ARG:H	6	0.2
(1,2382)	1:182:B:ILE:HD11	1:186:A:LEU:H	6	0.2
(1,2354)	1:206:B:LYS:HG3	1:210:B:LEU:H	9	0.2
(1,2353)	1:206:A:LYS:HG3	1:210:A:LEU:H	9	0.2
(1,2330)	1:199:B:GLN:HG3	1:196:B:ALA:H	4	0.2
(1,2329)	1:199:A:GLN:HG3	1:196:A:ALA:H	4	0.2
(1,2319)	1:210:A:LEU:HD11	1:210:A:LEU:HB2	9	0.2
(1,2319)	1:210:A:LEU:HD12	1:210:A:LEU:HB2	10	0.2
(1,2276)	1:202:B:GLU:HA	1:202:B:GLU:HB2	2	0.2
(1,2276)	1:202:B:GLU:HA	1:202:B:GLU:HB2	3	0.2
(1,2276)	1:202:B:GLU:HA	1:202:B:GLU:HB2	4	0.2
(1,2276)	1:202:B:GLU:HA	1:202:B:GLU:HB2	5	0.2
(1,2276)	1:202:B:GLU:HA	1:202:B:GLU:HB2	6	0.2
(1,2276)	1:202:B:GLU:HA	1:202:B:GLU:HB2	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2276)	1:202:B:GLU:HA	1:202:B:GLU:HB2	8	0.2
(1,2276)	1:202:B:GLU:HA	1:202:B:GLU:HB2	9	0.2
(1,2276)	1:202:B:GLU:HA	1:202:B:GLU:HB2	10	0.2
(1,2275)	1:202:A:GLU:HA	1:202:A:GLU:HB2	1	0.2
(1,2275)	1:202:A:GLU:HA	1:202:A:GLU:HB2	2	0.2
(1,2275)	1:202:A:GLU:HA	1:202:A:GLU:HB2	3	0.2
(1,2275)	1:202:A:GLU:HA	1:202:A:GLU:HB2	4	0.2
(1,2275)	1:202:A:GLU:HA	1:202:A:GLU:HB2	5	0.2
(1,2275)	1:202:A:GLU:HA	1:202:A:GLU:HB2	6	0.2
(1,2275)	1:202:A:GLU:HA	1:202:A:GLU:HB2	7	0.2
(1,2275)	1:202:A:GLU:HA	1:202:A:GLU:HB2	8	0.2
(1,2275)	1:202:A:GLU:HA	1:202:A:GLU:HB2	9	0.2
(1,2275)	1:202:A:GLU:HA	1:202:A:GLU:HB2	10	0.2
(1,2226)	1:208:B:TRP:HA	1:208:B:TRP:HE3	6	0.2
(1,2226)	1:208:B:TRP:HA	1:208:B:TRP:HE3	10	0.2
(1,2225)	1:208:A:TRP:HA	1:208:A:TRP:HE3	6	0.2
(1,2225)	1:208:A:TRP:HA	1:208:A:TRP:HE3	10	0.2
(1,2222)	1:208:B:TRP:HA	1:207:A:GLY:H	2	0.2
(1,2221)	1:208:A:TRP:HA	1:207:B:GLY:H	9	0.2
(1,2164)	1:189:B:ASN:HB3	1:186:B:LEU:HD22	8	0.2
(1,2163)	1:189:A:ASN:HB3	1:186:A:LEU:HD22	8	0.2
(1,2110)	1:177:B:VAL:HG22	1:179:B:TRP:HH2	10	0.2
(1,2109)	1:177:A:VAL:HG22	1:179:A:TRP:HH2	10	0.2
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG11	5	0.2
(1,1922)	1:179:B:TRP:H	1:179:B:TRP:HZ3	9	0.2
(1,1921)	1:179:A:TRP:H	1:179:A:TRP:HZ3	9	0.2
(1,1572)	1:192:B:ASN:HD22	1:192:B:ASN:HB2	7	0.2
(1,1571)	1:192:A:ASN:HD22	1:192:A:ASN:HB2	7	0.2
(1,1542)	1:206:B:LYS:H	1:206:B:LYS:HE3	7	0.2
(1,1541)	1:206:A:LYS:H	1:206:A:LYS:HE3	2	0.2
(1,1541)	1:206:A:LYS:H	1:206:A:LYS:HE3	7	0.2
(1,1530)	1:207:B:GLY:H	1:206:B:LYS:HB2	4	0.2
(1,1529)	1:207:A:GLY:H	1:206:A:LYS:HB2	4	0.2
(1,1434)	1:210:B:LEU:H	1:208:B:TRP:HB2	6	0.2
(1,1433)	1:210:A:LEU:H	1:208:A:TRP:HB2	1	0.2
(1,1409)	1:212:A:LYS:H	1:212:A:LYS:HB3	1	0.2
(1,1408)	1:212:B:LYS:H	1:203:A:ARG:HD3	8	0.2
(1,1353)	1:197:A:VAL:H	1:195:A:ALA:HB3	5	0.2
(1,1106)	1:176:B:THR:HG21	1:179:B:TRP:HD1	6	0.2
(1,1094)	1:191:B:GLU:HB2	1:191:B:GLU:H	2	0.2
(1,1094)	1:191:B:GLU:HB2	1:191:B:GLU:H	3	0.2
(1,1094)	1:191:B:GLU:HB2	1:191:B:GLU:H	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1094)	1:191:B:GLU:HB2	1:191:B:GLU:H	7	0.2
(1,1094)	1:191:B:GLU:HB2	1:191:B:GLU:H	8	0.2
(1,1094)	1:191:B:GLU:HB2	1:191:B:GLU:H	9	0.2
(1,1093)	1:191:A:GLU:HB2	1:191:A:GLU:H	2	0.2
(1,1093)	1:191:A:GLU:HB2	1:191:A:GLU:H	3	0.2
(1,1093)	1:191:A:GLU:HB2	1:191:A:GLU:H	6	0.2
(1,1093)	1:191:A:GLU:HB2	1:191:A:GLU:H	7	0.2
(1,1093)	1:191:A:GLU:HB2	1:191:A:GLU:H	8	0.2
(1,1093)	1:191:A:GLU:HB2	1:191:A:GLU:H	9	0.2
(1,1071)	1:175:A:LEU:HD12	1:201:B:MET:H	2	0.2
(1,1054)	1:199:B:GLN:HG3	1:175:A:LEU:HD13	1	0.2
(1,1053)	1:199:A:GLN:HG3	1:175:B:LEU:HD13	1	0.2
(1,1002)	1:199:B:GLN:H	1:197:B:VAL:HB	8	0.2
(1,1001)	1:199:A:GLN:H	1:197:A:VAL:HB	8	0.2
(1,916)	1:199:B:GLN:HG2	1:175:A:LEU:HD12	4	0.2
(1,915)	1:199:A:GLN:HG2	1:175:B:LEU:HD12	4	0.2
(1,860)	1:200:B:VAL:HA	1:175:A:LEU:HB3	2	0.2
(1,859)	1:200:A:VAL:HA	1:175:B:LEU:HB3	2	0.2
(1,859)	1:200:A:VAL:HA	1:175:B:LEU:HB3	5	0.2
(1,851)	1:182:A:ILE:HA	1:185:A:LEU:HB2	4	0.2
(1,851)	1:182:A:ILE:HA	1:185:A:LEU:HB2	8	0.2
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG22	6	0.2
(1,844)	1:176:B:THR:HA	1:177:B:VAL:HG23	10	0.2
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG22	6	0.2
(1,831)	1:182:A:ILE:HG23	1:179:A:TRP:HA	10	0.2
(1,822)	1:208:B:TRP:HA	1:203:A:ARG:HG3	1	0.2
(1,821)	1:208:A:TRP:HA	1:203:B:ARG:HG3	1	0.2
(1,722)	1:190:B:PHE:HA	1:189:B:ASN:HB3	10	0.2
(1,721)	1:190:A:PHE:HA	1:189:A:ASN:HB3	4	0.2
(1,721)	1:190:A:PHE:HA	1:189:A:ASN:HB3	5	0.2
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB2	1	0.2
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB3	2	0.2
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB1	5	0.2
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB1	6	0.2
(1,708)	1:195:B:ALA:HA	1:195:B:ALA:HB2	8	0.2
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB2	1	0.2
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB1	5	0.2
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB1	6	0.2
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB1	7	0.2
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB2	8	0.2
(1,698)	1:184:B:ALA:HA	1:183:B:GLU:HB3	7	0.2
(1,686)	1:192:B:ASN:HA	1:192:B:ASN:HB3	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,686)	1:192:B:ASN:HA	1:192:B:ASN:HB3	2	0.2
(1,686)	1:192:B:ASN:HA	1:192:B:ASN:HB3	3	0.2
(1,686)	1:192:B:ASN:HA	1:192:B:ASN:HB3	4	0.2
(1,686)	1:192:B:ASN:HA	1:192:B:ASN:HB3	6	0.2
(1,686)	1:192:B:ASN:HA	1:192:B:ASN:HB3	8	0.2
(1,686)	1:192:B:ASN:HA	1:192:B:ASN:HB3	9	0.2
(1,686)	1:192:B:ASN:HA	1:192:B:ASN:HB3	10	0.2
(1,685)	1:192:A:ASN:HA	1:192:A:ASN:HB3	1	0.2
(1,685)	1:192:A:ASN:HA	1:192:A:ASN:HB3	2	0.2
(1,685)	1:192:A:ASN:HA	1:192:A:ASN:HB3	3	0.2
(1,685)	1:192:A:ASN:HA	1:192:A:ASN:HB3	4	0.2
(1,685)	1:192:A:ASN:HA	1:192:A:ASN:HB3	7	0.2
(1,685)	1:192:A:ASN:HA	1:192:A:ASN:HB3	8	0.2
(1,685)	1:192:A:ASN:HA	1:192:A:ASN:HB3	9	0.2
(1,544)	1:199:B:GLN:HA	1:202:B:GLU:H	1	0.2
(1,544)	1:199:B:GLN:HA	1:202:B:GLU:H	10	0.2
(1,480)	1:192:B:ASN:H	1:192:B:ASN:HA	2	0.2
(1,480)	1:192:B:ASN:H	1:192:B:ASN:HA	8	0.2
(1,480)	1:192:B:ASN:H	1:192:B:ASN:HA	9	0.2
(1,479)	1:192:A:ASN:H	1:192:A:ASN:HA	2	0.2
(1,479)	1:192:A:ASN:H	1:192:A:ASN:HA	8	0.2
(1,479)	1:192:A:ASN:H	1:192:A:ASN:HA	9	0.2
(1,444)	1:192:B:ASN:H	1:192:B:ASN:HB2	3	0.2
(1,444)	1:192:B:ASN:H	1:192:B:ASN:HB2	10	0.2
(1,443)	1:192:A:ASN:H	1:192:A:ASN:HB2	3	0.2
(1,443)	1:192:A:ASN:H	1:192:A:ASN:HB2	10	0.2
(1,398)	1:175:B:LEU:HB2	1:190:A:PHE:HZ	8	0.2
(1,261)	1:175:A:LEU:HD12	1:199:B:GLN:HG3	6	0.2
(1,246)	1:200:B:VAL:HG13	1:197:B:VAL:HA	9	0.2
(1,245)	1:200:A:VAL:HG13	1:197:A:VAL:HA	9	0.2
(1,230)	1:204:B:LEU:HD12	1:177:A:VAL:HG21	2	0.2
(1,226)	1:177:B:VAL:HG21	1:200:A:VAL:HG11	2	0.2
(1,225)	1:177:A:VAL:HG21	1:200:B:VAL:HG11	2	0.2
(1,223)	1:177:A:VAL:HG21	1:204:B:LEU:HD12	2	0.2
(1,194)	1:201:B:MET:HE2	1:182:B:ILE:HD13	4	0.2
(1,77)	1:200:A:VAL:HG12	1:208:B:TRP:HZ3	4	0.2
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG13	9	0.2
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG11	3	0.2
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD22	6	0.2
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD22	6	0.2
(1,25)	1:201:A:MET:HE1	1:179:A:TRP:HB3	4	0.2
(1,4)	1:177:B:VAL:HG13	1:179:B:TRP:HE3	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2876)	1:205:B:GLN:H	1:177:A:VAL:HG22	1	0.19
(1,2876)	1:205:B:GLN:H	1:177:A:VAL:HG22	2	0.19
(1,2875)	1:205:A:GLN:H	1:177:B:VAL:HG22	1	0.19
(1,2875)	1:205:A:GLN:H	1:177:B:VAL:HG23	7	0.19
(1,2874)	1:204:B:LEU:H	1:182:B:ILE:HD13	7	0.19
(1,2870)	1:209:B:SER:H	1:206:B:LYS:HE3	3	0.19
(1,2789)	1:189:A:ASN:H	1:191:A:GLU:HA	6	0.19
(1,2771)	1:175:A:LEU:H	1:190:B:PHE:HZ	9	0.19
(1,2742)	1:196:B:ALA:H	1:175:A:LEU:HD13	7	0.19
(1,2626)	1:206:B:LYS:H	1:203:B:ARG:HG3	10	0.19
(1,2625)	1:206:A:LYS:H	1:203:A:ARG:HG3	10	0.19
(1,2606)	1:207:B:GLY:H	1:205:B:GLN:HA	10	0.19
(1,2605)	1:207:A:GLY:H	1:205:A:GLN:HA	10	0.19
(1,2590)	1:208:B:TRP:H	1:203:A:ARG:HG2	3	0.19
(1,2589)	1:208:A:TRP:H	1:203:B:ARG:HG2	4	0.19
(1,2563)	1:209:A:SER:H	1:210:A:LEU:HD23	1	0.19
(1,2554)	1:210:B:LEU:H	1:206:B:LYS:HE3	2	0.19
(1,2534)	1:181:B:ASP:H	1:185:A:LEU:HD12	10	0.19
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD12	7	0.19
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD12	10	0.19
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD12	7	0.19
(1,2512)	1:176:B:THR:H	1:174:B:GLU:HB3	6	0.19
(1,2488)	1:180:B:ASP:H	1:178:B:PRO:HG2	1	0.19
(1,2487)	1:180:A:ASP:H	1:178:A:PRO:HG2	1	0.19
(1,2487)	1:180:A:ASP:H	1:178:A:PRO:HG2	10	0.19
(1,2484)	1:180:B:ASP:H	1:182:B:ILE:HA	2	0.19
(1,2484)	1:180:B:ASP:H	1:182:B:ILE:HA	9	0.19
(1,2483)	1:180:A:ASP:H	1:182:A:ILE:HA	2	0.19
(1,2396)	1:207:B:GLY:HA3	1:206:B:LYS:HG2	7	0.19
(1,2395)	1:207:A:GLY:HA3	1:206:A:LYS:HG2	7	0.19
(1,2384)	1:202:B:GLU:HG3	1:203:B:ARG:H	6	0.19
(1,2342)	1:204:B:LEU:HG	1:182:A:ILE:HD12	4	0.19
(1,2326)	1:197:B:VAL:HG12	1:198:B:ARG:HA	1	0.19
(1,2325)	1:197:A:VAL:HG12	1:198:A:ARG:HA	1	0.19
(1,2320)	1:210:B:LEU:HD12	1:210:B:LEU:HB2	2	0.19
(1,2320)	1:210:B:LEU:HD11	1:210:B:LEU:HB2	3	0.19
(1,2320)	1:210:B:LEU:HD11	1:210:B:LEU:HB2	9	0.19
(1,2320)	1:210:B:LEU:HD12	1:210:B:LEU:HB2	10	0.19
(1,2319)	1:210:A:LEU:HD12	1:210:A:LEU:HB2	2	0.19
(1,2319)	1:210:A:LEU:HD11	1:210:A:LEU:HB2	3	0.19
(1,2286)	1:183:B:GLU:HB3	1:183:B:GLU:HA	1	0.19
(1,2286)	1:183:B:GLU:HB3	1:183:B:GLU:HA	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2286)	1:183:B:GLU:HB3	1:183:B:GLU:HA	3	0.19
(1,2286)	1:183:B:GLU:HB3	1:183:B:GLU:HA	4	0.19
(1,2286)	1:183:B:GLU:HB3	1:183:B:GLU:HA	5	0.19
(1,2286)	1:183:B:GLU:HB3	1:183:B:GLU:HA	7	0.19
(1,2286)	1:183:B:GLU:HB3	1:183:B:GLU:HA	8	0.19
(1,2286)	1:183:B:GLU:HB3	1:183:B:GLU:HA	9	0.19
(1,2286)	1:183:B:GLU:HB3	1:183:B:GLU:HA	10	0.19
(1,2285)	1:183:A:GLU:HB3	1:183:A:GLU:HA	1	0.19
(1,2285)	1:183:A:GLU:HB3	1:183:A:GLU:HA	2	0.19
(1,2285)	1:183:A:GLU:HB3	1:183:A:GLU:HA	3	0.19
(1,2285)	1:183:A:GLU:HB3	1:183:A:GLU:HA	4	0.19
(1,2285)	1:183:A:GLU:HB3	1:183:A:GLU:HA	5	0.19
(1,2285)	1:183:A:GLU:HB3	1:183:A:GLU:HA	7	0.19
(1,2285)	1:183:A:GLU:HB3	1:183:A:GLU:HA	8	0.19
(1,2285)	1:183:A:GLU:HB3	1:183:A:GLU:HA	9	0.19
(1,2285)	1:183:A:GLU:HB3	1:183:A:GLU:HA	10	0.19
(1,2254)	1:211:B:ALA:HA	1:206:A:LYS:HG2	3	0.19
(1,2108)	1:177:B:VAL:HG23	1:190:A:PHE:HE2	8	0.19
(1,2102)	1:204:B:LEU:HD12	1:179:B:TRP:HZ3	6	0.19
(1,2101)	1:204:A:LEU:HD12	1:179:A:TRP:HZ3	6	0.19
(1,2088)	1:202:B:GLU:H	1:200:B:VAL:HG22	9	0.19
(1,2087)	1:202:A:GLU:H	1:200:A:VAL:HG22	9	0.19
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG11	5	0.19
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG13	4	0.19
(1,1782)	1:175:B:LEU:H	1:177:B:VAL:HG21	7	0.19
(1,1781)	1:175:A:LEU:H	1:177:A:VAL:HG21	7	0.19
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG13	2	0.19
(1,1630)	1:203:B:ARG:H	1:179:B:TRP:HZ3	2	0.19
(1,1630)	1:203:B:ARG:H	1:179:B:TRP:HZ3	8	0.19
(1,1530)	1:207:B:GLY:H	1:206:B:LYS:HB2	3	0.19
(1,1530)	1:207:B:GLY:H	1:206:B:LYS:HB2	6	0.19
(1,1529)	1:207:A:GLY:H	1:206:A:LYS:HB2	3	0.19
(1,1529)	1:207:A:GLY:H	1:206:A:LYS:HB2	6	0.19
(1,1434)	1:210:B:LEU:H	1:208:B:TRP:HB2	1	0.19
(1,1434)	1:210:B:LEU:H	1:208:B:TRP:HB2	4	0.19
(1,1433)	1:210:A:LEU:H	1:208:A:TRP:HB2	4	0.19
(1,1410)	1:212:B:LYS:H	1:212:B:LYS:HB3	1	0.19
(1,1200)	1:203:B:ARG:HD3	1:212:A:LYS:HA	9	0.19
(1,1186)	1:175:B:LEU:HA	1:196:A:ALA:HB1	6	0.19
(1,1185)	1:175:A:LEU:HA	1:196:B:ALA:HB1	6	0.19
(1,1150)	1:178:B:PRO:HD3	1:177:B:VAL:HG23	8	0.19
(1,1149)	1:178:A:PRO:HD3	1:177:A:VAL:HG23	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1105)	1:176:A:THR:HG21	1:179:A:TRP:HD1	6	0.19
(1,1094)	1:191:B:GLU:HB2	1:191:B:GLU:H	1	0.19
(1,1094)	1:191:B:GLU:HB2	1:191:B:GLU:H	4	0.19
(1,1094)	1:191:B:GLU:HB2	1:191:B:GLU:H	10	0.19
(1,1093)	1:191:A:GLU:HB2	1:191:A:GLU:H	1	0.19
(1,1093)	1:191:A:GLU:HB2	1:191:A:GLU:H	4	0.19
(1,1093)	1:191:A:GLU:HB2	1:191:A:GLU:H	10	0.19
(1,1072)	1:175:B:LEU:HD11	1:201:A:MET:H	1	0.19
(1,1071)	1:175:A:LEU:HD11	1:201:B:MET:H	1	0.19
(1,860)	1:200:B:VAL:HA	1:175:A:LEU:HB3	4	0.19
(1,859)	1:200:A:VAL:HA	1:175:B:LEU:HB3	4	0.19
(1,852)	1:182:B:ILE:HA	1:185:B:LEU:HB2	4	0.19
(1,843)	1:176:A:THR:HA	1:177:A:VAL:HG23	10	0.19
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD21	6	0.19
(1,744)	1:184:B:ALA:HB1	1:181:B:ASP:HA	10	0.19
(1,743)	1:184:A:ALA:HB1	1:181:A:ASP:HA	10	0.19
(1,722)	1:190:B:PHE:HA	1:189:B:ASN:HB3	4	0.19
(1,722)	1:190:B:PHE:HA	1:189:B:ASN:HB3	5	0.19
(1,721)	1:190:A:PHE:HA	1:189:A:ASN:HB3	10	0.19
(1,707)	1:195:A:ALA:HA	1:195:A:ALA:HB3	2	0.19
(1,544)	1:199:B:GLN:HA	1:202:B:GLU:H	8	0.19
(1,543)	1:199:A:GLN:HA	1:202:A:GLU:H	1	0.19
(1,543)	1:199:A:GLN:HA	1:202:A:GLU:H	8	0.19
(1,543)	1:199:A:GLN:HA	1:202:A:GLU:H	10	0.19
(1,524)	1:191:B:GLU:H	1:191:B:GLU:HA	2	0.19
(1,524)	1:191:B:GLU:H	1:191:B:GLU:HA	8	0.19
(1,524)	1:191:B:GLU:H	1:191:B:GLU:HA	10	0.19
(1,523)	1:191:A:GLU:H	1:191:A:GLU:HA	2	0.19
(1,523)	1:191:A:GLU:H	1:191:A:GLU:HA	8	0.19
(1,523)	1:191:A:GLU:H	1:191:A:GLU:HA	10	0.19
(1,480)	1:192:B:ASN:H	1:192:B:ASN:HA	3	0.19
(1,480)	1:192:B:ASN:H	1:192:B:ASN:HA	10	0.19
(1,479)	1:192:A:ASN:H	1:192:A:ASN:HA	3	0.19
(1,479)	1:192:A:ASN:H	1:192:A:ASN:HA	6	0.19
(1,479)	1:192:A:ASN:H	1:192:A:ASN:HA	10	0.19
(1,360)	1:188:B:ASN:H	1:189:B:ASN:HB2	7	0.19
(1,359)	1:188:A:ASN:H	1:189:A:ASN:HB2	7	0.19
(1,234)	1:200:B:VAL:HG11	1:177:A:VAL:HG21	2	0.19
(1,233)	1:200:A:VAL:HG11	1:177:B:VAL:HG21	2	0.19
(1,230)	1:204:B:LEU:HD13	1:177:A:VAL:HG22	1	0.19
(1,229)	1:204:A:LEU:HD13	1:177:B:VAL:HG22	1	0.19
(1,224)	1:177:B:VAL:HG22	1:204:A:LEU:HD13	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:177:A:VAL:HG22	1:204:B:LEU:HD13	1	0.19
(1,78)	1:200:B:VAL:HG12	1:208:A:TRP:HZ3	8	0.19
(1,77)	1:200:A:VAL:HG13	1:208:B:TRP:HZ3	7	0.19
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG11	3	0.19
(1,34)	1:205:B:GLN:HE22	1:201:B:MET:HE1	1	0.19
(1,33)	1:205:A:GLN:HE22	1:201:A:MET:HE1	1	0.19
(1,26)	1:201:B:MET:HE3	1:179:B:TRP:HB3	2	0.19
(1,26)	1:201:B:MET:HE1	1:179:B:TRP:HB3	4	0.19
(1,25)	1:201:A:MET:HE3	1:179:A:TRP:HB3	2	0.19
(1,3)	1:177:A:VAL:HG13	1:179:A:TRP:HE3	8	0.19
(1,2873)	1:204:A:LEU:H	1:182:A:ILE:HD13	7	0.18
(1,2869)	1:209:A:SER:H	1:206:A:LYS:HE3	3	0.18
(1,2855)	1:174:A:GLU:H	1:196:B:ALA:HB2	5	0.18
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD13	1	0.18
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD12	9	0.18
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD13	1	0.18
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD12	9	0.18
(1,2790)	1:189:B:ASN:H	1:191:B:GLU:HA	6	0.18
(1,2790)	1:189:B:ASN:H	1:191:B:GLU:HA	8	0.18
(1,2789)	1:189:A:ASN:H	1:191:A:GLU:HA	8	0.18
(1,2738)	1:197:B:VAL:H	1:187:B:LYS:H	8	0.18
(1,2737)	1:197:A:VAL:H	1:187:A:LYS:H	1	0.18
(1,2737)	1:197:A:VAL:H	1:187:A:LYS:H	8	0.18
(1,2712)	1:199:B:GLN:HE22	1:195:B:ALA:HA	6	0.18
(1,2711)	1:199:A:GLN:HE22	1:195:A:ALA:HA	6	0.18
(1,2711)	1:199:A:GLN:HE22	1:195:A:ALA:HA	7	0.18
(1,2709)	1:199:A:GLN:HE22	1:175:B:LEU:HA	3	0.18
(1,2673)	1:202:A:GLU:H	1:179:A:TRP:HE3	8	0.18
(1,2605)	1:207:A:GLY:H	1:205:A:GLN:HA	3	0.18
(1,2590)	1:208:B:TRP:H	1:203:A:ARG:HG2	4	0.18
(1,2590)	1:208:B:TRP:H	1:203:A:ARG:HG2	9	0.18
(1,2589)	1:208:A:TRP:H	1:203:B:ARG:HG2	3	0.18
(1,2586)	1:179:B:TRP:HE1	1:205:B:GLN:HA	1	0.18
(1,2585)	1:179:A:TRP:HE1	1:205:A:GLN:HA	1	0.18
(1,2564)	1:209:B:SER:H	1:210:B:LEU:HD23	5	0.18
(1,2563)	1:209:A:SER:H	1:210:A:LEU:HD23	5	0.18
(1,2553)	1:210:A:LEU:H	1:206:A:LYS:HE3	2	0.18
(1,2501)	1:198:A:ARG:H	1:197:A:VAL:HG12	1	0.18
(1,2488)	1:180:B:ASP:H	1:178:B:PRO:HG2	10	0.18
(1,2483)	1:180:A:ASP:H	1:182:A:ILE:HA	9	0.18
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG22	2	0.18
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG22	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2384)	1:202:B:GLU:HG3	1:203:B:ARG:H	1	0.18
(1,2384)	1:202:B:GLU:HG3	1:203:B:ARG:H	8	0.18
(1,2383)	1:202:A:GLU:HG3	1:203:A:ARG:H	1	0.18
(1,2383)	1:202:A:GLU:HG3	1:203:A:ARG:H	8	0.18
(1,2370)	1:175:B:LEU:HG	1:199:A:GLN:HE22	4	0.18
(1,2354)	1:211:B:ALA:H	1:212:B:LYS:HG2	8	0.18
(1,2353)	1:211:A:ALA:H	1:212:A:LYS:HG2	8	0.18
(1,2320)	1:210:B:LEU:HD11	1:210:B:LEU:HB2	1	0.18
(1,2320)	1:210:B:LEU:HD12	1:210:B:LEU:HB2	4	0.18
(1,2320)	1:210:B:LEU:HD12	1:210:B:LEU:HB2	5	0.18
(1,2320)	1:210:B:LEU:HD11	1:210:B:LEU:HB2	6	0.18
(1,2319)	1:210:A:LEU:HD11	1:210:A:LEU:HB2	1	0.18
(1,2319)	1:210:A:LEU:HD12	1:210:A:LEU:HB2	4	0.18
(1,2319)	1:210:A:LEU:HD12	1:210:A:LEU:HB2	5	0.18
(1,2319)	1:210:A:LEU:HD11	1:210:A:LEU:HB2	6	0.18
(1,2319)	1:210:A:LEU:HD13	1:210:A:LEU:HB2	8	0.18
(1,2286)	1:201:B:MET:HE3	1:183:B:GLU:HA	6	0.18
(1,2285)	1:201:A:MET:HE3	1:183:A:GLU:HA	6	0.18
(1,2280)	1:194:B:GLN:HA	1:197:B:VAL:HB	1	0.18
(1,2280)	1:194:B:GLN:HA	1:197:B:VAL:HB	6	0.18
(1,2279)	1:194:A:GLN:HA	1:197:A:VAL:HB	1	0.18
(1,2253)	1:211:A:ALA:HA	1:206:B:LYS:HG2	3	0.18
(1,2225)	1:208:A:TRP:HA	1:208:A:TRP:HE3	4	0.18
(1,2222)	1:208:B:TRP:HA	1:207:A:GLY:H	9	0.18
(1,2221)	1:208:A:TRP:HA	1:207:B:GLY:H	7	0.18
(1,2194)	1:173:B:GLN:HA	1:174:B:GLU:H	6	0.18
(1,2193)	1:173:A:GLN:HA	1:174:A:GLU:H	6	0.18
(1,2173)	1:203:A:ARG:HD2	1:208:B:TRP:HZ3	3	0.18
(1,2158)	1:181:B:ASP:H	1:182:B:ILE:HB	1	0.18
(1,2118)	1:182:B:ILE:HD12	1:178:B:PRO:HD2	7	0.18
(1,2117)	1:182:A:ILE:HD12	1:178:A:PRO:HD2	7	0.18
(1,2102)	1:204:B:LEU:HD12	1:179:B:TRP:HZ3	5	0.18
(1,2101)	1:204:A:LEU:HD12	1:179:A:TRP:HZ3	5	0.18
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG13	4	0.18
(1,1998)	1:191:B:GLU:H	1:186:B:LEU:HD11	6	0.18
(1,1924)	1:179:B:TRP:H	1:205:B:GLN:HE22	7	0.18
(1,1923)	1:179:A:TRP:H	1:205:A:GLN:HE22	7	0.18
(1,1794)	1:193:B:ASP:H	1:188:B:ASN:HA	1	0.18
(1,1793)	1:193:A:ASP:H	1:188:A:ASN:HA	1	0.18
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG12	8	0.18
(1,1630)	1:203:B:ARG:H	1:179:B:TRP:HZ3	5	0.18
(1,1629)	1:203:A:ARG:H	1:179:A:TRP:HZ3	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1629)	1:203:A:ARG:H	1:179:A:TRP:HZ3	5	0.18
(1,1629)	1:203:A:ARG:H	1:179:A:TRP:HZ3	8	0.18
(1,1530)	1:207:B:GLY:H	1:206:B:LYS:HB2	8	0.18
(1,1529)	1:207:A:GLY:H	1:206:A:LYS:HB2	2	0.18
(1,1529)	1:207:A:GLY:H	1:206:A:LYS:HB2	8	0.18
(1,1262)	1:176:B:THR:HG22	1:177:B:VAL:HB	10	0.18
(1,1261)	1:176:A:THR:HG22	1:177:A:VAL:HB	10	0.18
(1,1192)	1:188:B:ASN:HA	1:191:B:GLU:HG2	4	0.18
(1,1191)	1:188:A:ASN:HA	1:191:A:GLU:HG2	4	0.18
(1,1150)	1:178:B:PRO:HD3	1:177:B:VAL:HG22	7	0.18
(1,1149)	1:178:A:PRO:HD3	1:177:A:VAL:HG22	7	0.18
(1,1094)	1:191:B:GLU:HB2	1:191:B:GLU:H	5	0.18
(1,1093)	1:191:A:GLU:HB2	1:191:A:GLU:H	5	0.18
(1,1071)	1:175:A:LEU:HD11	1:201:B:MET:H	5	0.18
(1,1002)	1:199:B:GLN:H	1:197:B:VAL:HB	9	0.18
(1,1001)	1:199:A:GLN:H	1:197:A:VAL:HB	9	0.18
(1,1000)	1:199:B:GLN:HE22	1:199:B:GLN:HG2	5	0.18
(1,1000)	1:199:B:GLN:HE22	1:199:B:GLN:HG2	9	0.18
(1,999)	1:199:A:GLN:HE22	1:199:A:GLN:HG2	5	0.18
(1,971)	1:204:A:LEU:HD22	1:182:B:ILE:HD11	9	0.18
(1,874)	1:185:B:LEU:HD13	1:188:B:ASN:HB2	5	0.18
(1,852)	1:182:B:ILE:HA	1:185:B:LEU:HB2	10	0.18
(1,851)	1:182:A:ILE:HA	1:185:A:LEU:HB2	10	0.18
(1,782)	1:206:B:LYS:HG2	1:206:B:LYS:HA	7	0.18
(1,781)	1:206:A:LYS:HG2	1:206:A:LYS:HA	7	0.18
(1,745)	1:181:A:ASP:HA	1:185:B:LEU:HD21	8	0.18
(1,744)	1:184:B:ALA:HB1	1:181:B:ASP:HA	3	0.18
(1,743)	1:184:A:ALA:HB1	1:181:A:ASP:HA	3	0.18
(1,738)	1:201:B:MET:HA	1:200:B:VAL:HG22	7	0.18
(1,737)	1:201:A:MET:HA	1:200:A:VAL:HG22	7	0.18
(1,730)	1:186:B:LEU:HA	1:186:B:LEU:HG	1	0.18
(1,730)	1:186:B:LEU:HA	1:186:B:LEU:HG	3	0.18
(1,730)	1:186:B:LEU:HA	1:186:B:LEU:HG	4	0.18
(1,730)	1:186:B:LEU:HA	1:186:B:LEU:HG	8	0.18
(1,729)	1:186:A:LEU:HA	1:186:A:LEU:HG	1	0.18
(1,729)	1:186:A:LEU:HA	1:186:A:LEU:HG	3	0.18
(1,729)	1:186:A:LEU:HA	1:186:A:LEU:HG	4	0.18
(1,729)	1:186:A:LEU:HA	1:186:A:LEU:HG	8	0.18
(1,722)	1:190:B:PHE:HA	1:189:B:ASN:HB3	3	0.18
(1,721)	1:190:A:PHE:HA	1:189:A:ASN:HB3	3	0.18
(1,590)	1:209:B:SER:HB3	1:208:B:TRP:H	10	0.18
(1,524)	1:191:B:GLU:H	1:191:B:GLU:HA	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:191:B:GLU:H	1:191:B:GLU:HA	4	0.18
(1,523)	1:191:A:GLU:H	1:191:A:GLU:HA	3	0.18
(1,523)	1:191:A:GLU:H	1:191:A:GLU:HA	4	0.18
(1,523)	1:191:A:GLU:H	1:191:A:GLU:HA	9	0.18
(1,480)	1:192:B:ASN:H	1:192:B:ASN:HA	1	0.18
(1,480)	1:192:B:ASN:H	1:192:B:ASN:HA	6	0.18
(1,479)	1:192:A:ASN:H	1:192:A:ASN:HA	1	0.18
(1,360)	1:188:B:ASN:H	1:189:B:ASN:HB2	4	0.18
(1,360)	1:188:B:ASN:H	1:189:B:ASN:HB2	10	0.18
(1,359)	1:188:A:ASN:H	1:189:A:ASN:HB2	4	0.18
(1,359)	1:188:A:ASN:H	1:189:A:ASN:HB2	10	0.18
(1,308)	1:199:B:GLN:HB3	1:200:B:VAL:HG11	3	0.18
(1,307)	1:199:A:GLN:HB3	1:200:A:VAL:HG11	3	0.18
(1,78)	1:200:B:VAL:HG13	1:208:A:TRP:HZ3	7	0.18
(1,68)	1:198:B:ARG:H	1:197:B:VAL:HG12	7	0.18
(1,67)	1:198:A:ARG:H	1:197:A:VAL:HG12	7	0.18
(1,41)	1:196:A:ALA:H	1:195:A:ALA:HB3	10	0.18
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB3	5	0.18
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB3	5	0.18
(1,2876)	1:205:B:GLN:H	1:177:B:VAL:HG22	4	0.17
(1,2875)	1:205:A:GLN:H	1:177:B:VAL:HG22	2	0.17
(1,2875)	1:205:A:GLN:H	1:177:A:VAL:HG22	4	0.17
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD11	2	0.17
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD11	2	0.17
(1,2800)	1:186:B:LEU:H	1:197:B:VAL:HG11	7	0.17
(1,2799)	1:186:A:LEU:H	1:197:A:VAL:HG11	7	0.17
(1,2790)	1:189:B:ASN:H	1:191:B:GLU:HA	10	0.17
(1,2789)	1:189:A:ASN:H	1:191:A:GLU:HA	10	0.17
(1,2772)	1:175:B:LEU:H	1:190:A:PHE:HZ	9	0.17
(1,2768)	1:175:B:LEU:H	1:173:B:GLN:HB3	4	0.17
(1,2738)	1:197:B:VAL:H	1:187:B:LYS:H	1	0.17
(1,2674)	1:202:B:GLU:H	1:179:B:TRP:HE3	8	0.17
(1,2606)	1:207:B:GLY:H	1:205:B:GLN:HA	3	0.17
(1,2606)	1:207:B:GLY:H	1:205:B:GLN:HA	4	0.17
(1,2526)	1:212:B:LYS:H	1:210:B:LEU:HB2	5	0.17
(1,2525)	1:212:A:LYS:H	1:210:A:LEU:HB2	5	0.17
(1,2502)	1:198:B:ARG:H	1:197:B:VAL:HG12	1	0.17
(1,2501)	1:198:A:ARG:H	1:197:A:VAL:HG11	5	0.17
(1,2483)	1:180:A:ASP:H	1:178:A:PRO:HD2	8	0.17
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD23	1	0.17
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD23	8	0.17
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD23	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD23	8	0.17
(1,2396)	1:207:B:GLY:HA3	1:206:B:LYS:HG2	10	0.17
(1,2395)	1:207:A:GLY:HA3	1:206:A:LYS:HG2	10	0.17
(1,2384)	1:202:B:GLU:HG3	1:203:B:ARG:H	4	0.17
(1,2383)	1:202:A:GLU:HG3	1:203:A:ARG:H	4	0.17
(1,2369)	1:175:A:LEU:HG	1:199:B:GLN:HE22	4	0.17
(1,2342)	1:204:B:LEU:HG	1:182:A:ILE:HD13	5	0.17
(1,2341)	1:204:A:LEU:HG	1:182:B:ILE:HD13	5	0.17
(1,2330)	1:199:B:GLN:HG3	1:196:B:ALA:H	2	0.17
(1,2329)	1:199:A:GLN:HG3	1:196:A:ALA:H	2	0.17
(1,2320)	1:210:B:LEU:HD13	1:210:B:LEU:HB2	8	0.17
(1,2288)	1:182:B:ILE:HG22	1:183:B:GLU:HA	2	0.17
(1,2287)	1:182:A:ILE:HG22	1:183:A:GLU:HA	2	0.17
(1,2279)	1:194:A:GLN:HA	1:197:A:VAL:HB	6	0.17
(1,2226)	1:208:B:TRP:HA	1:208:B:TRP:HE3	4	0.17
(1,2226)	1:208:B:TRP:HA	1:208:B:TRP:HE3	7	0.17
(1,2225)	1:208:A:TRP:HA	1:208:A:TRP:HE3	7	0.17
(1,2222)	1:208:B:TRP:HA	1:207:A:GLY:H	1	0.17
(1,2222)	1:208:B:TRP:HA	1:207:A:GLY:H	7	0.17
(1,2221)	1:208:A:TRP:HA	1:207:B:GLY:H	1	0.17
(1,2158)	1:181:B:ASP:H	1:182:B:ILE:HB	8	0.17
(1,2157)	1:181:A:ASP:H	1:182:A:ILE:HB	1	0.17
(1,2140)	1:206:B:LYS:HD3	1:203:B:ARG:HA	8	0.17
(1,2139)	1:206:A:LYS:HD3	1:203:A:ARG:HA	8	0.17
(1,2138)	1:187:B:LYS:HD3	1:184:B:ALA:HA	3	0.17
(1,2137)	1:187:A:LYS:HD3	1:184:A:ALA:HA	3	0.17
(1,2097)	1:204:A:LEU:HD23	1:208:B:TRP:H	2	0.17
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD11	6	0.17
(1,1986)	1:173:A:GLN:H	1:175:A:LEU:HD12	9	0.17
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG13	2	0.17
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG11	9	0.17
(1,1738)	1:195:B:ALA:H	1:194:B:GLN:HB3	2	0.17
(1,1737)	1:195:A:ALA:H	1:194:A:GLN:HB3	2	0.17
(1,1693)	1:189:A:ASN:HD22	1:182:B:ILE:HD12	2	0.17
(1,1644)	1:201:B:MET:H	1:186:B:LEU:HA	3	0.17
(1,1542)	1:206:B:LYS:H	1:206:B:LYS:HE3	5	0.17
(1,1541)	1:206:A:LYS:H	1:206:A:LYS:HE3	5	0.17
(1,1541)	1:206:A:LYS:H	1:206:A:LYS:HE3	8	0.17
(1,1530)	1:207:B:GLY:H	1:206:B:LYS:HB2	2	0.17
(1,1530)	1:207:B:GLY:H	1:206:B:LYS:HB2	5	0.17
(1,1529)	1:207:A:GLY:H	1:206:A:LYS:HB2	5	0.17
(1,1434)	1:210:B:LEU:H	1:208:B:TRP:HB2	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1433)	1:210:A:LEU:H	1:208:A:TRP:HB2	3	0.17
(1,1398)	1:202:B:GLU:H	1:200:B:VAL:HG12	7	0.17
(1,1397)	1:202:A:GLU:H	1:200:A:VAL:HG12	7	0.17
(1,1320)	1:204:B:LEU:H	1:179:B:TRP:HE3	7	0.17
(1,1319)	1:204:A:LEU:H	1:179:A:TRP:HE3	7	0.17
(1,1185)	1:175:A:LEU:HA	1:196:B:ALA:HB3	3	0.17
(1,1184)	1:199:B:GLN:HA	1:175:A:LEU:HD13	10	0.17
(1,1072)	1:175:B:LEU:HD11	1:201:A:MET:H	3	0.17
(1,1062)	1:189:B:ASN:HB2	1:191:B:GLU:H	9	0.17
(1,1061)	1:189:A:ASN:HB2	1:191:A:GLU:H	9	0.17
(1,1002)	1:199:B:GLN:H	1:197:B:VAL:HB	5	0.17
(1,1002)	1:199:B:GLN:H	1:197:B:VAL:HB	6	0.17
(1,1001)	1:199:A:GLN:H	1:197:A:VAL:HB	5	0.17
(1,1001)	1:199:A:GLN:H	1:197:A:VAL:HB	6	0.17
(1,1000)	1:199:B:GLN:HE22	1:199:B:GLN:HG2	1	0.17
(1,1000)	1:199:B:GLN:HE22	1:199:B:GLN:HG2	2	0.17
(1,1000)	1:199:B:GLN:HE22	1:199:B:GLN:HG2	3	0.17
(1,1000)	1:199:B:GLN:HE22	1:199:B:GLN:HG2	4	0.17
(1,1000)	1:199:B:GLN:HE22	1:199:B:GLN:HG2	6	0.17
(1,1000)	1:199:B:GLN:HE22	1:199:B:GLN:HG2	7	0.17
(1,1000)	1:199:B:GLN:HE22	1:199:B:GLN:HG2	8	0.17
(1,1000)	1:199:B:GLN:HE22	1:199:B:GLN:HG2	10	0.17
(1,999)	1:199:A:GLN:HE22	1:199:A:GLN:HG2	1	0.17
(1,999)	1:199:A:GLN:HE22	1:199:A:GLN:HG2	2	0.17
(1,999)	1:199:A:GLN:HE22	1:199:A:GLN:HG2	3	0.17
(1,999)	1:199:A:GLN:HE22	1:199:A:GLN:HG2	4	0.17
(1,999)	1:199:A:GLN:HE22	1:199:A:GLN:HG2	6	0.17
(1,999)	1:199:A:GLN:HE22	1:199:A:GLN:HG2	7	0.17
(1,999)	1:199:A:GLN:HE22	1:199:A:GLN:HG2	8	0.17
(1,999)	1:199:A:GLN:HE22	1:199:A:GLN:HG2	9	0.17
(1,999)	1:199:A:GLN:HE22	1:199:A:GLN:HG2	10	0.17
(1,972)	1:204:B:LEU:HD22	1:182:A:ILE:HD11	9	0.17
(1,874)	1:185:B:LEU:HD12	1:188:B:ASN:HB2	2	0.17
(1,873)	1:185:A:LEU:HD12	1:188:A:ASN:HB2	2	0.17
(1,873)	1:185:A:LEU:HD13	1:188:A:ASN:HB2	5	0.17
(1,859)	1:200:A:VAL:HA	1:175:B:LEU:HB3	3	0.17
(1,852)	1:182:B:ILE:HA	1:185:B:LEU:HB2	1	0.17
(1,851)	1:182:A:ILE:HA	1:185:A:LEU:HB2	1	0.17
(1,822)	1:208:B:TRP:HA	1:203:A:ARG:HG3	3	0.17
(1,792)	1:202:B:GLU:HA	1:202:B:GLU:HG3	5	0.17
(1,791)	1:202:A:GLU:HA	1:202:A:GLU:HG3	7	0.17
(1,782)	1:206:B:LYS:HG2	1:206:B:LYS:HA	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:206:A:LYS:HG2	1:206:A:LYS:HA	4	0.17
(1,776)	1:173:B:GLN:HB2	1:173:B:GLN:HA	1	0.17
(1,776)	1:173:B:GLN:HB2	1:173:B:GLN:HA	2	0.17
(1,776)	1:173:B:GLN:HB2	1:173:B:GLN:HA	5	0.17
(1,776)	1:173:B:GLN:HB2	1:173:B:GLN:HA	8	0.17
(1,776)	1:173:B:GLN:HB2	1:173:B:GLN:HA	9	0.17
(1,776)	1:173:B:GLN:HB2	1:173:B:GLN:HA	10	0.17
(1,775)	1:173:A:GLN:HB2	1:173:A:GLN:HA	1	0.17
(1,775)	1:173:A:GLN:HB2	1:173:A:GLN:HA	2	0.17
(1,775)	1:173:A:GLN:HB2	1:173:A:GLN:HA	4	0.17
(1,775)	1:173:A:GLN:HB2	1:173:A:GLN:HA	5	0.17
(1,775)	1:173:A:GLN:HB2	1:173:A:GLN:HA	8	0.17
(1,775)	1:173:A:GLN:HB2	1:173:A:GLN:HA	9	0.17
(1,775)	1:173:A:GLN:HB2	1:173:A:GLN:HA	10	0.17
(1,746)	1:181:B:ASP:HA	1:185:A:LEU:HD21	8	0.17
(1,730)	1:186:B:LEU:HA	1:186:B:LEU:HG	2	0.17
(1,730)	1:186:B:LEU:HA	1:186:B:LEU:HG	5	0.17
(1,730)	1:186:B:LEU:HA	1:186:B:LEU:HG	6	0.17
(1,730)	1:186:B:LEU:HA	1:186:B:LEU:HG	7	0.17
(1,730)	1:186:B:LEU:HA	1:186:B:LEU:HG	9	0.17
(1,730)	1:186:B:LEU:HA	1:186:B:LEU:HG	10	0.17
(1,729)	1:186:A:LEU:HA	1:186:A:LEU:HG	2	0.17
(1,729)	1:186:A:LEU:HA	1:186:A:LEU:HG	5	0.17
(1,729)	1:186:A:LEU:HA	1:186:A:LEU:HG	6	0.17
(1,729)	1:186:A:LEU:HA	1:186:A:LEU:HG	7	0.17
(1,729)	1:186:A:LEU:HA	1:186:A:LEU:HG	9	0.17
(1,729)	1:186:A:LEU:HA	1:186:A:LEU:HG	10	0.17
(1,721)	1:190:A:PHE:HA	1:189:A:ASN:HB3	9	0.17
(1,589)	1:209:A:SER:HB3	1:208:A:TRP:H	10	0.17
(1,524)	1:191:B:GLU:H	1:191:B:GLU:HA	6	0.17
(1,524)	1:191:B:GLU:H	1:191:B:GLU:HA	9	0.17
(1,523)	1:191:A:GLU:H	1:191:A:GLU:HA	6	0.17
(1,444)	1:192:B:ASN:H	1:192:B:ASN:HB2	2	0.17
(1,444)	1:192:B:ASN:H	1:192:B:ASN:HB2	6	0.17
(1,443)	1:192:A:ASN:H	1:192:A:ASN:HB2	6	0.17
(1,360)	1:188:B:ASN:H	1:189:B:ASN:HB2	5	0.17
(1,359)	1:188:A:ASN:H	1:189:A:ASN:HB2	5	0.17
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD12	7	0.17
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD13	8	0.17
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD13	8	0.17
(1,50)	1:199:B:GLN:HE22	1:195:B:ALA:HB1	4	0.17
(1,42)	1:196:B:ALA:H	1:195:B:ALA:HB3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:196:A:ALA:H	1:195:A:ALA:HB1	8	0.17
(1,4)	1:177:B:VAL:HG11	1:179:B:TRP:HE3	5	0.17
(1,3)	1:177:A:VAL:HG11	1:179:A:TRP:HE3	5	0.17
(1,2856)	1:174:B:GLU:H	1:196:A:ALA:HB2	5	0.16
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD11	7	0.16
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD13	4	0.16
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD11	7	0.16
(1,2771)	1:175:A:LEU:H	1:190:B:PHE:HZ	4	0.16
(1,2771)	1:175:A:LEU:H	1:190:B:PHE:HZ	10	0.16
(1,2767)	1:175:A:LEU:H	1:173:A:GLN:HB3	4	0.16
(1,2738)	1:197:B:VAL:H	1:187:B:LYS:H	3	0.16
(1,2737)	1:197:A:VAL:H	1:187:A:LYS:H	3	0.16
(1,2712)	1:199:B:GLN:HE22	1:195:B:ALA:HA	7	0.16
(1,2704)	1:200:B:VAL:H	1:190:B:PHE:HE2	7	0.16
(1,2703)	1:200:A:VAL:H	1:190:A:PHE:HE2	7	0.16
(1,2673)	1:202:A:GLU:H	1:179:A:TRP:HE3	4	0.16
(1,2606)	1:207:B:GLY:H	1:205:B:GLN:HA	2	0.16
(1,2605)	1:207:A:GLY:H	1:205:A:GLN:HA	2	0.16
(1,2605)	1:207:A:GLY:H	1:205:A:GLN:HA	4	0.16
(1,2590)	1:208:B:TRP:H	1:203:A:ARG:HG2	2	0.16
(1,2572)	1:208:B:TRP:HE1	1:203:A:ARG:HB3	6	0.16
(1,2566)	1:208:B:TRP:HE1	1:209:B:SER:HA	9	0.16
(1,2565)	1:208:A:TRP:HE1	1:209:A:SER:HA	9	0.16
(1,2526)	1:212:B:LYS:H	1:210:B:LEU:HB2	2	0.16
(1,2526)	1:212:B:LYS:H	1:210:B:LEU:HB2	8	0.16
(1,2525)	1:212:A:LYS:H	1:210:A:LEU:HB2	8	0.16
(1,2502)	1:198:B:ARG:H	1:197:B:VAL:HG11	5	0.16
(1,2484)	1:180:B:ASP:H	1:178:B:PRO:HD2	3	0.16
(1,2484)	1:180:B:ASP:H	1:178:B:PRO:HD2	5	0.16
(1,2484)	1:180:B:ASP:H	1:178:B:PRO:HD2	8	0.16
(1,2483)	1:180:A:ASP:H	1:178:A:PRO:HD2	3	0.16
(1,2483)	1:180:A:ASP:H	1:178:A:PRO:HD2	5	0.16
(1,2470)	1:204:B:LEU:H	1:179:B:TRP:HZ3	2	0.16
(1,2469)	1:204:A:LEU:H	1:179:A:TRP:HZ3	2	0.16
(1,2384)	1:202:B:GLU:HG3	1:203:B:ARG:H	7	0.16
(1,2383)	1:202:A:GLU:HG3	1:203:A:ARG:H	7	0.16
(1,2281)	1:202:A:GLU:HB2	1:199:A:GLN:HA	9	0.16
(1,2222)	1:208:B:TRP:HA	1:207:A:GLY:H	4	0.16
(1,2222)	1:208:B:TRP:HA	1:207:A:GLY:H	8	0.16
(1,2221)	1:208:A:TRP:HA	1:207:B:GLY:H	4	0.16
(1,2221)	1:208:A:TRP:HA	1:207:B:GLY:H	8	0.16
(1,2174)	1:203:B:ARG:HD2	1:208:A:TRP:HZ3	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2157)	1:181:A:ASP:H	1:182:A:ILE:HB	8	0.16
(1,2102)	1:204:B:LEU:HD12	1:179:B:TRP:HZ3	3	0.16
(1,2101)	1:204:A:LEU:HD12	1:179:A:TRP:HZ3	3	0.16
(1,1998)	1:191:B:GLU:H	1:186:B:LEU:HD11	5	0.16
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD11	5	0.16
(1,1985)	1:173:B:GLN:H	1:175:B:LEU:HD12	9	0.16
(1,1922)	1:179:B:TRP:H	1:179:B:TRP:HZ3	10	0.16
(1,1921)	1:179:A:TRP:H	1:179:A:TRP:HZ3	10	0.16
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG11	10	0.16
(1,1677)	1:199:A:GLN:HE22	1:198:A:ARG:HD3	9	0.16
(1,1643)	1:201:A:MET:H	1:186:A:LEU:HA	3	0.16
(1,1542)	1:206:B:LYS:H	1:206:B:LYS:HE3	1	0.16
(1,1542)	1:206:B:LYS:H	1:206:B:LYS:HE3	8	0.16
(1,1541)	1:206:A:LYS:H	1:206:A:LYS:HE3	1	0.16
(1,1530)	1:207:B:GLY:H	1:206:B:LYS:HB2	1	0.16
(1,1529)	1:207:A:GLY:H	1:206:A:LYS:HB2	1	0.16
(1,1434)	1:210:B:LEU:H	1:208:B:TRP:HB2	10	0.16
(1,1433)	1:210:A:LEU:H	1:208:A:TRP:HB2	10	0.16
(1,1199)	1:203:A:ARG:HD3	1:212:B:LYS:HA	9	0.16
(1,1185)	1:175:A:LEU:HA	1:196:B:ALA:HB1	4	0.16
(1,1184)	1:199:B:GLN:HA	1:175:A:LEU:HD12	4	0.16
(1,1183)	1:199:A:GLN:HA	1:175:B:LEU:HD13	10	0.16
(1,1150)	1:178:B:PRO:HD3	1:177:B:VAL:HG21	10	0.16
(1,1149)	1:178:A:PRO:HD3	1:177:A:VAL:HG21	10	0.16
(1,1118)	1:175:B:LEU:HD23	1:208:B:TRP:HH2	6	0.16
(1,1117)	1:175:A:LEU:HD23	1:208:A:TRP:HH2	6	0.16
(1,1115)	1:175:A:LEU:HD21	1:199:B:GLN:H	9	0.16
(1,1110)	1:201:B:MET:H	1:197:B:VAL:HG12	7	0.16
(1,1109)	1:201:A:MET:H	1:197:A:VAL:HG12	7	0.16
(1,1082)	1:206:B:LYS:H	1:206:B:LYS:HG3	7	0.16
(1,1082)	1:206:B:LYS:H	1:206:B:LYS:HG3	10	0.16
(1,1081)	1:206:A:LYS:H	1:206:A:LYS:HG3	7	0.16
(1,1072)	1:175:B:LEU:HD11	1:201:A:MET:H	5	0.16
(1,1002)	1:199:B:GLN:H	1:197:B:VAL:HB	3	0.16
(1,1001)	1:199:A:GLN:H	1:197:A:VAL:HB	3	0.16
(1,874)	1:185:B:LEU:HD12	1:188:B:ASN:HB2	9	0.16
(1,860)	1:200:B:VAL:HA	1:175:A:LEU:HB3	3	0.16
(1,821)	1:208:A:TRP:HA	1:203:B:ARG:HG3	3	0.16
(1,804)	1:203:B:ARG:HA	1:203:B:ARG:HG2	8	0.16
(1,803)	1:203:A:ARG:HA	1:203:A:ARG:HG2	8	0.16
(1,792)	1:202:B:GLU:HA	1:202:B:GLU:HG3	7	0.16
(1,791)	1:202:A:GLU:HA	1:202:A:GLU:HG3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	1:202:A:GLU:HA	1:202:A:GLU:HG3	5	0.16
(1,776)	1:173:B:GLN:HB2	1:173:B:GLN:HA	3	0.16
(1,776)	1:173:B:GLN:HB2	1:173:B:GLN:HA	4	0.16
(1,744)	1:184:B:ALA:HB3	1:181:B:ASP:HA	6	0.16
(1,743)	1:184:A:ALA:HB3	1:181:A:ASP:HA	6	0.16
(1,722)	1:190:B:PHE:HA	1:189:B:ASN:HB3	9	0.16
(1,698)	1:184:B:ALA:HA	1:183:B:GLU:HB3	1	0.16
(1,697)	1:184:A:ALA:HA	1:183:A:GLU:HB3	1	0.16
(1,524)	1:191:B:GLU:H	1:191:B:GLU:HA	1	0.16
(1,443)	1:192:A:ASN:H	1:192:A:ASN:HB2	2	0.16
(1,226)	1:177:B:VAL:HG23	1:200:A:VAL:HG13	8	0.16
(1,218)	1:210:B:LEU:HD11	1:211:A:ALA:HA	6	0.16
(1,217)	1:210:A:LEU:HD11	1:211:B:ALA:HA	6	0.16
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD12	1	0.16
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD12	1	0.16
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD12	7	0.16
(1,76)	1:199:B:GLN:H	1:200:B:VAL:HG12	7	0.16
(1,75)	1:199:A:GLN:H	1:200:A:VAL:HG12	7	0.16
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB1	1	0.16
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB1	1	0.16
(1,2876)	1:205:B:GLN:H	1:177:A:VAL:HG23	9	0.15
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD13	4	0.15
(1,2790)	1:189:B:ASN:H	1:191:B:GLU:HA	4	0.15
(1,2789)	1:189:A:ASN:H	1:191:A:GLU:HA	4	0.15
(1,2762)	1:175:B:LEU:H	1:175:B:LEU:HD11	8	0.15
(1,2751)	1:194:A:GLN:HE21	1:192:A:ASN:HB3	10	0.15
(1,2738)	1:197:B:VAL:H	1:187:B:LYS:H	10	0.15
(1,2737)	1:197:A:VAL:H	1:187:A:LYS:H	6	0.15
(1,2737)	1:197:A:VAL:H	1:187:A:LYS:H	10	0.15
(1,2710)	1:199:B:GLN:HE22	1:175:A:LEU:HA	3	0.15
(1,2709)	1:199:A:GLN:HE22	1:175:B:LEU:HA	4	0.15
(1,2674)	1:202:B:GLU:H	1:179:B:TRP:HE3	4	0.15
(1,2674)	1:202:B:GLU:H	1:179:B:TRP:HE3	6	0.15
(1,2673)	1:202:A:GLU:H	1:179:A:TRP:HE3	6	0.15
(1,2606)	1:207:B:GLY:H	1:205:B:GLN:HA	5	0.15
(1,2606)	1:207:B:GLY:H	1:205:B:GLN:HA	6	0.15
(1,2605)	1:207:A:GLY:H	1:205:A:GLN:HA	5	0.15
(1,2605)	1:207:A:GLY:H	1:205:A:GLN:HA	6	0.15
(1,2589)	1:208:A:TRP:H	1:203:B:ARG:HG2	2	0.15
(1,2586)	1:179:B:TRP:HE1	1:205:B:GLN:HA	2	0.15
(1,2586)	1:179:B:TRP:HE1	1:205:B:GLN:HA	8	0.15
(1,2585)	1:179:A:TRP:HE1	1:205:A:GLN:HA	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2566)	1:208:B:TRP:HE1	1:209:B:SER:HA	6	0.15
(1,2565)	1:208:A:TRP:HE1	1:209:A:SER:HA	6	0.15
(1,2526)	1:212:B:LYS:H	1:210:B:LEU:HB2	3	0.15
(1,2525)	1:212:A:LYS:H	1:210:A:LEU:HB2	3	0.15
(1,2518)	1:205:B:GLN:H	1:204:B:LEU:HD11	9	0.15
(1,2517)	1:205:A:GLN:H	1:204:A:LEU:HD11	9	0.15
(1,2516)	1:205:B:GLN:H	1:204:B:LEU:HB3	5	0.15
(1,2515)	1:205:A:GLN:H	1:204:A:LEU:HB3	3	0.15
(1,2515)	1:205:A:GLN:H	1:204:A:LEU:HB3	5	0.15
(1,2470)	1:204:B:LEU:H	1:179:B:TRP:HZ3	8	0.15
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG22	10	0.15
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG22	10	0.15
(1,2436)	1:201:B:MET:HB2	1:200:B:VAL:HG21	3	0.15
(1,2435)	1:201:A:MET:HB2	1:200:A:VAL:HG21	3	0.15
(1,2393)	1:211:A:ALA:HA	1:207:B:GLY:HA2	4	0.15
(1,2384)	1:202:B:GLU:HG3	1:203:B:ARG:H	10	0.15
(1,2383)	1:202:A:GLU:HG3	1:203:A:ARG:H	10	0.15
(1,2342)	1:204:B:LEU:HG	1:182:A:ILE:HD12	8	0.15
(1,2326)	1:197:B:VAL:HG11	1:198:B:ARG:HA	5	0.15
(1,2282)	1:202:B:GLU:HB2	1:199:B:GLN:HA	9	0.15
(1,2280)	1:194:B:GLN:HA	1:197:B:VAL:HB	4	0.15
(1,2279)	1:194:A:GLN:HA	1:197:A:VAL:HB	4	0.15
(1,2226)	1:208:B:TRP:HA	1:208:B:TRP:HE3	5	0.15
(1,2226)	1:208:B:TRP:HA	1:208:B:TRP:HE3	8	0.15
(1,2225)	1:208:A:TRP:HA	1:208:A:TRP:HE3	5	0.15
(1,2225)	1:208:A:TRP:HA	1:208:A:TRP:HE3	8	0.15
(1,2173)	1:203:A:ARG:HD2	1:208:B:TRP:HZ3	5	0.15
(1,2157)	1:181:A:ASP:H	1:182:A:ILE:HB	6	0.15
(1,2138)	1:187:B:LYS:HD3	1:184:B:ALA:HA	6	0.15
(1,2137)	1:187:A:LYS:HD3	1:184:A:ALA:HA	6	0.15
(1,2137)	1:187:A:LYS:HD3	1:184:A:ALA:HA	7	0.15
(1,2107)	1:177:A:VAL:HG21	1:190:B:PHE:HE2	4	0.15
(1,2107)	1:177:A:VAL:HG23	1:190:B:PHE:HE2	8	0.15
(1,2098)	1:204:B:LEU:HD21	1:208:A:TRP:H	1	0.15
(1,2097)	1:204:A:LEU:HD21	1:208:B:TRP:H	1	0.15
(1,1998)	1:191:B:GLU:H	1:186:B:LEU:HD12	1	0.15
(1,1998)	1:191:B:GLU:H	1:186:B:LEU:HD12	3	0.15
(1,1998)	1:191:B:GLU:H	1:186:B:LEU:HD12	8	0.15
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD12	1	0.15
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG12	8	0.15
(1,1736)	1:195:B:ALA:H	1:194:B:GLN:HG3	10	0.15
(1,1735)	1:195:A:ALA:H	1:194:A:GLN:HG3	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1694)	1:189:B:ASN:HD22	1:182:A:ILE:HD11	1	0.15
(1,1694)	1:189:B:ASN:HD22	1:182:A:ILE:HD12	2	0.15
(1,1678)	1:199:B:GLN:HE22	1:198:B:ARG:HD3	9	0.15
(1,1407)	1:212:A:LYS:H	1:203:B:ARG:HD3	8	0.15
(1,1398)	1:202:B:GLU:H	1:200:B:VAL:HG11	3	0.15
(1,1378)	1:180:B:ASP:H	1:183:B:GLU:HA	9	0.15
(1,1377)	1:180:A:ASP:H	1:183:A:GLU:HA	9	0.15
(1,1192)	1:188:B:ASN:HA	1:191:B:GLU:HG2	2	0.15
(1,1191)	1:188:A:ASN:HA	1:191:A:GLU:HG2	2	0.15
(1,1183)	1:199:A:GLN:HA	1:175:B:LEU:HD12	4	0.15
(1,1109)	1:201:A:MET:H	1:197:A:VAL:HG13	10	0.15
(1,1082)	1:206:B:LYS:H	1:206:B:LYS:HG3	2	0.15
(1,1081)	1:206:A:LYS:H	1:206:A:LYS:HG3	2	0.15
(1,1081)	1:206:A:LYS:H	1:206:A:LYS:HG3	10	0.15
(1,873)	1:185:A:LEU:HD12	1:188:A:ASN:HB2	9	0.15
(1,821)	1:208:A:TRP:HA	1:203:B:ARG:HG3	9	0.15
(1,792)	1:202:B:GLU:HA	1:202:B:GLU:HG3	4	0.15
(1,791)	1:202:A:GLU:HA	1:202:A:GLU:HG3	10	0.15
(1,782)	1:206:B:LYS:HG2	1:206:B:LYS:HA	3	0.15
(1,781)	1:206:A:LYS:HG2	1:206:A:LYS:HA	3	0.15
(1,775)	1:173:A:GLN:HB2	1:173:A:GLN:HA	3	0.15
(1,714)	1:175:B:LEU:HB2	1:175:B:LEU:HA	1	0.15
(1,714)	1:175:B:LEU:HB2	1:175:B:LEU:HA	2	0.15
(1,714)	1:175:B:LEU:HB2	1:175:B:LEU:HA	3	0.15
(1,714)	1:175:B:LEU:HB2	1:175:B:LEU:HA	4	0.15
(1,714)	1:175:B:LEU:HB2	1:175:B:LEU:HA	7	0.15
(1,714)	1:175:B:LEU:HB2	1:175:B:LEU:HA	8	0.15
(1,714)	1:175:B:LEU:HB2	1:175:B:LEU:HA	9	0.15
(1,714)	1:175:B:LEU:HB2	1:175:B:LEU:HA	10	0.15
(1,713)	1:175:A:LEU:HB2	1:175:A:LEU:HA	1	0.15
(1,713)	1:175:A:LEU:HB2	1:175:A:LEU:HA	2	0.15
(1,713)	1:175:A:LEU:HB2	1:175:A:LEU:HA	3	0.15
(1,713)	1:175:A:LEU:HB2	1:175:A:LEU:HA	4	0.15
(1,713)	1:175:A:LEU:HB2	1:175:A:LEU:HA	7	0.15
(1,713)	1:175:A:LEU:HB2	1:175:A:LEU:HA	8	0.15
(1,713)	1:175:A:LEU:HB2	1:175:A:LEU:HA	9	0.15
(1,713)	1:175:A:LEU:HB2	1:175:A:LEU:HA	10	0.15
(1,589)	1:209:A:SER:HB3	1:208:A:TRP:H	3	0.15
(1,543)	1:199:A:GLN:HA	1:202:A:GLU:H	2	0.15
(1,523)	1:191:A:GLU:H	1:191:A:GLU:HA	1	0.15
(1,444)	1:192:B:ASN:H	1:192:B:ASN:HB2	8	0.15
(1,444)	1:192:B:ASN:H	1:192:B:ASN:HB2	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,443)	1:192:A:ASN:H	1:192:A:ASN:HB2	8	0.15
(1,443)	1:192:A:ASN:H	1:192:A:ASN:HB2	9	0.15
(1,397)	1:175:A:LEU:HB2	1:190:B:PHE:HZ	8	0.15
(1,307)	1:199:A:GLN:HB3	1:200:A:VAL:HG12	1	0.15
(1,260)	1:185:B:LEU:HD21	1:178:A:PRO:HB2	9	0.15
(1,259)	1:185:A:LEU:HD21	1:178:B:PRO:HB2	9	0.15
(1,225)	1:177:A:VAL:HG23	1:200:B:VAL:HG13	8	0.15
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD11	2	0.15
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD13	3	0.15
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD13	5	0.15
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD11	2	0.15
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD13	5	0.15
(1,86)	1:197:B:VAL:HG23	1:190:B:PHE:HD2	7	0.15
(1,85)	1:197:A:VAL:HG23	1:190:A:PHE:HD2	7	0.15
(1,42)	1:196:B:ALA:H	1:195:B:ALA:HB1	8	0.15
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB1	3	0.15
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB1	3	0.15
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB1	2	0.15
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB1	3	0.15
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB2	4	0.15
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB1	10	0.15
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB1	2	0.15
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB1	3	0.15
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB2	4	0.15
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB1	10	0.15
(1,4)	1:177:B:VAL:HG13	1:179:B:TRP:HE3	2	0.15
(1,3)	1:177:A:VAL:HG13	1:179:A:TRP:HE3	2	0.15
(1,2875)	1:205:A:GLN:H	1:177:B:VAL:HG23	9	0.14
(1,2869)	1:209:A:SER:H	1:206:A:LYS:HE3	1	0.14
(1,2818)	1:183:B:GLU:H	1:182:B:ILE:HG12	1	0.14
(1,2817)	1:183:A:GLU:H	1:182:A:ILE:HG12	1	0.14
(1,2802)	1:186:B:LEU:H	1:185:B:LEU:HD22	2	0.14
(1,2802)	1:186:B:LEU:H	1:185:B:LEU:HD22	5	0.14
(1,2801)	1:186:A:LEU:H	1:185:A:LEU:HD22	2	0.14
(1,2801)	1:186:A:LEU:H	1:185:A:LEU:HD22	5	0.14
(1,2790)	1:189:B:ASN:H	1:191:B:GLU:HA	1	0.14
(1,2761)	1:175:A:LEU:H	1:175:A:LEU:HD11	8	0.14
(1,2752)	1:194:B:GLN:HE21	1:192:B:ASN:HB3	10	0.14
(1,2738)	1:197:B:VAL:H	1:187:B:LYS:H	6	0.14
(1,2737)	1:197:A:VAL:H	1:187:A:LYS:H	4	0.14
(1,2704)	1:200:B:VAL:H	1:190:B:PHE:HE2	8	0.14
(1,2703)	1:200:A:VAL:H	1:190:A:PHE:HE2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2585)	1:179:A:TRP:HE1	1:205:A:GLN:HA	8	0.14
(1,2571)	1:208:A:TRP:HE1	1:203:B:ARG:HB3	6	0.14
(1,2564)	1:209:B:SER:H	1:210:B:LEU:HD21	10	0.14
(1,2563)	1:209:A:SER:H	1:210:A:LEU:HD21	10	0.14
(1,2553)	1:210:A:LEU:H	1:206:A:LYS:HE3	8	0.14
(1,2532)	1:211:B:ALA:H	1:210:B:LEU:HB3	4	0.14
(1,2532)	1:211:B:ALA:H	1:210:B:LEU:HB3	6	0.14
(1,2532)	1:211:B:ALA:H	1:210:B:LEU:HB3	9	0.14
(1,2531)	1:211:A:ALA:H	1:210:A:LEU:HB3	4	0.14
(1,2531)	1:211:A:ALA:H	1:210:A:LEU:HB3	6	0.14
(1,2531)	1:211:A:ALA:H	1:210:A:LEU:HB3	7	0.14
(1,2531)	1:211:A:ALA:H	1:210:A:LEU:HB3	9	0.14
(1,2525)	1:212:A:LYS:H	1:210:A:LEU:HB2	2	0.14
(1,2516)	1:205:B:GLN:H	1:204:B:LEU:HB3	2	0.14
(1,2516)	1:205:B:GLN:H	1:204:B:LEU:HB3	3	0.14
(1,2516)	1:205:B:GLN:H	1:204:B:LEU:HB3	4	0.14
(1,2516)	1:205:B:GLN:H	1:204:B:LEU:HB3	8	0.14
(1,2515)	1:205:A:GLN:H	1:204:A:LEU:HB3	2	0.14
(1,2515)	1:205:A:GLN:H	1:204:A:LEU:HB3	4	0.14
(1,2515)	1:205:A:GLN:H	1:204:A:LEU:HB3	8	0.14
(1,2502)	1:198:B:ARG:H	1:197:B:VAL:HG12	2	0.14
(1,2501)	1:198:A:ARG:H	1:197:A:VAL:HG12	2	0.14
(1,2487)	1:180:A:ASP:H	1:178:A:PRO:HG2	6	0.14
(1,2484)	1:180:B:ASP:H	1:178:B:PRO:HD2	1	0.14
(1,2483)	1:180:A:ASP:H	1:178:A:PRO:HD2	1	0.14
(1,2470)	1:204:B:LEU:H	1:179:B:TRP:HZ3	5	0.14
(1,2469)	1:204:A:LEU:H	1:179:A:TRP:HZ3	8	0.14
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD23	6	0.14
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD23	6	0.14
(1,2330)	1:199:B:GLN:HG3	1:196:B:ALA:H	5	0.14
(1,2325)	1:197:A:VAL:HG11	1:198:A:ARG:HA	5	0.14
(1,2280)	1:194:B:GLN:HA	1:197:B:VAL:HB	3	0.14
(1,2280)	1:194:B:GLN:HA	1:197:B:VAL:HB	9	0.14
(1,2279)	1:194:A:GLN:HA	1:197:A:VAL:HB	3	0.14
(1,2279)	1:194:A:GLN:HA	1:197:A:VAL:HB	9	0.14
(1,2256)	1:196:B:ALA:HA	1:175:A:LEU:HD21	4	0.14
(1,2255)	1:196:A:ALA:HA	1:175:B:LEU:HD22	3	0.14
(1,2255)	1:196:A:ALA:HA	1:175:B:LEU:HD21	8	0.14
(1,2254)	1:211:B:ALA:HA	1:206:A:LYS:HG2	6	0.14
(1,2253)	1:211:A:ALA:HA	1:206:B:LYS:HG2	6	0.14
(1,2253)	1:211:A:ALA:HA	1:206:B:LYS:HG2	9	0.14
(1,2226)	1:208:B:TRP:HA	1:208:B:TRP:HE3	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2225)	1:208:A:TRP:HA	1:208:A:TRP:HE3	1	0.14
(1,2158)	1:181:B:ASP:H	1:182:B:ILE:HB	6	0.14
(1,2157)	1:181:A:ASP:H	1:182:A:ILE:HB	3	0.14
(1,2138)	1:187:B:LYS:HD3	1:184:B:ALA:HA	7	0.14
(1,2109)	1:177:A:VAL:HG22	1:179:A:TRP:HH2	1	0.14
(1,2106)	1:177:B:VAL:HG22	1:208:B:TRP:HZ3	1	0.14
(1,2105)	1:177:A:VAL:HG22	1:208:A:TRP:HZ3	1	0.14
(1,2098)	1:204:B:LEU:HD22	1:208:A:TRP:H	10	0.14
(1,2097)	1:204:A:LEU:HD22	1:208:B:TRP:H	3	0.14
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD12	3	0.14
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD12	8	0.14
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG11	10	0.14
(1,1693)	1:189:A:ASN:HD22	1:182:B:ILE:HD11	1	0.14
(1,1693)	1:189:A:ASN:HD22	1:182:B:ILE:HD12	3	0.14
(1,1693)	1:189:A:ASN:HD22	1:182:B:ILE:HD12	5	0.14
(1,1541)	1:206:A:LYS:H	1:206:A:LYS:HE3	3	0.14
(1,1530)	1:207:B:GLY:H	1:206:B:LYS:HB2	10	0.14
(1,1529)	1:207:A:GLY:H	1:206:A:LYS:HB2	10	0.14
(1,1410)	1:212:B:LYS:H	1:212:B:LYS:HB3	7	0.14
(1,1409)	1:212:A:LYS:H	1:212:A:LYS:HB3	7	0.14
(1,1398)	1:202:B:GLU:H	1:200:B:VAL:HG11	4	0.14
(1,1397)	1:202:A:GLU:H	1:200:A:VAL:HG11	3	0.14
(1,1150)	1:178:B:PRO:HD3	1:177:B:VAL:HG21	4	0.14
(1,1149)	1:178:A:PRO:HD3	1:177:A:VAL:HG21	4	0.14
(1,1110)	1:201:B:MET:H	1:197:B:VAL:HG13	10	0.14
(1,1082)	1:206:B:LYS:H	1:206:B:LYS:HG3	3	0.14
(1,1082)	1:206:B:LYS:H	1:206:B:LYS:HG3	4	0.14
(1,1082)	1:206:B:LYS:H	1:206:B:LYS:HG3	5	0.14
(1,1082)	1:206:B:LYS:H	1:206:B:LYS:HG3	8	0.14
(1,1081)	1:206:A:LYS:H	1:206:A:LYS:HG3	3	0.14
(1,1081)	1:206:A:LYS:H	1:206:A:LYS:HG3	4	0.14
(1,1081)	1:206:A:LYS:H	1:206:A:LYS:HG3	5	0.14
(1,1081)	1:206:A:LYS:H	1:206:A:LYS:HG3	8	0.14
(1,1071)	1:175:A:LEU:HD11	1:201:B:MET:H	3	0.14
(1,1050)	1:212:B:LYS:HB3	1:212:B:LYS:HE3	3	0.14
(1,1049)	1:212:A:LYS:HB3	1:212:A:LYS:HE3	3	0.14
(1,1030)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	7	0.14
(1,1002)	1:199:B:GLN:H	1:197:B:VAL:HB	4	0.14
(1,1001)	1:199:A:GLN:H	1:197:A:VAL:HB	4	0.14
(1,948)	1:197:B:VAL:HG12	1:197:B:VAL:HB	3	0.14
(1,948)	1:197:B:VAL:HG12	1:197:B:VAL:HB	7	0.14
(1,948)	1:197:B:VAL:HG11	1:197:B:VAL:HB	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,947)	1:197:A:VAL:HG13	1:197:A:VAL:HB	3	0.14
(1,947)	1:197:A:VAL:HG12	1:197:A:VAL:HB	7	0.14
(1,947)	1:197:A:VAL:HG11	1:197:A:VAL:HB	8	0.14
(1,947)	1:197:A:VAL:HG11	1:197:A:VAL:HB	9	0.14
(1,874)	1:185:B:LEU:HD11	1:188:B:ASN:HB2	10	0.14
(1,873)	1:185:A:LEU:HD11	1:188:A:ASN:HB2	10	0.14
(1,792)	1:202:B:GLU:HA	1:202:B:GLU:HG3	1	0.14
(1,792)	1:202:B:GLU:HA	1:202:B:GLU:HG3	3	0.14
(1,792)	1:202:B:GLU:HA	1:202:B:GLU:HG3	10	0.14
(1,791)	1:202:A:GLU:HA	1:202:A:GLU:HG3	1	0.14
(1,791)	1:202:A:GLU:HA	1:202:A:GLU:HG3	3	0.14
(1,782)	1:206:B:LYS:HG2	1:206:B:LYS:HA	6	0.14
(1,781)	1:206:A:LYS:HG2	1:206:A:LYS:HA	6	0.14
(1,776)	1:173:B:GLN:HB2	1:173:B:GLN:HA	7	0.14
(1,775)	1:173:A:GLN:HB2	1:173:A:GLN:HA	7	0.14
(1,722)	1:190:B:PHE:HA	1:189:B:ASN:HB3	2	0.14
(1,722)	1:190:B:PHE:HA	1:189:B:ASN:HB3	6	0.14
(1,721)	1:190:A:PHE:HA	1:189:A:ASN:HB3	2	0.14
(1,714)	1:175:B:LEU:HB2	1:175:B:LEU:HA	5	0.14
(1,714)	1:175:B:LEU:HB2	1:175:B:LEU:HA	6	0.14
(1,713)	1:175:A:LEU:HB2	1:175:A:LEU:HA	5	0.14
(1,713)	1:175:A:LEU:HB2	1:175:A:LEU:HA	6	0.14
(1,590)	1:209:B:SER:HB3	1:208:B:TRP:H	3	0.14
(1,590)	1:209:B:SER:HB3	1:208:B:TRP:H	9	0.14
(1,544)	1:199:B:GLN:HA	1:202:B:GLU:H	2	0.14
(1,444)	1:192:B:ASN:H	1:192:B:ASN:HB2	4	0.14
(1,443)	1:192:A:ASN:H	1:192:A:ASN:HB2	4	0.14
(1,359)	1:188:A:ASN:H	1:189:A:ASN:HB2	8	0.14
(1,308)	1:199:B:GLN:HB3	1:200:B:VAL:HG12	1	0.14
(1,233)	1:200:A:VAL:HG13	1:177:B:VAL:HG23	8	0.14
(1,226)	1:177:B:VAL:HG21	1:200:A:VAL:HG11	1	0.14
(1,225)	1:177:A:VAL:HG21	1:200:B:VAL:HG11	1	0.14
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD13	3	0.14
(1,86)	1:197:B:VAL:HG23	1:190:B:PHE:HD2	5	0.14
(1,85)	1:197:A:VAL:HG23	1:190:A:PHE:HD2	5	0.14
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD23	9	0.14
(1,42)	1:196:B:ALA:H	1:195:B:ALA:HB3	1	0.14
(1,42)	1:196:B:ALA:H	1:195:B:ALA:HB1	3	0.14
(1,41)	1:196:A:ALA:H	1:195:A:ALA:HB3	1	0.14
(1,41)	1:196:A:ALA:H	1:195:A:ALA:HB1	3	0.14
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB3	2	0.14
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB3	6	0.14
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB3	8	0.14
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB3	2	0.14
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB2	4	0.14
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB3	8	0.14
(1,2870)	1:209:B:SER:H	1:206:B:LYS:HE3	1	0.13
(1,2869)	1:209:A:SER:H	1:206:A:LYS:HE3	4	0.13
(1,2789)	1:189:A:ASN:H	1:191:A:GLU:HA	1	0.13
(1,2756)	1:194:B:GLN:HE22	1:187:B:LYS:HE2	7	0.13
(1,2738)	1:197:B:VAL:H	1:187:B:LYS:H	2	0.13
(1,2738)	1:197:B:VAL:H	1:187:B:LYS:H	4	0.13
(1,2738)	1:197:B:VAL:H	1:187:B:LYS:H	5	0.13
(1,2737)	1:197:A:VAL:H	1:187:A:LYS:H	2	0.13
(1,2737)	1:197:A:VAL:H	1:187:A:LYS:H	5	0.13
(1,2722)	1:189:B:ASN:HD22	1:178:A:PRO:HG2	9	0.13
(1,2710)	1:199:B:GLN:HE22	1:175:A:LEU:HA	4	0.13
(1,2674)	1:202:B:GLU:H	1:179:B:TRP:HE3	10	0.13
(1,2673)	1:202:A:GLU:H	1:179:A:TRP:HE3	10	0.13
(1,2668)	1:205:B:GLN:H	1:201:B:MET:HE3	7	0.13
(1,2667)	1:205:A:GLN:H	1:201:A:MET:HE3	7	0.13
(1,2588)	1:208:B:TRP:H	1:204:B:LEU:HB3	1	0.13
(1,2587)	1:208:A:TRP:H	1:204:A:LEU:HB3	1	0.13
(1,2554)	1:210:B:LEU:H	1:206:B:LYS:HE3	8	0.13
(1,2532)	1:211:B:ALA:H	1:210:B:LEU:HB3	7	0.13
(1,2532)	1:211:B:ALA:H	1:210:B:LEU:HB3	10	0.13
(1,2531)	1:211:A:ALA:H	1:210:A:LEU:HB3	10	0.13
(1,2516)	1:205:B:GLN:H	1:204:B:LEU:HB3	6	0.13
(1,2515)	1:205:A:GLN:H	1:204:A:LEU:HB3	6	0.13
(1,2515)	1:205:A:GLN:H	1:204:A:LEU:HB3	10	0.13
(1,2502)	1:198:B:ARG:H	1:197:B:VAL:HG12	3	0.13
(1,2502)	1:198:B:ARG:H	1:197:B:VAL:HG12	6	0.13
(1,2502)	1:198:B:ARG:H	1:197:B:VAL:HG13	9	0.13
(1,2501)	1:198:A:ARG:H	1:197:A:VAL:HG12	3	0.13
(1,2501)	1:198:A:ARG:H	1:197:A:VAL:HG13	9	0.13
(1,2488)	1:180:B:ASP:H	1:178:B:PRO:HG2	6	0.13
(1,2484)	1:180:B:ASP:H	1:178:B:PRO:HD2	4	0.13
(1,2483)	1:180:A:ASP:H	1:178:A:PRO:HD2	4	0.13
(1,2470)	1:204:B:LEU:H	1:179:B:TRP:HZ3	4	0.13
(1,2469)	1:204:A:LEU:H	1:179:A:TRP:HZ3	4	0.13
(1,2469)	1:204:A:LEU:H	1:179:A:TRP:HZ3	5	0.13
(1,2466)	1:184:B:ALA:H	1:185:A:LEU:HD23	2	0.13
(1,2465)	1:184:A:ALA:H	1:185:B:LEU:HD23	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2394)	1:211:B:ALA:HA	1:207:A:GLY:HA2	4	0.13
(1,2383)	1:202:A:GLU:HG3	1:203:A:ARG:H	3	0.13
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD11	6	0.13
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD11	6	0.13
(1,2329)	1:199:A:GLN:HG3	1:196:A:ALA:H	5	0.13
(1,2280)	1:194:B:GLN:HA	1:197:B:VAL:HB	10	0.13
(1,2279)	1:194:A:GLN:HA	1:197:A:VAL:HB	10	0.13
(1,2186)	1:192:B:ASN:HD22	1:192:B:ASN:HB3	7	0.13
(1,2185)	1:192:A:ASN:HD22	1:192:A:ASN:HB3	7	0.13
(1,2158)	1:181:B:ASP:H	1:182:B:ILE:HB	3	0.13
(1,2154)	1:205:B:GLN:HG2	1:205:B:GLN:H	10	0.13
(1,2140)	1:206:B:LYS:HD3	1:203:B:ARG:HA	1	0.13
(1,2139)	1:206:A:LYS:HD3	1:203:A:ARG:HA	1	0.13
(1,2110)	1:177:B:VAL:HG22	1:179:B:TRP:HH2	1	0.13
(1,2107)	1:177:A:VAL:HG22	1:190:B:PHE:HE2	5	0.13
(1,2098)	1:204:B:LEU:HD23	1:208:A:TRP:H	2	0.13
(1,2081)	1:175:A:LEU:HD23	1:190:B:PHE:HZ	6	0.13
(1,2000)	1:191:B:GLU:H	1:188:B:ASN:HD21	8	0.13
(1,1999)	1:191:A:GLU:H	1:188:A:ASN:HD21	8	0.13
(1,1985)	1:173:B:GLN:H	1:175:B:LEU:HD12	1	0.13
(1,1924)	1:179:B:TRP:H	1:205:B:GLN:HE22	6	0.13
(1,1923)	1:179:A:TRP:H	1:205:A:GLN:HE22	6	0.13
(1,1922)	1:179:B:TRP:H	1:179:B:TRP:HZ3	7	0.13
(1,1921)	1:179:A:TRP:H	1:179:A:TRP:HZ3	7	0.13
(1,1794)	1:193:B:ASP:H	1:188:B:ASN:HA	8	0.13
(1,1793)	1:193:A:ASP:H	1:188:A:ASN:HA	8	0.13
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG11	9	0.13
(1,1771)	1:175:A:LEU:H	1:200:B:VAL:HG12	6	0.13
(1,1694)	1:189:B:ASN:HD22	1:182:A:ILE:HD12	3	0.13
(1,1678)	1:199:B:GLN:HE22	1:198:B:ARG:HD3	1	0.13
(1,1630)	1:203:B:ARG:H	1:179:B:TRP:HZ3	3	0.13
(1,1629)	1:203:A:ARG:H	1:179:A:TRP:HZ3	3	0.13
(1,1542)	1:206:B:LYS:H	1:206:B:LYS:HE3	3	0.13
(1,1542)	1:206:B:LYS:H	1:206:B:LYS:HE3	10	0.13
(1,1541)	1:206:A:LYS:H	1:206:A:LYS:HE3	10	0.13
(1,1408)	1:212:B:LYS:H	1:203:A:ARG:HD3	3	0.13
(1,1407)	1:212:A:LYS:H	1:203:B:ARG:HD3	6	0.13
(1,1398)	1:202:B:GLU:H	1:200:B:VAL:HG13	5	0.13
(1,1397)	1:202:A:GLU:H	1:200:A:VAL:HG11	4	0.13
(1,1397)	1:202:A:GLU:H	1:200:A:VAL:HG13	5	0.13
(1,1378)	1:180:B:ASP:H	1:183:B:GLU:HA	1	0.13
(1,1377)	1:180:A:ASP:H	1:183:A:GLU:HA	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1186)	1:175:B:LEU:HA	1:196:A:ALA:HB1	4	0.13
(1,1108)	1:197:B:VAL:HG11	1:190:B:PHE:HD2	7	0.13
(1,1082)	1:206:B:LYS:H	1:206:B:LYS:HG3	1	0.13
(1,1082)	1:206:B:LYS:H	1:206:B:LYS:HG3	9	0.13
(1,1081)	1:206:A:LYS:H	1:206:A:LYS:HG3	1	0.13
(1,1081)	1:206:A:LYS:H	1:206:A:LYS:HG3	9	0.13
(1,1062)	1:189:B:ASN:HB2	1:191:B:GLU:H	5	0.13
(1,1061)	1:189:A:ASN:HB2	1:191:A:GLU:H	3	0.13
(1,1061)	1:189:A:ASN:HB2	1:191:A:GLU:H	5	0.13
(1,1050)	1:212:B:LYS:HB3	1:212:B:LYS:HE3	7	0.13
(1,1049)	1:212:A:LYS:HB3	1:212:A:LYS:HE3	7	0.13
(1,1029)	1:182:A:ILE:HD11	1:178:A:PRO:HB2	7	0.13
(1,1002)	1:199:B:GLN:H	1:197:B:VAL:HB	2	0.13
(1,1002)	1:199:B:GLN:H	1:197:B:VAL:HB	7	0.13
(1,1001)	1:199:A:GLN:H	1:197:A:VAL:HB	7	0.13
(1,948)	1:197:B:VAL:HG12	1:197:B:VAL:HB	1	0.13
(1,948)	1:197:B:VAL:HG12	1:197:B:VAL:HB	2	0.13
(1,948)	1:197:B:VAL:HG11	1:197:B:VAL:HB	4	0.13
(1,948)	1:197:B:VAL:HG11	1:197:B:VAL:HB	5	0.13
(1,948)	1:197:B:VAL:HG12	1:197:B:VAL:HB	6	0.13
(1,948)	1:197:B:VAL:HG11	1:197:B:VAL:HB	9	0.13
(1,948)	1:197:B:VAL:HG13	1:197:B:VAL:HB	10	0.13
(1,947)	1:197:A:VAL:HG12	1:197:A:VAL:HB	1	0.13
(1,947)	1:197:A:VAL:HG12	1:197:A:VAL:HB	2	0.13
(1,947)	1:197:A:VAL:HG11	1:197:A:VAL:HB	4	0.13
(1,947)	1:197:A:VAL:HG11	1:197:A:VAL:HB	5	0.13
(1,947)	1:197:A:VAL:HG12	1:197:A:VAL:HB	6	0.13
(1,947)	1:197:A:VAL:HG13	1:197:A:VAL:HB	10	0.13
(1,869)	1:188:A:ASN:HB3	1:187:A:LYS:HB3	2	0.13
(1,822)	1:208:B:TRP:HA	1:203:A:ARG:HG3	6	0.13
(1,822)	1:208:B:TRP:HA	1:203:A:ARG:HG3	9	0.13
(1,791)	1:202:A:GLU:HA	1:202:A:GLU:HG3	6	0.13
(1,782)	1:206:B:LYS:HG2	1:206:B:LYS:HA	2	0.13
(1,782)	1:206:B:LYS:HG2	1:206:B:LYS:HA	5	0.13
(1,782)	1:206:B:LYS:HG2	1:206:B:LYS:HA	8	0.13
(1,781)	1:206:A:LYS:HG2	1:206:A:LYS:HA	5	0.13
(1,781)	1:206:A:LYS:HG2	1:206:A:LYS:HA	8	0.13
(1,721)	1:190:A:PHE:HA	1:189:A:ASN:HB3	6	0.13
(1,648)	1:195:B:ALA:HB1	1:198:B:ARG:HD3	2	0.13
(1,589)	1:209:A:SER:HB3	1:208:A:TRP:H	9	0.13
(1,438)	1:188:B:ASN:HD22	1:188:B:ASN:HB3	1	0.13
(1,438)	1:188:B:ASN:HD22	1:188:B:ASN:HB3	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:188:B:ASN:HD22	1:188:B:ASN:HB3	3	0.13
(1,438)	1:188:B:ASN:HD22	1:188:B:ASN:HB3	4	0.13
(1,438)	1:188:B:ASN:HD22	1:188:B:ASN:HB3	6	0.13
(1,438)	1:188:B:ASN:HD22	1:188:B:ASN:HB3	7	0.13
(1,438)	1:188:B:ASN:HD22	1:188:B:ASN:HB3	9	0.13
(1,437)	1:188:A:ASN:HD22	1:188:A:ASN:HB3	2	0.13
(1,437)	1:188:A:ASN:HD22	1:188:A:ASN:HB3	3	0.13
(1,437)	1:188:A:ASN:HD22	1:188:A:ASN:HB3	4	0.13
(1,437)	1:188:A:ASN:HD22	1:188:A:ASN:HB3	6	0.13
(1,437)	1:188:A:ASN:HD22	1:188:A:ASN:HB3	7	0.13
(1,437)	1:188:A:ASN:HD22	1:188:A:ASN:HB3	9	0.13
(1,437)	1:188:A:ASN:HD22	1:188:A:ASN:HB3	10	0.13
(1,360)	1:188:B:ASN:H	1:189:B:ASN:HB2	1	0.13
(1,360)	1:188:B:ASN:H	1:189:B:ASN:HB2	6	0.13
(1,360)	1:188:B:ASN:H	1:189:B:ASN:HB2	8	0.13
(1,246)	1:200:B:VAL:HG13	1:197:B:VAL:HA	5	0.13
(1,234)	1:200:B:VAL:HG13	1:177:A:VAL:HG23	8	0.13
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD11	4	0.13
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD13	6	0.13
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD11	4	0.13
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD13	6	0.13
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD11	10	0.13
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD11	10	0.13
(1,72)	1:175:B:LEU:H	1:175:B:LEU:HD22	10	0.13
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD23	9	0.13
(1,71)	1:175:A:LEU:H	1:175:A:LEU:HD22	10	0.13
(1,49)	1:199:A:GLN:HE22	1:195:A:ALA:HB1	4	0.13
(1,42)	1:196:B:ALA:H	1:195:B:ALA:HB2	6	0.13
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB2	1	0.13
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB2	5	0.13
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB2	1	0.13
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB2	5	0.13
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB3	6	0.13
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB3	8	0.13
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB2	9	0.13
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB3	8	0.13
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB2	9	0.13
(1,2870)	1:209:B:SER:H	1:206:B:LYS:HE3	4	0.12
(1,2818)	1:183:B:GLU:H	1:182:B:ILE:HG12	2	0.12
(1,2818)	1:183:B:GLU:H	1:182:B:ILE:HG12	3	0.12
(1,2818)	1:183:B:GLU:H	1:182:B:ILE:HG12	4	0.12
(1,2818)	1:183:B:GLU:H	1:182:B:ILE:HG12	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2818)	1:183:B:GLU:H	1:182:B:ILE:HG12	6	0.12
(1,2817)	1:183:A:GLU:H	1:182:A:ILE:HG12	2	0.12
(1,2817)	1:183:A:GLU:H	1:182:A:ILE:HG12	3	0.12
(1,2817)	1:183:A:GLU:H	1:182:A:ILE:HG12	4	0.12
(1,2817)	1:183:A:GLU:H	1:182:A:ILE:HG12	6	0.12
(1,2802)	1:186:B:LEU:H	1:185:B:LEU:HD22	6	0.12
(1,2801)	1:186:A:LEU:H	1:185:A:LEU:HD22	6	0.12
(1,2772)	1:175:B:LEU:H	1:190:A:PHE:HZ	8	0.12
(1,2772)	1:175:B:LEU:H	1:190:A:PHE:HZ	10	0.12
(1,2755)	1:194:A:GLN:HE22	1:187:A:LYS:HE2	7	0.12
(1,2735)	1:189:A:ASN:HD21	1:186:A:LEU:HB2	7	0.12
(1,2721)	1:189:A:ASN:HD22	1:178:B:PRO:HG2	9	0.12
(1,2610)	1:207:B:GLY:H	1:203:B:ARG:HG3	10	0.12
(1,2606)	1:207:B:GLY:H	1:205:B:GLN:HA	7	0.12
(1,2605)	1:207:A:GLY:H	1:205:A:GLN:HA	7	0.12
(1,2588)	1:208:B:TRP:H	1:204:B:LEU:HB3	2	0.12
(1,2587)	1:208:A:TRP:H	1:204:A:LEU:HB3	2	0.12
(1,2564)	1:209:B:SER:H	1:210:B:LEU:HD22	8	0.12
(1,2564)	1:209:B:SER:H	1:210:B:LEU:HD21	9	0.12
(1,2563)	1:209:A:SER:H	1:210:A:LEU:HD22	8	0.12
(1,2532)	1:211:B:ALA:H	1:210:B:LEU:HB3	1	0.12
(1,2516)	1:205:B:GLN:H	1:204:B:LEU:HB3	10	0.12
(1,2501)	1:198:A:ARG:H	1:197:A:VAL:HG12	6	0.12
(1,2470)	1:204:B:LEU:H	1:179:B:TRP:HZ3	9	0.12
(1,2469)	1:204:A:LEU:H	1:179:A:TRP:HZ3	9	0.12
(1,2384)	1:202:B:GLU:HG3	1:203:B:ARG:H	3	0.12
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD12	5	0.12
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD11	4	0.12
(1,2341)	1:204:A:LEU:HG	1:182:B:ILE:HD11	6	0.12
(1,2326)	1:197:B:VAL:HG12	1:198:B:ARG:HA	3	0.12
(1,2325)	1:197:A:VAL:HG12	1:198:A:ARG:HA	3	0.12
(1,2288)	1:182:B:ILE:HG22	1:183:B:GLU:HA	10	0.12
(1,2287)	1:182:A:ILE:HG22	1:183:A:GLU:HA	10	0.12
(1,2256)	1:196:B:ALA:HA	1:175:A:LEU:HD21	8	0.12
(1,2226)	1:208:B:TRP:HA	1:208:B:TRP:HE3	2	0.12
(1,2225)	1:208:A:TRP:HA	1:208:A:TRP:HE3	2	0.12
(1,2222)	1:208:B:TRP:HA	1:207:A:GLY:H	6	0.12
(1,2221)	1:208:A:TRP:HA	1:207:B:GLY:H	5	0.12
(1,2194)	1:173:B:GLN:HA	1:174:B:GLU:H	3	0.12
(1,2194)	1:173:B:GLN:HA	1:174:B:GLU:H	9	0.12
(1,2193)	1:173:A:GLN:HA	1:174:A:GLU:H	9	0.12
(1,2153)	1:205:A:GLN:HG2	1:205:A:GLN:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2118)	1:182:B:ILE:HD13	1:178:B:PRO:HD2	9	0.12
(1,2117)	1:182:A:ILE:HD13	1:178:A:PRO:HD2	9	0.12
(1,2110)	1:177:B:VAL:HG22	1:179:B:TRP:HH2	2	0.12
(1,2109)	1:177:A:VAL:HG22	1:179:A:TRP:HH2	2	0.12
(1,2108)	1:177:B:VAL:HG21	1:190:A:PHE:HE2	4	0.12
(1,2108)	1:177:B:VAL:HG22	1:190:A:PHE:HE2	5	0.12
(1,2107)	1:177:A:VAL:HG22	1:190:B:PHE:HE2	9	0.12
(1,2106)	1:177:B:VAL:HG22	1:208:B:TRP:HZ3	4	0.12
(1,2105)	1:177:A:VAL:HG22	1:208:A:TRP:HZ3	4	0.12
(1,2102)	1:204:B:LEU:HD11	1:179:B:TRP:HZ3	10	0.12
(1,2101)	1:204:A:LEU:HD11	1:179:A:TRP:HZ3	10	0.12
(1,2098)	1:204:B:LEU:HD22	1:208:A:TRP:H	3	0.12
(1,2058)	1:179:B:TRP:H	1:177:B:VAL:HG13	3	0.12
(1,2057)	1:179:A:TRP:H	1:177:A:VAL:HG13	3	0.12
(1,1986)	1:173:A:GLN:H	1:175:A:LEU:HD12	1	0.12
(1,1772)	1:175:B:LEU:H	1:200:A:VAL:HG12	6	0.12
(1,1694)	1:189:B:ASN:HD22	1:182:A:ILE:HD11	4	0.12
(1,1694)	1:189:B:ASN:HD22	1:182:A:ILE:HD12	5	0.12
(1,1644)	1:201:B:MET:H	1:186:B:LEU:HA	4	0.12
(1,1644)	1:201:B:MET:H	1:186:B:LEU:HA	8	0.12
(1,1643)	1:201:A:MET:H	1:186:A:LEU:HA	8	0.12
(1,1398)	1:202:B:GLU:H	1:200:B:VAL:HG11	6	0.12
(1,1398)	1:202:B:GLU:H	1:200:B:VAL:HG11	8	0.12
(1,1397)	1:202:A:GLU:H	1:200:A:VAL:HG11	6	0.12
(1,1397)	1:202:A:GLU:H	1:200:A:VAL:HG11	8	0.12
(1,1298)	1:191:B:GLU:H	1:187:B:LYS:HG3	7	0.12
(1,1297)	1:191:A:GLU:H	1:187:A:LYS:HG3	7	0.12
(1,1150)	1:178:B:PRO:HD3	1:177:B:VAL:HG21	1	0.12
(1,1149)	1:178:A:PRO:HD3	1:177:A:VAL:HG21	1	0.12
(1,1107)	1:197:A:VAL:HG11	1:190:A:PHE:HD2	7	0.12
(1,1082)	1:206:B:LYS:H	1:206:B:LYS:HG3	6	0.12
(1,1081)	1:206:A:LYS:H	1:206:A:LYS:HG3	6	0.12
(1,1062)	1:189:B:ASN:HB2	1:191:B:GLU:H	3	0.12
(1,1062)	1:189:B:ASN:HB2	1:191:B:GLU:H	8	0.12
(1,1030)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	3	0.12
(1,1029)	1:182:A:ILE:HD11	1:178:A:PRO:HB2	3	0.12
(1,1002)	1:199:B:GLN:H	1:197:B:VAL:HB	10	0.12
(1,1001)	1:199:A:GLN:H	1:197:A:VAL:HB	2	0.12
(1,1001)	1:199:A:GLN:H	1:197:A:VAL:HB	10	0.12
(1,958)	1:204:B:LEU:HD11	1:204:B:LEU:HD21	3	0.12
(1,958)	1:204:B:LEU:HD12	1:204:B:LEU:HD23	9	0.12
(1,957)	1:204:A:LEU:HD11	1:204:A:LEU:HD21	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:199:B:GLN:HG2	1:175:A:LEU:HD13	10	0.12
(1,915)	1:199:A:GLN:HG2	1:175:B:LEU:HD13	10	0.12
(1,873)	1:185:A:LEU:HD11	1:188:A:ASN:HB2	3	0.12
(1,870)	1:188:B:ASN:HB3	1:187:B:LYS:HB3	2	0.12
(1,821)	1:208:A:TRP:HA	1:203:B:ARG:HG3	6	0.12
(1,792)	1:202:B:GLU:HA	1:202:B:GLU:HG3	6	0.12
(1,781)	1:206:A:LYS:HG2	1:206:A:LYS:HA	2	0.12
(1,648)	1:195:B:ALA:HB1	1:198:B:ARG:HD3	7	0.12
(1,647)	1:195:A:ALA:HB1	1:198:A:ARG:HD3	2	0.12
(1,647)	1:195:A:ALA:HB1	1:198:A:ARG:HD3	7	0.12
(1,644)	1:199:B:GLN:H	1:198:B:ARG:HD3	1	0.12
(1,438)	1:188:B:ASN:HD22	1:188:B:ASN:HB3	5	0.12
(1,438)	1:188:B:ASN:HD22	1:188:B:ASN:HB3	10	0.12
(1,437)	1:188:A:ASN:HD22	1:188:A:ASN:HB3	1	0.12
(1,437)	1:188:A:ASN:HD22	1:188:A:ASN:HB3	5	0.12
(1,398)	1:175:B:LEU:HB2	1:190:A:PHE:HZ	7	0.12
(1,359)	1:188:A:ASN:H	1:189:A:ASN:HB2	1	0.12
(1,359)	1:188:A:ASN:H	1:189:A:ASN:HB2	3	0.12
(1,359)	1:188:A:ASN:H	1:189:A:ASN:HB2	6	0.12
(1,308)	1:199:B:GLN:HB3	1:200:B:VAL:HG11	8	0.12
(1,307)	1:199:A:GLN:HB3	1:200:A:VAL:HG11	8	0.12
(1,260)	1:185:B:LEU:HD21	1:178:A:PRO:HB2	6	0.12
(1,256)	1:185:B:LEU:HD21	1:182:A:ILE:HA	4	0.12
(1,245)	1:200:A:VAL:HG13	1:197:A:VAL:HA	5	0.12
(1,234)	1:200:B:VAL:HG11	1:177:A:VAL:HG21	1	0.12
(1,233)	1:200:A:VAL:HG11	1:177:B:VAL:HG21	1	0.12
(1,230)	1:204:B:LEU:HD13	1:177:A:VAL:HG21	10	0.12
(1,223)	1:177:A:VAL:HG21	1:204:B:LEU:HD13	10	0.12
(1,194)	1:201:B:MET:HE3	1:182:B:ILE:HD13	8	0.12
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD11	9	0.12
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD11	9	0.12
(1,98)	1:188:B:ASN:HD22	1:185:B:LEU:HD12	9	0.12
(1,97)	1:188:A:ASN:HD22	1:185:A:LEU:HD12	9	0.12
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB2	7	0.12
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB2	9	0.12
(1,38)	1:184:B:ALA:H	1:184:B:ALA:HB1	10	0.12
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB2	7	0.12
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB2	9	0.12
(1,37)	1:184:A:ALA:H	1:184:A:ALA:HB1	10	0.12
(1,4)	1:177:B:VAL:HG13	1:179:B:TRP:HE3	3	0.12
(1,2855)	1:174:A:GLU:H	1:196:B:ALA:HB1	9	0.11
(1,2832)	1:181:B:ASP:H	1:177:B:VAL:HA	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2831)	1:181:A:ASP:H	1:177:A:VAL:HA	5	0.11
(1,2831)	1:181:A:ASP:H	1:177:A:VAL:HA	7	0.11
(1,2818)	1:183:B:GLU:H	1:182:B:ILE:HG12	8	0.11
(1,2817)	1:183:A:GLU:H	1:182:A:ILE:HG12	5	0.11
(1,2817)	1:183:A:GLU:H	1:182:A:ILE:HG12	8	0.11
(1,2810)	1:184:B:ALA:H	1:182:B:ILE:HD13	8	0.11
(1,2809)	1:184:A:ALA:H	1:182:A:ILE:HD13	8	0.11
(1,2772)	1:175:B:LEU:H	1:190:A:PHE:HZ	4	0.11
(1,2754)	1:194:B:GLN:HE22	1:192:B:ASN:HB3	10	0.11
(1,2753)	1:194:A:GLN:HE22	1:192:A:ASN:HB3	10	0.11
(1,2736)	1:189:B:ASN:HD21	1:186:B:LEU:HB2	7	0.11
(1,2704)	1:200:B:VAL:H	1:190:B:PHE:HE2	2	0.11
(1,2704)	1:200:B:VAL:H	1:190:B:PHE:HE2	5	0.11
(1,2703)	1:200:A:VAL:H	1:190:A:PHE:HE2	2	0.11
(1,2686)	1:203:B:ARG:H	1:203:B:ARG:HG3	10	0.11
(1,2685)	1:203:A:ARG:H	1:203:A:ARG:HG3	10	0.11
(1,2609)	1:207:A:GLY:H	1:203:A:ARG:HG3	10	0.11
(1,2606)	1:207:B:GLY:H	1:205:B:GLN:HA	1	0.11
(1,2605)	1:207:A:GLY:H	1:205:A:GLN:HA	1	0.11
(1,2605)	1:207:A:GLY:H	1:205:A:GLN:HA	8	0.11
(1,2588)	1:208:B:TRP:H	1:204:B:LEU:HB3	7	0.11
(1,2587)	1:208:A:TRP:H	1:204:A:LEU:HB3	7	0.11
(1,2586)	1:179:B:TRP:HE1	1:205:B:GLN:HA	3	0.11
(1,2563)	1:209:A:SER:H	1:210:A:LEU:HD21	9	0.11
(1,2560)	1:209:B:SER:H	1:206:B:LYS:HG2	6	0.11
(1,2559)	1:209:A:SER:H	1:206:A:LYS:HG2	4	0.11
(1,2559)	1:209:A:SER:H	1:206:A:LYS:HG2	6	0.11
(1,2531)	1:211:A:ALA:H	1:210:A:LEU:HB3	1	0.11
(1,2526)	1:212:B:LYS:H	1:210:B:LEU:HB2	1	0.11
(1,2526)	1:212:B:LYS:H	1:210:B:LEU:HB2	4	0.11
(1,2525)	1:212:A:LYS:H	1:210:A:LEU:HB2	1	0.11
(1,2525)	1:212:A:LYS:H	1:210:A:LEU:HB2	4	0.11
(1,2512)	1:176:B:THR:H	1:174:B:GLU:HB3	2	0.11
(1,2511)	1:176:A:THR:H	1:174:A:GLU:HB3	2	0.11
(1,2462)	1:184:B:ALA:H	1:182:B:ILE:HG22	7	0.11
(1,2370)	1:175:B:LEU:HG	1:199:A:GLN:HE22	2	0.11
(1,2369)	1:175:A:LEU:HG	1:199:B:GLN:HE22	2	0.11
(1,2344)	1:178:B:PRO:HG3	1:182:B:ILE:HD11	4	0.11
(1,2343)	1:178:A:PRO:HG3	1:182:A:ILE:HD12	5	0.11
(1,2341)	1:204:A:LEU:HG	1:182:B:ILE:HD12	8	0.11
(1,2292)	1:182:B:ILE:HG21	1:182:B:ILE:HA	10	0.11
(1,2291)	1:182:A:ILE:HG21	1:182:A:ILE:HA	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2258)	1:188:B:ASN:HB3	1:188:B:ASN:HA	8	0.11
(1,2257)	1:188:A:ASN:HB3	1:188:A:ASN:HA	8	0.11
(1,2256)	1:196:B:ALA:HA	1:175:A:LEU:HD22	3	0.11
(1,2255)	1:196:A:ALA:HA	1:175:B:LEU:HD21	4	0.11
(1,2254)	1:211:B:ALA:HA	1:206:A:LYS:HG2	9	0.11
(1,2222)	1:208:B:TRP:HA	1:207:A:GLY:H	5	0.11
(1,2194)	1:173:B:GLN:HA	1:174:B:GLU:H	1	0.11
(1,2193)	1:173:A:GLN:HA	1:174:A:GLU:H	3	0.11
(1,2184)	1:187:B:LYS:H	1:188:B:ASN:HB3	4	0.11
(1,2158)	1:181:B:ASP:H	1:182:B:ILE:HB	4	0.11
(1,2157)	1:181:A:ASP:H	1:182:A:ILE:HB	4	0.11
(1,2154)	1:205:B:GLN:HG2	1:205:B:GLN:H	5	0.11
(1,2154)	1:205:B:GLN:HG2	1:205:B:GLN:H	8	0.11
(1,2153)	1:205:A:GLN:HG2	1:205:A:GLN:H	5	0.11
(1,2153)	1:205:A:GLN:HG2	1:205:A:GLN:H	8	0.11
(1,2106)	1:177:B:VAL:HG22	1:208:B:TRP:HE3	10	0.11
(1,1997)	1:191:A:GLU:H	1:186:A:LEU:HD11	10	0.11
(1,1955)	1:177:A:VAL:H	1:182:A:ILE:HD13	1	0.11
(1,1924)	1:179:B:TRP:H	1:205:B:GLN:HE22	5	0.11
(1,1923)	1:179:A:TRP:H	1:205:A:GLN:HE22	5	0.11
(1,1921)	1:179:A:TRP:H	1:179:A:TRP:HZ3	2	0.11
(1,1918)	1:180:B:ASP:H	1:179:B:TRP:HD1	10	0.11
(1,1648)	1:201:B:MET:H	1:200:B:VAL:HG13	5	0.11
(1,1647)	1:201:A:MET:H	1:200:A:VAL:HG13	5	0.11
(1,1643)	1:201:A:MET:H	1:186:A:LEU:HA	4	0.11
(1,1630)	1:203:B:ARG:H	1:179:B:TRP:HZ3	6	0.11
(1,1500)	1:179:B:TRP:HE1	1:180:B:ASP:H	10	0.11
(1,1408)	1:212:B:LYS:H	1:203:A:ARG:HD3	2	0.11
(1,1407)	1:212:A:LYS:H	1:203:B:ARG:HD3	3	0.11
(1,1062)	1:189:B:ASN:HB2	1:191:B:GLU:H	2	0.11
(1,1062)	1:189:B:ASN:HB2	1:191:B:GLU:H	6	0.11
(1,1062)	1:189:B:ASN:HB2	1:191:B:GLU:H	10	0.11
(1,1061)	1:189:A:ASN:HB2	1:191:A:GLU:H	2	0.11
(1,1061)	1:189:A:ASN:HB2	1:191:A:GLU:H	8	0.11
(1,1030)	1:182:B:ILE:HD11	1:178:B:PRO:HB2	1	0.11
(1,1029)	1:182:A:ILE:HD11	1:178:A:PRO:HB2	1	0.11
(1,958)	1:204:B:LEU:HD13	1:204:B:LEU:HD23	1	0.11
(1,958)	1:204:B:LEU:HD12	1:204:B:LEU:HD22	2	0.11
(1,958)	1:204:B:LEU:HD12	1:204:B:LEU:HD22	4	0.11
(1,958)	1:204:B:LEU:HD11	1:204:B:LEU:HD22	5	0.11
(1,958)	1:204:B:LEU:HD11	1:204:B:LEU:HD23	6	0.11
(1,958)	1:204:B:LEU:HD11	1:204:B:LEU:HD21	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:204:B:LEU:HD13	1:204:B:LEU:HD21	10	0.11
(1,957)	1:204:A:LEU:HD13	1:204:A:LEU:HD23	1	0.11
(1,957)	1:204:A:LEU:HD12	1:204:A:LEU:HD22	2	0.11
(1,957)	1:204:A:LEU:HD12	1:204:A:LEU:HD22	4	0.11
(1,957)	1:204:A:LEU:HD11	1:204:A:LEU:HD22	5	0.11
(1,957)	1:204:A:LEU:HD11	1:204:A:LEU:HD23	6	0.11
(1,957)	1:204:A:LEU:HD11	1:204:A:LEU:HD21	8	0.11
(1,957)	1:204:A:LEU:HD12	1:204:A:LEU:HD23	9	0.11
(1,957)	1:204:A:LEU:HD13	1:204:A:LEU:HD21	10	0.11
(1,918)	1:173:B:GLN:HG2	1:175:B:LEU:HD11	4	0.11
(1,917)	1:173:A:GLN:HG2	1:175:A:LEU:HD11	4	0.11
(1,874)	1:185:B:LEU:HD11	1:188:B:ASN:HB2	3	0.11
(1,859)	1:200:A:VAL:HA	1:175:B:LEU:HB3	10	0.11
(1,822)	1:208:B:TRP:HA	1:203:A:ARG:HG3	7	0.11
(1,821)	1:208:A:TRP:HA	1:203:B:ARG:HG3	7	0.11
(1,808)	1:208:B:TRP:HA	1:211:B:ALA:HB3	3	0.11
(1,807)	1:208:A:TRP:HA	1:211:A:ALA:HB3	3	0.11
(1,803)	1:203:A:ARG:HA	1:203:A:ARG:HG2	7	0.11
(1,744)	1:184:B:ALA:HB2	1:181:B:ASP:HA	7	0.11
(1,743)	1:184:A:ALA:HB2	1:181:A:ASP:HA	7	0.11
(1,743)	1:184:A:ALA:HB3	1:181:A:ASP:HA	8	0.11
(1,722)	1:190:B:PHE:HA	1:189:B:ASN:HB3	1	0.11
(1,721)	1:190:A:PHE:HA	1:189:A:ASN:HB3	1	0.11
(1,643)	1:199:A:GLN:H	1:198:A:ARG:HD3	1	0.11
(1,590)	1:209:B:SER:HB3	1:208:B:TRP:H	1	0.11
(1,544)	1:199:B:GLN:HA	1:202:B:GLU:H	6	0.11
(1,543)	1:199:A:GLN:HA	1:202:A:GLU:H	6	0.11
(1,360)	1:188:B:ASN:H	1:189:B:ASN:HB2	3	0.11
(1,259)	1:185:A:LEU:HD21	1:178:B:PRO:HB2	3	0.11
(1,259)	1:185:A:LEU:HD21	1:178:B:PRO:HB2	6	0.11
(1,253)	1:175:A:LEU:HD13	1:196:B:ALA:HA	9	0.11
(1,246)	1:200:B:VAL:HG13	1:197:B:VAL:HA	10	0.11
(1,245)	1:200:A:VAL:HG13	1:197:A:VAL:HA	10	0.11
(1,229)	1:204:A:LEU:HD13	1:177:B:VAL:HG21	10	0.11
(1,224)	1:177:B:VAL:HG21	1:204:A:LEU:HD13	10	0.11
(1,216)	1:176:B:THR:HG22	1:176:B:THR:HB	2	0.11
(1,216)	1:176:B:THR:HG23	1:176:B:THR:HB	5	0.11
(1,216)	1:176:B:THR:HG21	1:176:B:THR:HB	6	0.11
(1,216)	1:176:B:THR:HG22	1:176:B:THR:HB	9	0.11
(1,216)	1:176:B:THR:HG23	1:176:B:THR:HB	10	0.11
(1,215)	1:176:A:THR:HG22	1:176:A:THR:HB	2	0.11
(1,215)	1:176:A:THR:HG21	1:176:A:THR:HB	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:176:A:THR:HG21	1:176:A:THR:HB	4	0.11
(1,215)	1:176:A:THR:HG23	1:176:A:THR:HB	5	0.11
(1,215)	1:176:A:THR:HG21	1:176:A:THR:HB	6	0.11
(1,215)	1:176:A:THR:HG23	1:176:A:THR:HB	7	0.11
(1,193)	1:201:A:MET:HE3	1:182:A:ILE:HD13	8	0.11
(1,120)	1:204:B:LEU:H	1:204:B:LEU:HD12	10	0.11
(1,119)	1:204:A:LEU:H	1:204:A:LEU:HD12	10	0.11
(1,44)	1:195:B:ALA:H	1:195:B:ALA:HB2	7	0.11
(1,43)	1:195:A:ALA:H	1:195:A:ALA:HB2	7	0.11
(1,41)	1:196:A:ALA:H	1:195:A:ALA:HB2	6	0.11
(1,36)	1:196:B:ALA:H	1:196:B:ALA:HB2	6	0.11
(1,35)	1:196:A:ALA:H	1:196:A:ALA:HB2	6	0.11
(1,4)	1:177:B:VAL:HG13	1:179:B:TRP:HE3	4	0.11
(1,3)	1:177:A:VAL:HG13	1:179:A:TRP:HE3	3	0.11
(1,3)	1:177:A:VAL:HG13	1:179:A:TRP:HE3	4	0.11
(1,2832)	1:181:B:ASP:H	1:177:B:VAL:HA	5	0.1
(1,2832)	1:181:B:ASP:H	1:177:B:VAL:HA	6	0.1
(1,2818)	1:183:B:GLU:H	1:182:B:ILE:HG12	10	0.1
(1,2814)	1:183:B:GLU:H	1:182:B:ILE:HG13	10	0.1
(1,2813)	1:183:A:GLU:H	1:182:A:ILE:HG13	10	0.1
(1,2703)	1:200:A:VAL:H	1:190:A:PHE:HE2	5	0.1
(1,2606)	1:207:B:GLY:H	1:205:B:GLN:HA	8	0.1
(1,2588)	1:208:B:TRP:H	1:204:B:LEU:HB3	3	0.1
(1,2560)	1:209:B:SER:H	1:206:B:LYS:HG2	4	0.1
(1,2532)	1:211:B:ALA:H	1:210:B:LEU:HB3	2	0.1
(1,2526)	1:212:B:LYS:H	1:210:B:LEU:HB2	6	0.1
(1,2525)	1:212:A:LYS:H	1:210:A:LEU:HB2	6	0.1
(1,2516)	1:205:B:GLN:H	1:204:B:LEU:HB3	1	0.1
(1,2516)	1:205:B:GLN:H	1:204:B:LEU:HB3	7	0.1
(1,2515)	1:205:A:GLN:H	1:204:A:LEU:HB3	1	0.1
(1,2483)	1:180:A:ASP:H	1:182:A:ILE:HA	10	0.1
(1,2461)	1:184:A:ALA:H	1:182:A:ILE:HG22	7	0.1
(1,2342)	1:204:B:LEU:HG	1:182:A:ILE:HD13	2	0.1
(1,2256)	1:196:B:ALA:HA	1:175:A:LEU:HD21	10	0.1
(1,2222)	1:208:B:TRP:HA	1:207:A:GLY:H	10	0.1
(1,2221)	1:208:A:TRP:HA	1:207:B:GLY:H	10	0.1
(1,2193)	1:173:A:GLN:HA	1:174:A:GLU:H	1	0.1
(1,2118)	1:182:B:ILE:HD11	1:178:B:PRO:HD2	10	0.1
(1,2117)	1:182:A:ILE:HD11	1:178:A:PRO:HD2	10	0.1
(1,2105)	1:177:A:VAL:HG22	1:208:A:TRP:HE3	10	0.1
(1,2097)	1:204:A:LEU:HD22	1:208:B:TRP:H	10	0.1
(1,1982)	1:173:A:GLN:H	1:173:A:GLN:HG3	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1981)	1:173:B:GLN:H	1:173:B:GLN:HG3	4	0.1
(1,1956)	1:177:B:VAL:H	1:182:B:ILE:HD13	1	0.1
(1,1922)	1:179:B:TRP:H	1:179:B:TRP:HZ3	2	0.1
(1,1917)	1:180:A:ASP:H	1:179:A:TRP:HD1	10	0.1
(1,1648)	1:201:B:MET:H	1:200:B:VAL:HG11	4	0.1
(1,1648)	1:201:B:MET:H	1:200:B:VAL:HG11	8	0.1
(1,1647)	1:201:A:MET:H	1:200:A:VAL:HG11	4	0.1
(1,1647)	1:201:A:MET:H	1:200:A:VAL:HG11	8	0.1
(1,1644)	1:201:B:MET:H	1:186:B:LEU:HA	5	0.1
(1,1643)	1:201:A:MET:H	1:186:A:LEU:HA	5	0.1
(1,1578)	1:192:B:ASN:HD21	1:193:B:ASP:HA	1	0.1
(1,1577)	1:192:A:ASN:HD21	1:193:A:ASP:HA	1	0.1
(1,1553)	1:173:A:GLN:HE21	1:175:A:LEU:HB3	6	0.1
(1,1378)	1:180:B:ASP:H	1:183:B:GLU:HA	5	0.1
(1,1377)	1:180:A:ASP:H	1:183:A:GLU:HA	5	0.1
(1,1196)	1:188:B:ASN:HA	1:191:B:GLU:HB2	10	0.1
(1,1116)	1:175:B:LEU:HD21	1:199:A:GLN:H	9	0.1
(1,1115)	1:175:A:LEU:HD23	1:199:B:GLN:H	10	0.1
(1,1061)	1:189:A:ASN:HB2	1:191:A:GLU:H	6	0.1
(1,1061)	1:189:A:ASN:HB2	1:191:A:GLU:H	10	0.1
(1,996)	1:199:B:GLN:HG2	1:199:B:GLN:H	10	0.1
(1,995)	1:199:A:GLN:HG2	1:199:A:GLN:H	10	0.1
(1,957)	1:204:A:LEU:HD13	1:204:A:LEU:HD23	7	0.1
(1,860)	1:200:B:VAL:HA	1:175:A:LEU:HB3	10	0.1
(1,822)	1:208:B:TRP:HA	1:203:A:ARG:HG3	4	0.1
(1,804)	1:203:B:ARG:HA	1:203:B:ARG:HG2	7	0.1
(1,744)	1:184:B:ALA:HB2	1:181:B:ASP:HA	1	0.1
(1,744)	1:184:B:ALA:HB3	1:181:B:ASP:HA	8	0.1
(1,743)	1:184:A:ALA:HB2	1:181:A:ASP:HA	1	0.1
(1,724)	1:190:B:PHE:HA	1:191:B:GLU:HG2	3	0.1
(1,589)	1:209:A:SER:HB3	1:208:A:TRP:H	1	0.1
(1,343)	1:191:A:GLU:HG2	1:190:A:PHE:H	7	0.1
(1,260)	1:185:B:LEU:HD21	1:178:A:PRO:HB2	3	0.1
(1,246)	1:200:B:VAL:HG12	1:197:B:VAL:HA	1	0.1
(1,216)	1:176:B:THR:HG22	1:176:B:THR:HB	1	0.1
(1,216)	1:176:B:THR:HG21	1:176:B:THR:HB	3	0.1
(1,216)	1:176:B:THR:HG21	1:176:B:THR:HB	4	0.1
(1,216)	1:176:B:THR:HG23	1:176:B:THR:HB	7	0.1
(1,216)	1:176:B:THR:HG22	1:176:B:THR:HB	8	0.1
(1,215)	1:176:A:THR:HG22	1:176:A:THR:HB	8	0.1
(1,215)	1:176:A:THR:HG22	1:176:A:THR:HB	9	0.1
(1,215)	1:176:A:THR:HG23	1:176:A:THR:HB	10	0.1

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

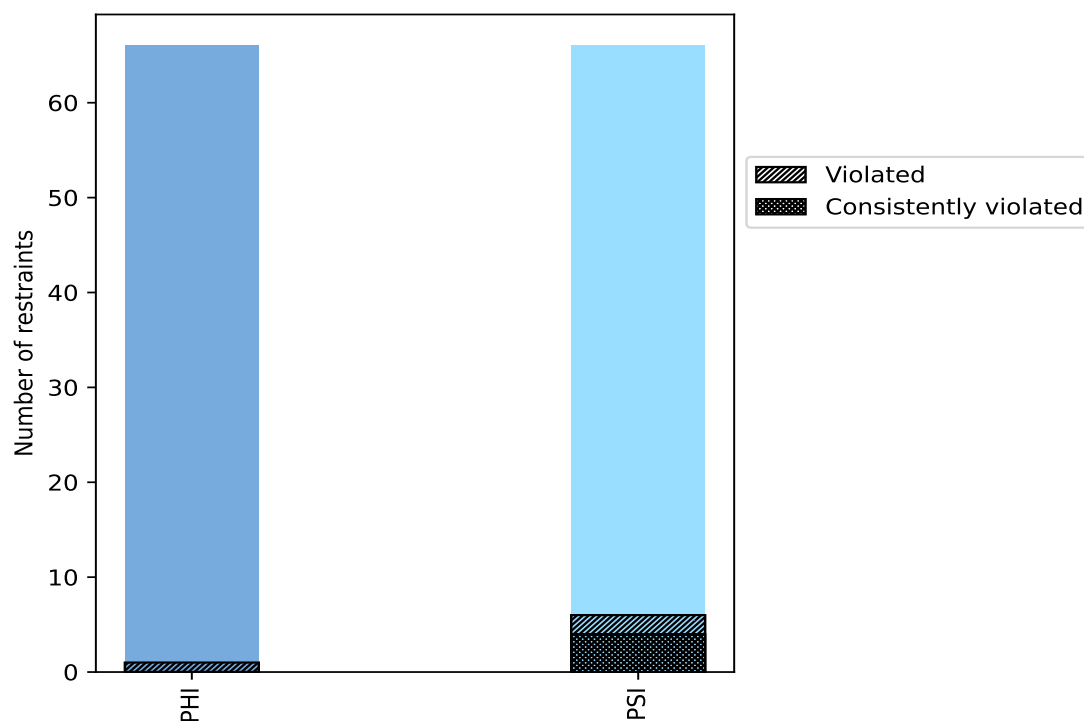
### 10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PHI	66	50.0	1	1.5	0.8	0	0.0	0.0
PSI	66	50.0	6	9.1	4.5	4	6.1	3.0
Total	132	100.0	7	5.3	5.3	4	3.0	3.0

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

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



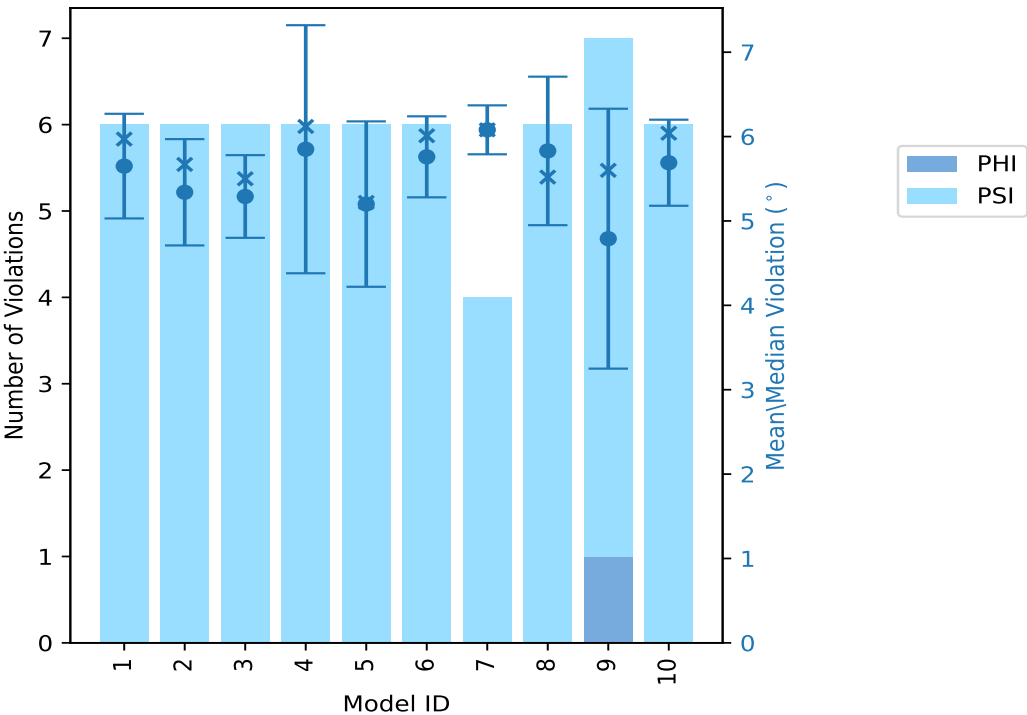
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	6	6	5.65	6.23	0.62	5.97
2	0	6	6	5.34	6.0	0.63	5.67
3	0	6	6	5.29	5.79	0.49	5.5
4	0	6	6	5.85	7.53	1.47	6.12
5	0	6	6	5.2	6.4	0.98	5.22
6	0	6	6	5.76	6.27	0.48	6.01
7	0	4	4	6.08	6.37	0.29	6.08
8	0	6	6	5.83	7.07	0.88	5.52
9	1	6	7	4.79	5.68	1.54	5.6
10	0	6	6	5.69	6.08	0.51	6.04

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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



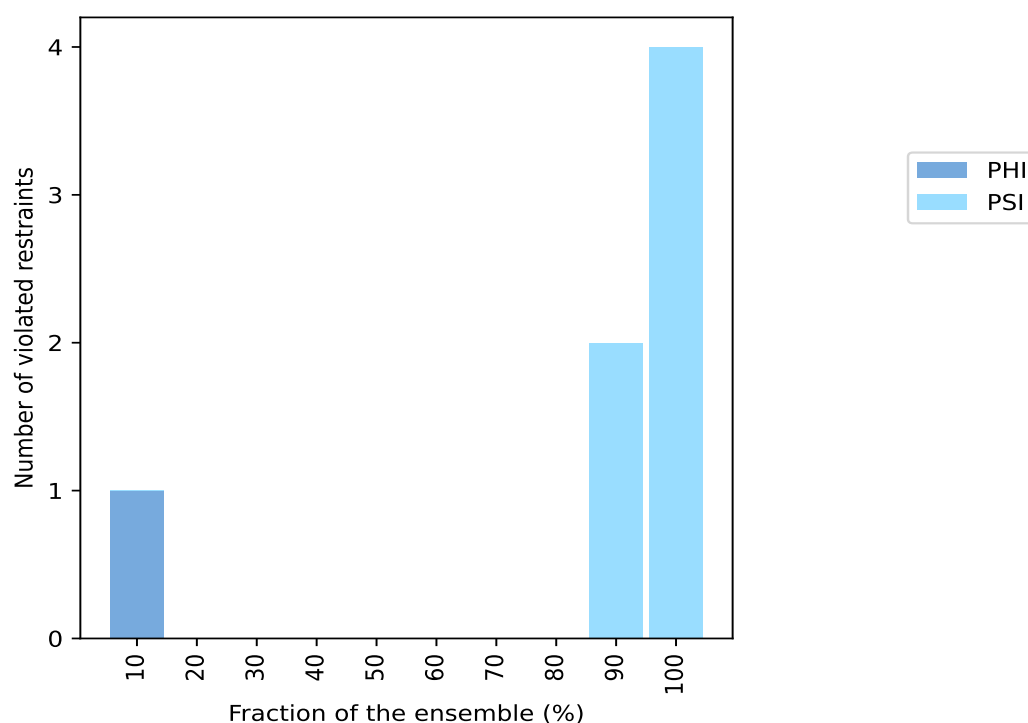
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

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

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

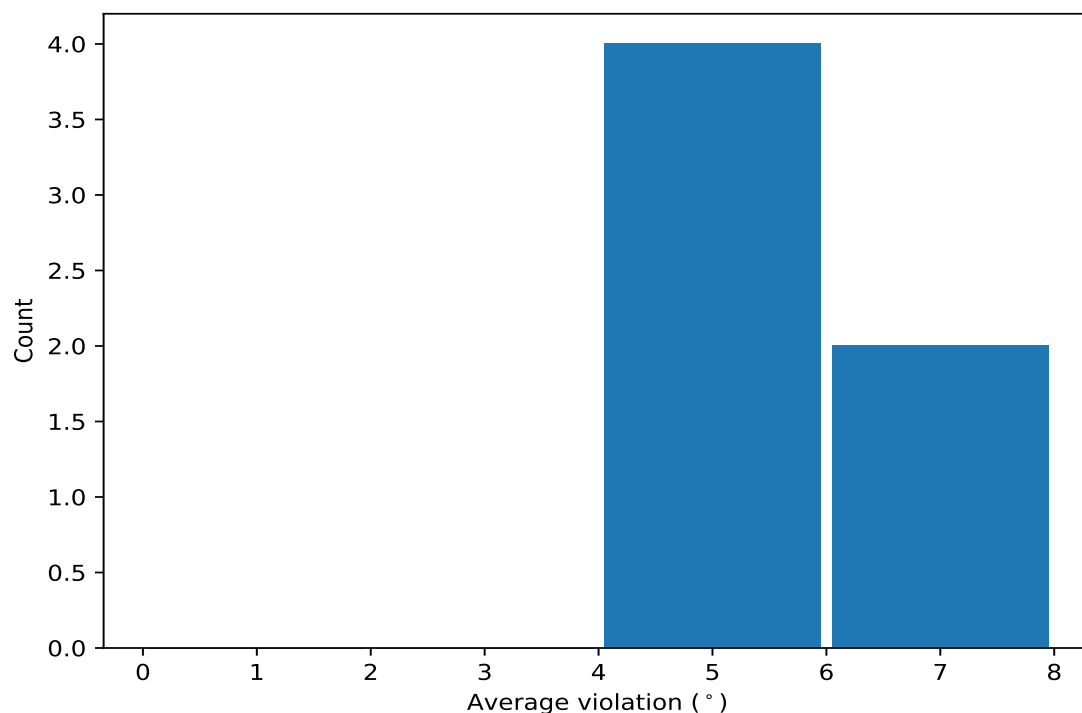
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

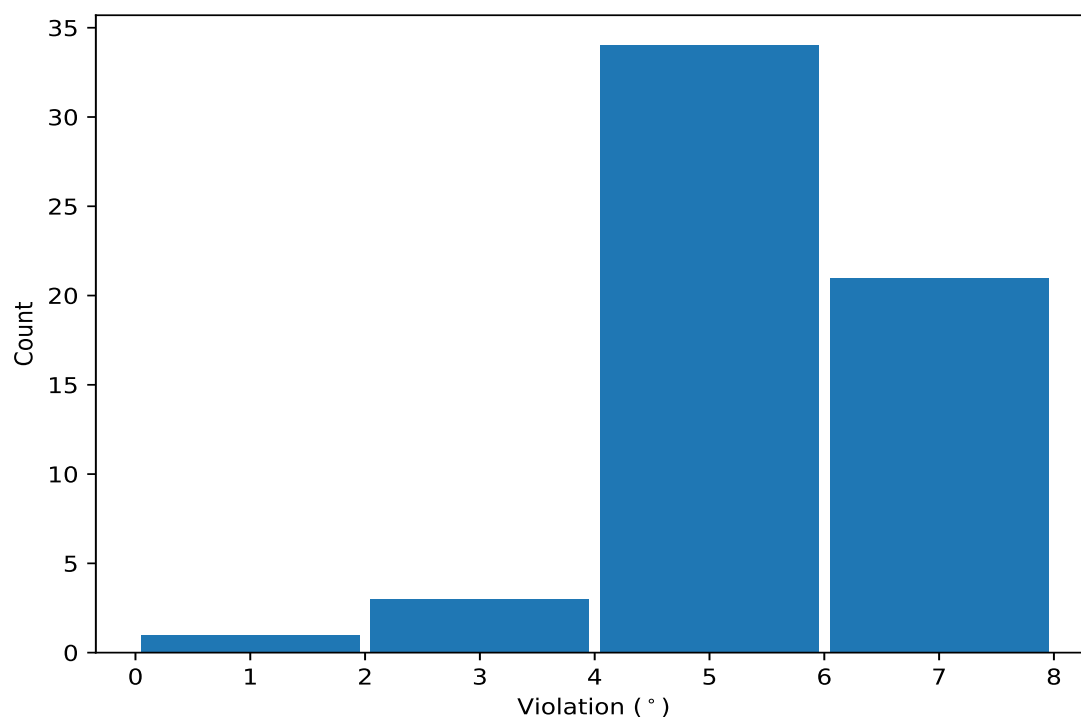
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	10	6.27	0.57	6.22
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	10	6.27	0.56	6.16
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	10	5.81	0.31	5.88
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	10	5.74	0.27	5.8
(1,32)	1:191:A:GLU:N	1:191:A:GLU:CA	1:191:A:GLU:C	1:192:A:ASN:N	9	4.67	0.41	4.7
(1,98)	1:191:B:GLU:N	1:191:B:GLU:CA	1:191:B:GLU:C	1:192:B:ASN:N	9	4.61	0.42	4.75

<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 (°)
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	4	7.53
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	4	7.46
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	8	7.07
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	8	6.94
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	5	6.4
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	5	6.37
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	7	6.37
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	7	6.35
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	6	6.27
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	1	6.23
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	4	6.17
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	1	6.16
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	1	6.1
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	6	6.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	4	6.08
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	10	6.08
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	6	6.08
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	10	6.06
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	10	6.04
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	10	6.03
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	2	6.0
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	6	5.94
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	1	5.84
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	7	5.81
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	2	5.79
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	3	5.79
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	7	5.77
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	3	5.72
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	2	5.7
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	9	5.68
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	8	5.65
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	2	5.64
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	3	5.63
(1,72)	1:178:B:PRO:N	1:178:B:PRO:CA	1:178:B:PRO:C	1:179:B:TRP:N	9	5.63
(1,6)	1:178:A:PRO:N	1:178:A:PRO:CA	1:178:A:PRO:C	1:179:A:TRP:N	9	5.63
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	9	5.6
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	8	5.39
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	3	5.36
(1,30)	1:190:A:PHE:N	1:190:A:PHE:CA	1:190:A:PHE:C	1:191:A:GLU:N	5	5.24
(1,96)	1:190:B:PHE:N	1:190:B:PHE:CA	1:190:B:PHE:C	1:191:B:GLU:N	5	5.2
(1,32)	1:191:A:GLU:N	1:191:A:GLU:CA	1:191:A:GLU:C	1:192:A:ASN:N	8	5.17
(1,98)	1:191:B:GLU:N	1:191:B:GLU:CA	1:191:B:GLU:C	1:192:B:ASN:N	6	5.15
(1,32)	1:191:A:GLU:N	1:191:A:GLU:CA	1:191:A:GLU:C	1:192:A:ASN:N	6	5.03
(1,32)	1:191:A:GLU:N	1:191:A:GLU:CA	1:191:A:GLU:C	1:192:A:ASN:N	10	5.02
(1,32)	1:191:A:GLU:N	1:191:A:GLU:CA	1:191:A:GLU:C	1:192:A:ASN:N	9	4.96
(1,98)	1:191:B:GLU:N	1:191:B:GLU:CA	1:191:B:GLU:C	1:192:B:ASN:N	10	4.92
(1,98)	1:191:B:GLU:N	1:191:B:GLU:CA	1:191:B:GLU:C	1:192:B:ASN:N	9	4.91
(1,98)	1:191:B:GLU:N	1:191:B:GLU:CA	1:191:B:GLU:C	1:192:B:ASN:N	1	4.88
(1,98)	1:191:B:GLU:N	1:191:B:GLU:CA	1:191:B:GLU:C	1:192:B:ASN:N	8	4.75
(1,32)	1:191:A:GLU:N	1:191:A:GLU:CA	1:191:A:GLU:C	1:192:A:ASN:N	1	4.7
(1,32)	1:191:A:GLU:N	1:191:A:GLU:CA	1:191:A:GLU:C	1:192:A:ASN:N	3	4.67
(1,98)	1:191:B:GLU:N	1:191:B:GLU:CA	1:191:B:GLU:C	1:192:B:ASN:N	3	4.58
(1,32)	1:191:A:GLU:N	1:191:A:GLU:CA	1:191:A:GLU:C	1:192:A:ASN:N	2	4.5
(1,98)	1:191:B:GLU:N	1:191:B:GLU:CA	1:191:B:GLU:C	1:192:B:ASN:N	2	4.44
(1,32)	1:191:A:GLU:N	1:191:A:GLU:CA	1:191:A:GLU:C	1:192:A:ASN:N	5	4.14
(1,98)	1:191:B:GLU:N	1:191:B:GLU:CA	1:191:B:GLU:C	1:192:B:ASN:N	4	3.97
(1,32)	1:191:A:GLU:N	1:191:A:GLU:CA	1:191:A:GLU:C	1:192:A:ASN:N	4	3.87
(1,98)	1:191:B:GLU:N	1:191:B:GLU:CA	1:191:B:GLU:C	1:192:B:ASN:N	5	3.86
(1,7)	1:178:A:PRO:C	1:179:A:TRP:N	1:179:A:TRP:CA	1:179:A:TRP:C	9	1.1