Full wwPDB NMR Structure Validation Report (i)

Dec 12, 2023 – 02:11 PM JST

PDB ID	:	8HQB
BMRB ID	:	36528
Title	:	NMR Structure of OsCIE1-Ubox
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Deposited on	:	2022-12-13

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

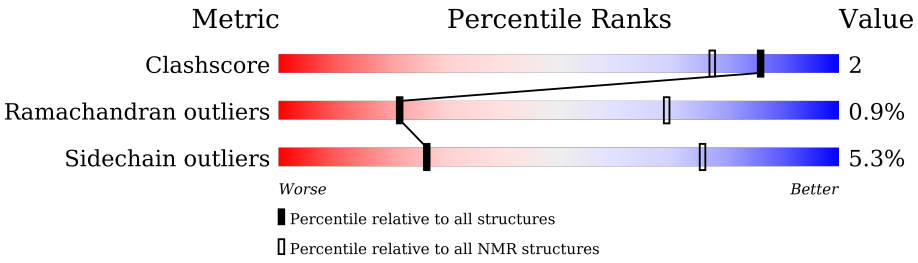
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	80	91% 5% ·
1	B	80	81% 6% · 11%

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:227-A:303, B:227-B:276, B:283-B:303 (148)	1.09	7

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2504 atoms, of which 1254 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called U-box domain-containing protein 12.

Mol	Chain	Residues	Atoms						Trace
1	A	80	Total	C	H	N	O	S	0
			1252	395	627	104	120	6	
1	B	80	Total	C	H	N	O	S	0
			1252	395	627	104	120	6	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	GLY	-	expression tag	UNP Q5VRH9
A	225	ALA	-	expression tag	UNP Q5VRH9
A	226	MET	-	expression tag	UNP Q5VRH9
B	224	GLY	-	expression tag	UNP Q5VRH9
B	225	ALA	-	expression tag	UNP Q5VRH9
B	226	MET	-	expression tag	UNP Q5VRH9

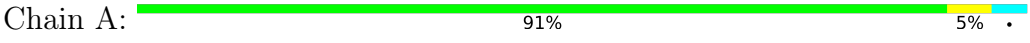
4 Residue-property plots

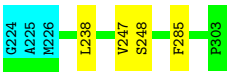
4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: U-box domain-containing protein 12

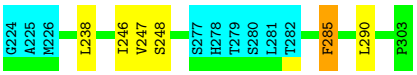
Chain A:





• Molecule 1: U-box domain-containing protein 12

Chain B:



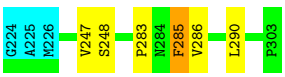
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

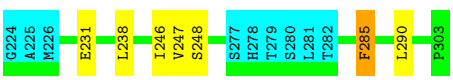
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

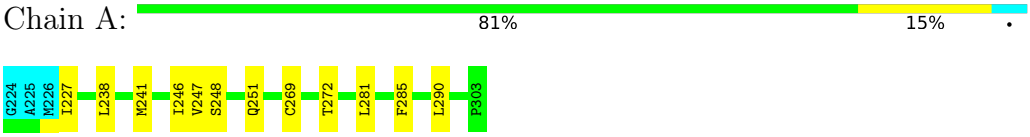
Chain B:



4.2.2 Score per residue for model 2

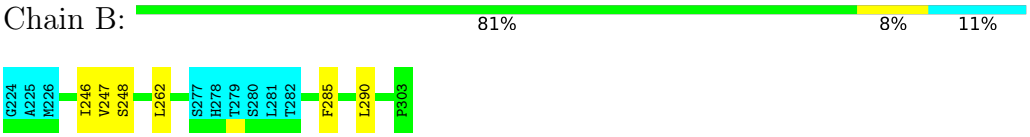
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

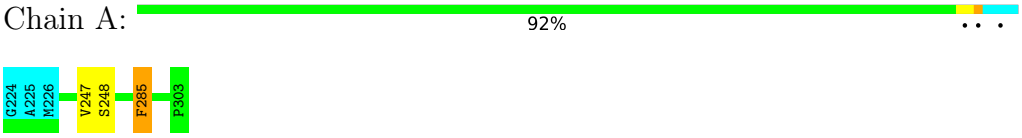
Chain B:



4.2.3 Score per residue for model 3

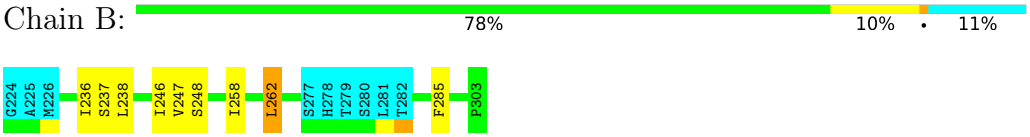
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

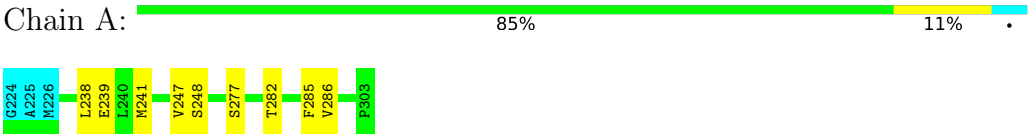
Chain B:



4.2.4 Score per residue for model 4

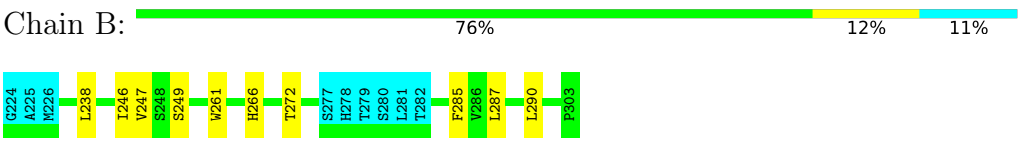
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

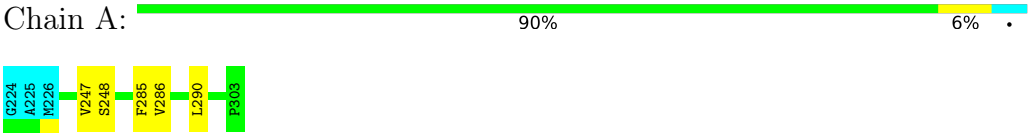
Chain B:



4.2.5 Score per residue for model 5

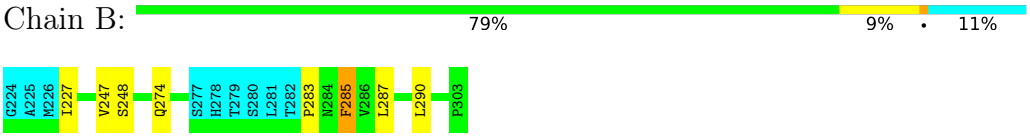
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

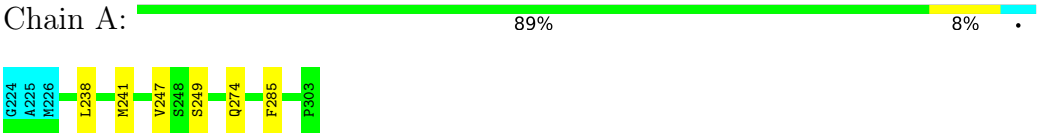
Chain B:



4.2.6 Score per residue for model 6

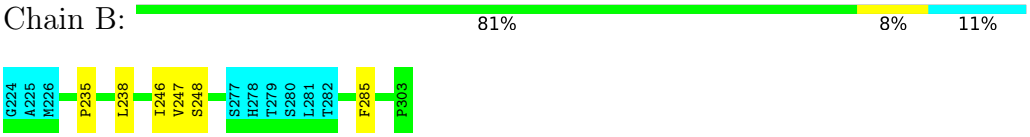
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

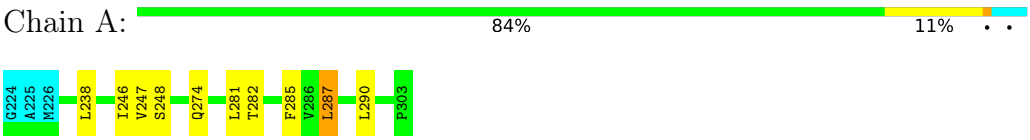
Chain B:



4.2.7 Score per residue for model 7 (medoid)

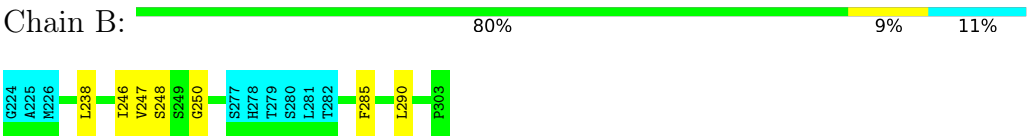
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

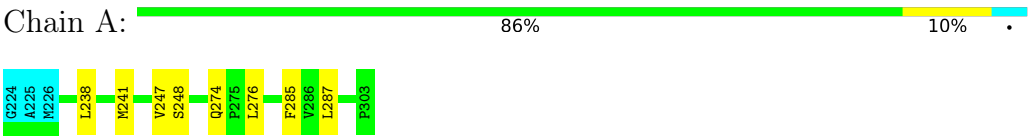
Chain B:



4.2.8 Score per residue for model 8

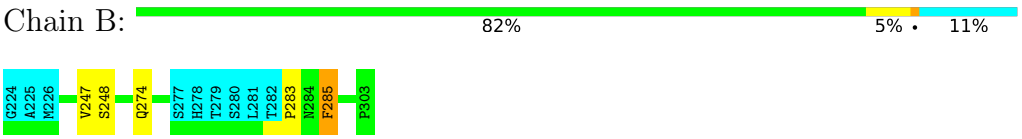
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

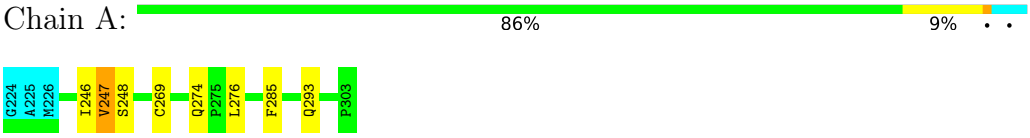
Chain B:



4.2.9 Score per residue for model 9

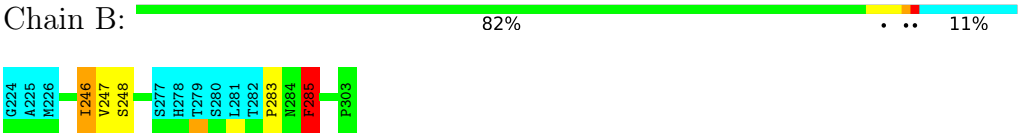
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

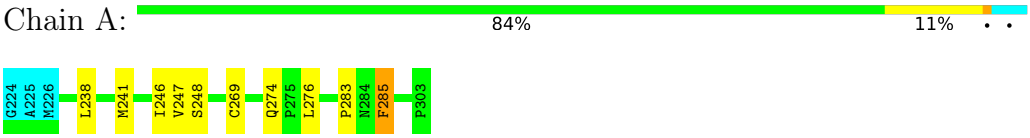
Chain B:



4.2.10 Score per residue for model 10

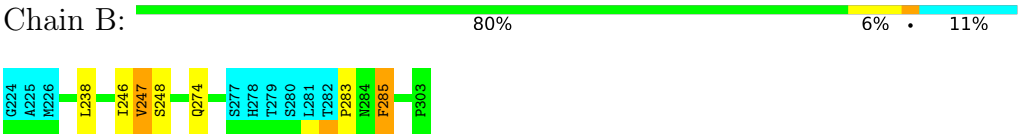
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

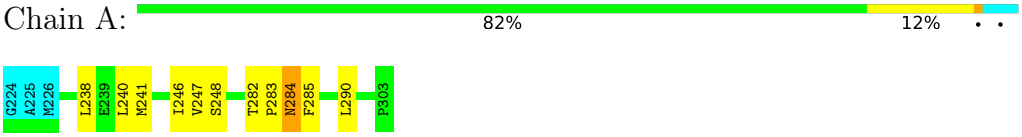
Chain B:



4.2.11 Score per residue for model 11

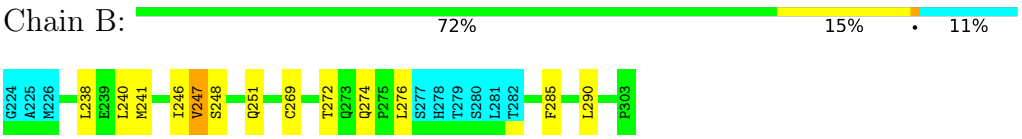
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

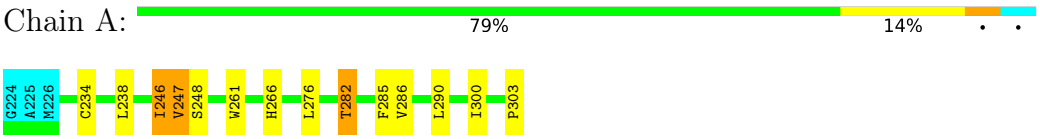
Chain B:



4.2.12 Score per residue for model 12

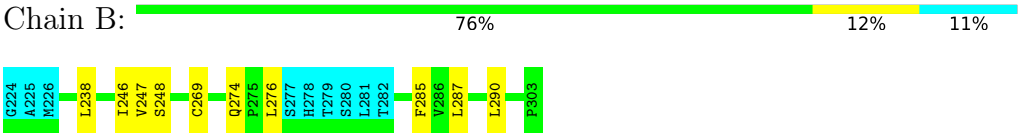
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

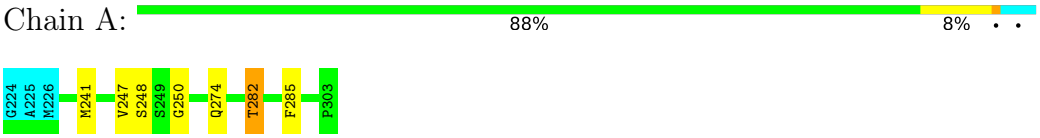
Chain B:



4.2.13 Score per residue for model 13

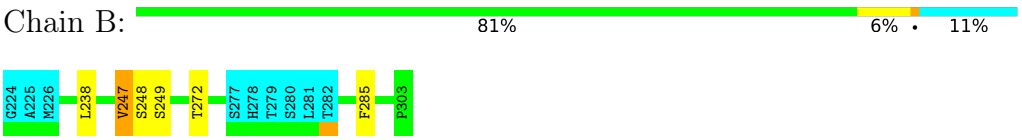
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

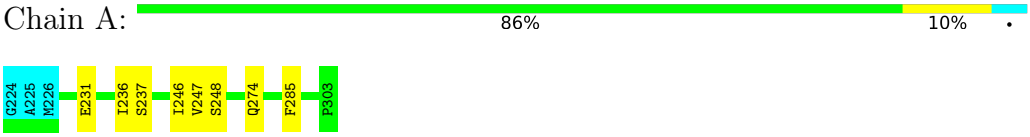
Chain B:



4.2.14 Score per residue for model 14

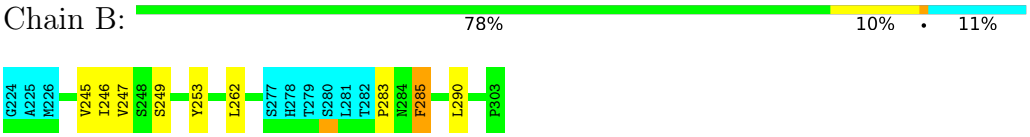
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

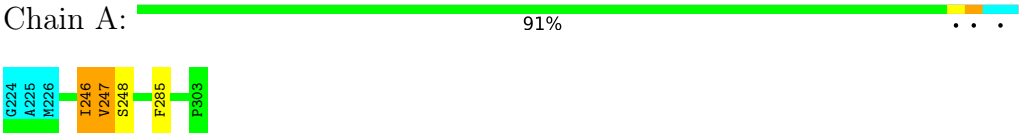
Chain B:



4.2.15 Score per residue for model 15

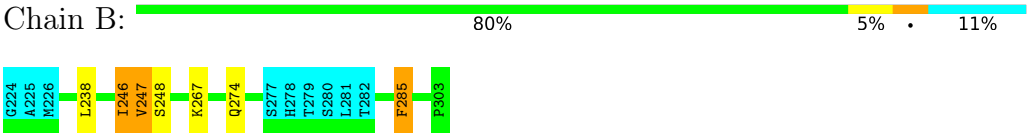
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

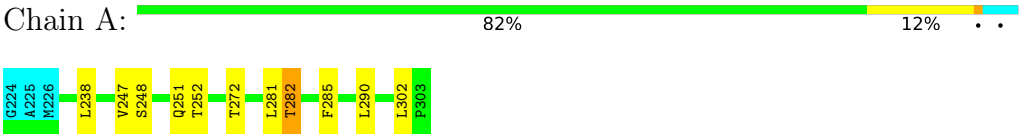
Chain B:



4.2.16 Score per residue for model 16

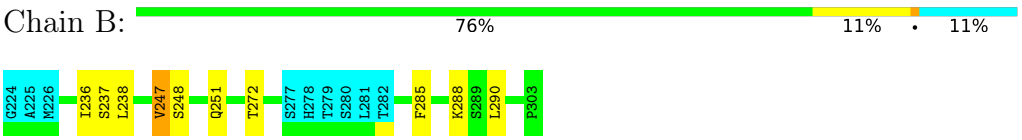
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

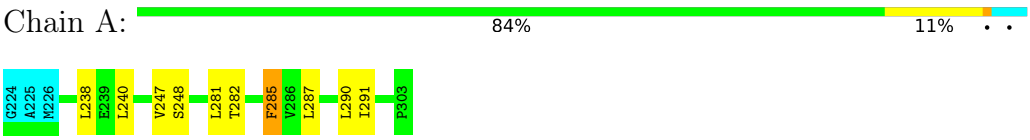
Chain B:



4.2.17 Score per residue for model 17

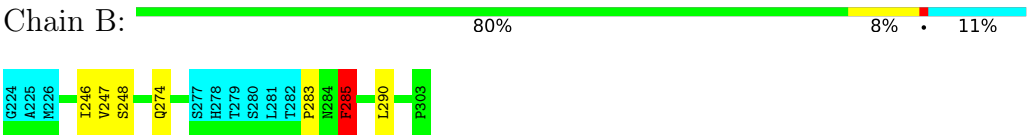
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

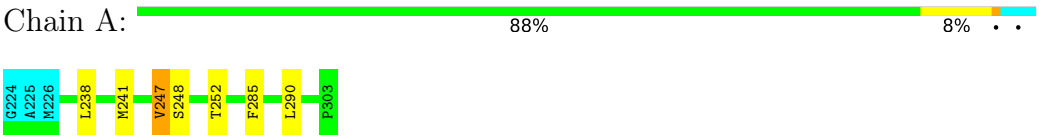
Chain B:



4.2.18 Score per residue for model 18

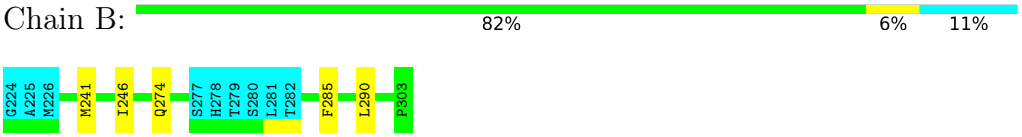
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

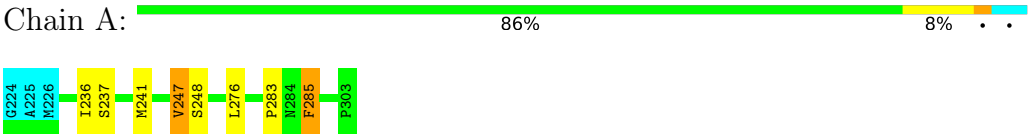
Chain B:



4.2.19 Score per residue for model 19

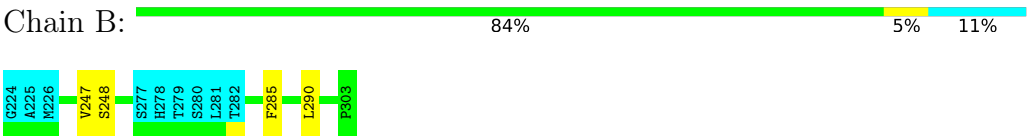
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

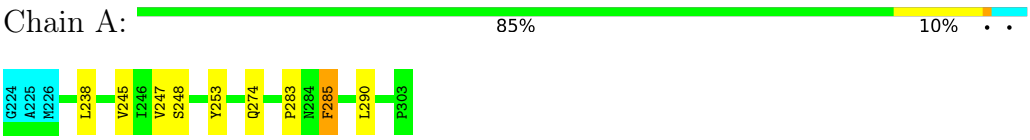
Chain B:



4.2.20 Score per residue for model 20

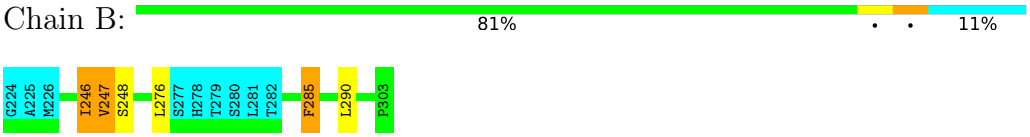
• Molecule 1: U-box domain-containing protein 12

Chain A:



• Molecule 1: U-box domain-containing protein 12

Chain B:



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1007
Number of shifts mapped to atoms	1007
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

6 Model quality

6.1 Standard geometry

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

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	608	607	605	3±2
1	B	564	564	563	3±1
All	All	23440	23420	23360	100

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:290:LEU:CD1	1:B:290:LEU:HD13	0.65	2.22	5	3
1:B:246:ILE:HG21	1:B:285:PHE:CZ	0.64	2.27	10	2
1:A:290:LEU:HD13	1:B:290:LEU:HD13	0.63	1.69	5	9
1:B:247:VAL:HG13	1:B:249:SER:H	0.58	1.59	14	1
1:B:251:GLN:OE1	1:B:272:THR:HG23	0.57	1.99	16	1
1:B:249:SER:OG	1:B:272:THR:HG21	0.56	2.00	13	2
1:B:251:GLN:CD	1:B:272:THR:HG23	0.55	2.22	11	1
1:A:240:LEU:HD23	1:A:241:MET:N	0.55	2.16	11	1
1:A:248:SER:HB2	1:A:276:LEU:HD22	0.53	1.80	12	1
1:B:246:ILE:HG21	1:B:285:PHE:CE2	0.53	2.39	9	2
1:B:246:ILE:HD12	1:B:285:PHE:HZ	0.52	1.64	20	2
1:A:286:VAL:HG11	1:B:287:LEU:HD13	0.52	1.80	4	2
1:A:251:GLN:NE2	1:A:272:THR:HG23	0.50	2.20	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:251:GLN:NE2	1:B:272:THR:HG23	0.49	2.22	11	1
1:A:282:THR:HG23	1:B:248:SER:O	0.48	2.07	16	2
1:B:269:CYS:SG	1:B:276:LEU:HD11	0.48	2.49	11	1
1:A:285:PHE:CE2	1:B:246:ILE:HD11	0.47	2.43	17	1
1:A:247:VAL:HG13	1:A:248:SER:N	0.47	2.25	19	5
1:B:247:VAL:HG13	1:B:248:SER:N	0.47	2.24	11	6
1:A:246:ILE:HD11	1:B:246:ILE:HD11	0.47	1.86	15	1
1:A:285:PHE:CZ	1:B:246:ILE:HD11	0.47	2.45	3	1
1:A:246:ILE:HD12	1:A:247:VAL:O	0.47	2.09	12	1
1:A:247:VAL:HG11	1:A:269:CYS:SG	0.45	2.51	2	1
1:A:287:LEU:HD13	1:A:287:LEU:C	0.45	2.32	17	1
1:B:258:ILE:O	1:B:262:LEU:HD12	0.44	2.13	3	1
1:B:247:VAL:HG11	1:B:269:CYS:SG	0.44	2.53	12	1
1:A:281:LEU:O	1:A:282:THR:C	0.44	2.55	16	2
1:A:247:VAL:HG12	1:A:248:SER:N	0.43	2.28	5	7
1:B:245:VAL:HG22	1:B:253:TYR:O	0.43	2.13	14	1
1:A:247:VAL:HG22	1:A:248:SER:N	0.43	2.29	16	6
1:B:247:VAL:HG12	1:B:248:SER:N	0.43	2.29	9	9
1:A:269:CYS:SG	1:A:276:LEU:HD21	0.43	2.54	10	2
1:A:252:THR:HG23	1:A:252:THR:O	0.43	2.14	16	1
1:B:247:VAL:HG22	1:B:248:SER:N	0.43	2.29	8	2
1:B:236:ILE:HG23	1:B:237:SER:N	0.43	2.28	16	2
1:A:247:VAL:HG22	1:A:248:SER:H	0.43	1.74	4	1
1:A:286:VAL:HG13	1:B:231:GLU:HB3	0.42	1.91	1	1
1:A:283:PRO:O	1:A:284:ASN:C	0.42	2.57	11	1
1:A:286:VAL:HG11	1:B:287:LEU:HD21	0.42	1.92	5	1
1:A:247:VAL:HG13	1:A:249:SER:H	0.42	1.74	6	1
1:A:245:VAL:HG22	1:A:253:TYR:O	0.42	2.15	20	1
1:A:251:GLN:CD	1:A:272:THR:HG23	0.42	2.35	2	1
1:A:246:ILE:HG21	1:B:285:PHE:CZ	0.42	2.50	15	1
1:A:252:THR:O	1:A:252:THR:HG23	0.41	2.15	18	1
1:A:287:LEU:O	1:A:287:LEU:HD23	0.41	2.16	7	1
1:A:236:ILE:HG23	1:A:237:SER:N	0.41	2.30	14	2
1:A:246:ILE:HG21	1:B:285:PHE:CE1	0.41	2.51	15	1
1:A:231:GLU:CB	1:B:290:LEU:HD21	0.41	2.46	14	1
1:B:261:TRP:CD1	1:B:266:HIS:CG	0.40	3.09	4	1
1:A:282:THR:HG22	1:B:250:GLY:CA	0.40	2.47	7	1
1:A:261:TRP:CD1	1:A:266:HIS:CG	0.40	3.10	12	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	76/80 (95%)	71±1 (93±2%)	4±1 (6±1%)	1±1 (1±1%)	21 69
1	B	70/80 (88%)	66±1 (95±2%)	3±1 (4±1%)	1±1 (1±1%)	21 69
All	All	2920/3200 (91%)	2748 (94%)	145 (5%)	27 (1%)	21 69

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	285	PHE	6
1	B	283	PRO	6
1	A	283	PRO	4
1	A	285	PHE	4
1	A	282	THR	2
1	A	281	LEU	1
1	A	277	SER	1
1	B	235	PRO	1
1	A	238	LEU	1
1	A	284	ASN	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	73/74 (99%)	69±2 (95±2%)	4±2 (5±2%)	26 75
1	B	67/74 (91%)	63±1 (95±2%)	4±1 (5±2%)	26 75
All	All	2800/2960 (95%)	2651 (95%)	149 (5%)	26 75

All 32 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	285	PHE	20
1	B	285	PHE	20
1	B	246	ILE	12
1	B	238	LEU	11
1	A	238	LEU	11
1	A	241	MET	8
1	A	246	ILE	8
1	B	274	GLN	8
1	A	274	GLN	8
1	B	247	VAL	7
1	A	247	VAL	5
1	A	282	THR	4
1	B	262	LEU	3
1	B	290	LEU	2
1	A	287	LEU	2
1	A	276	LEU	2
1	B	241	MET	2
1	B	276	LEU	2
1	A	227	ILE	1
1	A	239	GLU	1
1	B	227	ILE	1
1	A	281	LEU	1
1	A	293	GLN	1
1	B	240	LEU	1
1	A	234	CYS	1
1	A	300	ILE	1
1	A	303	PRO	1
1	B	267	LYS	1
1	A	302	LEU	1
1	B	288	LYS	1
1	A	240	LEU	1
1	A	291	ILE	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_ output*

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	1007
Number of shifts mapped to atoms	1007
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 86 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	225	ALA	HB2	1.388	.	.
1	A	225	ALA	HB3	1.388	.	.
1	A	226	MET	HE2	1.47	.	.
1	A	226	MET	HE3	1.47	.	.
1	A	227	ILE	HD12	0.824	.	.
1	A	227	ILE	HD13	0.824	.	.
1	A	227	ILE	HG22	0.805	.	.
1	A	227	ILE	HG23	0.805	.	.
1	A	228	ILE	HD12	0.907	.	.
1	A	228	ILE	HD13	0.907	.	.
1	A	228	ILE	HG22	0.653	.	.
1	A	228	ILE	HG23	0.653	.	.
1	A	236	ILE	HD12	0.251	.	.
1	A	236	ILE	HD13	0.251	.	.
1	A	236	ILE	HG22	0.842	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	236	ILE	HG23	0.842	.	.
1	A	238	LEU	HD12	0.807	.	.
1	A	238	LEU	HD13	0.807	.	.
1	A	238	LEU	HD22	1.102	.	.
1	A	238	LEU	HD23	1.102	.	.
1	A	240	LEU	HD12	0.664	.	.
1	A	240	LEU	HD13	0.664	.	.
1	A	240	LEU	HD22	0.907	.	.
1	A	240	LEU	HD23	0.907	.	.
1	A	241	MET	HE2	1.656	.	.
1	A	241	MET	HE3	1.656	.	.
1	A	245	VAL	HG12	0.686	.	.
1	A	245	VAL	HG13	0.686	.	.
1	A	245	VAL	HG22	0.921	.	.
1	A	245	VAL	HG23	0.921	.	.
1	A	246	ILE	HD12	0.886	.	.
1	A	246	ILE	HD13	0.886	.	.
1	A	246	ILE	HG22	0.788	.	.
1	A	246	ILE	HG23	0.788	.	.
1	A	247	VAL	HG12	0.996	.	.
1	A	247	VAL	HG13	0.996	.	.
1	A	247	VAL	HG22	0.996	.	.
1	A	247	VAL	HG23	0.996	.	.
1	A	252	THR	HG22	1.079	.	.
1	A	252	THR	HG23	1.079	.	.
1	A	258	ILE	HD12	0.197	.	.
1	A	258	ILE	HD13	0.197	.	.
1	A	258	ILE	HG22	0.703	.	.
1	A	258	ILE	HG23	0.703	.	.
1	A	262	LEU	HD12	0.927	.	.
1	A	262	LEU	HD13	0.927	.	.
1	A	262	LEU	HD22	0.927	.	.
1	A	262	LEU	HD23	0.927	.	.
1	A	268	THR	HG22	0.99	.	.
1	A	268	THR	HG23	0.99	.	.
1	A	272	THR	HG22	1.202	.	.
1	A	272	THR	HG23	1.202	.	.
1	A	276	LEU	HD12	0.781	.	.
1	A	276	LEU	HD13	0.781	.	.
1	A	276	LEU	HD22	0.978	.	.
1	A	276	LEU	HD23	0.978	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	279	THR	HG22	1.335	.	.
1	A	279	THR	HG23	1.335	.	.
1	A	282	THR	HG22	1.262	.	.
1	A	282	THR	HG23	1.262	.	.
1	A	286	VAL	HG12	1.086	.	.
1	A	286	VAL	HG13	1.086	.	.
1	A	286	VAL	HG22	1.086	.	.
1	A	286	VAL	HG23	1.086	.	.
1	A	287	LEU	HD12	1.075	.	.
1	A	287	LEU	HD13	1.075	.	.
1	A	287	LEU	HD22	1.075	.	.
1	A	287	LEU	HD23	1.075	.	.
1	A	290	LEU	HD12	0.743	.	.
1	A	290	LEU	HD13	0.743	.	.
1	A	290	LEU	HD22	0.927	.	.
1	A	290	LEU	HD23	0.927	.	.
1	A	291	ILE	HD12	0.659	.	.
1	A	291	ILE	HD13	0.659	.	.
1	A	291	ILE	HG22	0.885	.	.
1	A	291	ILE	HG23	0.885	.	.
1	A	297	ALA	HB2	1.351	.	.
1	A	297	ALA	HB3	1.351	.	.
1	A	300	ILE	HD12	0.907	.	.
1	A	300	ILE	HD13	0.907	.	.
1	A	300	ILE	HG22	0.907	.	.
1	A	300	ILE	HG23	0.907	.	.
1	A	302	LEU	HD12	0.934	.	.
1	A	302	LEU	HD13	0.934	.	.
1	A	302	LEU	HD22	0.934	.	.
1	A	302	LEU	HD23	0.934	.	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	75	-0.35 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	68	0.21 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	63	-0.40 ± 0.20	None needed (< 0.5 ppm)
^{15}N	67	0.22 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 45%, i.e. 901 atoms were assigned a chemical shift out of a possible 2016. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	342/718 (48%)	141/288 (49%)	135/296 (46%)	66/134 (49%)
Sidechain	506/1168 (43%)	357/761 (47%)	146/371 (39%)	3/36 (8%)
Aromatic	53/130 (41%)	27/64 (42%)	24/56 (43%)	2/10 (20%)
Overall	901/2016 (45%)	525/1113 (47%)	305/723 (42%)	71/180 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 920 atoms were assigned a chemical shift out of a possible 2148. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	349/780 (45%)	144/314 (46%)	138/320 (43%)	67/146 (46%)
Sidechain	518/1230 (42%)	367/804 (46%)	148/390 (38%)	3/36 (8%)
Aromatic	53/138 (38%)	27/68 (40%)	24/58 (41%)	2/12 (17%)
Overall	920/2148 (43%)	538/1186 (45%)	310/768 (40%)	72/194 (37%)

7.1.4 Statistically unusual chemical shifts (i)

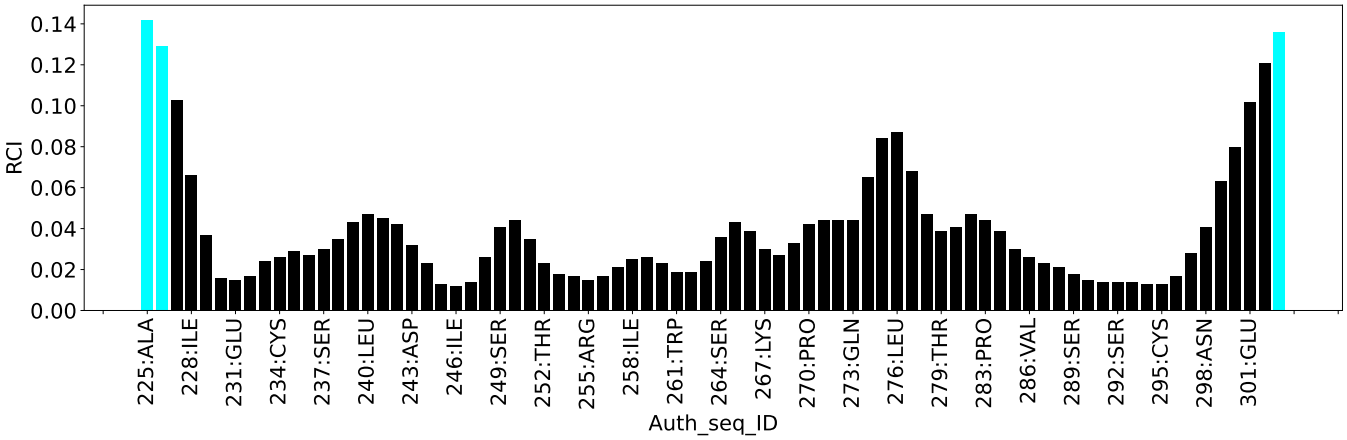
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	255	ARG	CD	33.94	38.57 – 47.75	-10.1
1	A	246	ILE	CG1	14.85	19.24 – 36.26	-7.6
1	A	261	TRP	CZ3	109.66	113.48 – 129.28	-7.4
1	A	270	PRO	HG2	-0.20	0.41 – 3.45	-7.0
1	A	270	PRO	HG3	-0.20	0.33 – 3.48	-6.7
1	A	232	PHE	CD2	123.72	125.53 – 137.61	-6.5
1	A	232	PHE	CD1	123.72	125.33 – 137.83	-6.3
1	A	235	PRO	CG	33.69	21.69 – 32.72	5.9
1	A	239	GLU	CG	29.55	30.20 – 42.01	-5.5
1	A	253	TYR	CE2	111.56	111.68 – 124.17	-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	2381
Intra-residue (|i-j|=0)	1028
Sequential (|i-j|=1)	577
Medium range (|i-j|>1 and |i-j|<5)	346
Long range (|i-j|≥5)	374
Inter-chain	56
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	14.9
Number of long range restraints per residue[1]	2.3

[1]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)	32.6	0.2
0.2-0.5 (Medium)	13.6	0.46
>0.5 (Large)	1.4	1.18

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

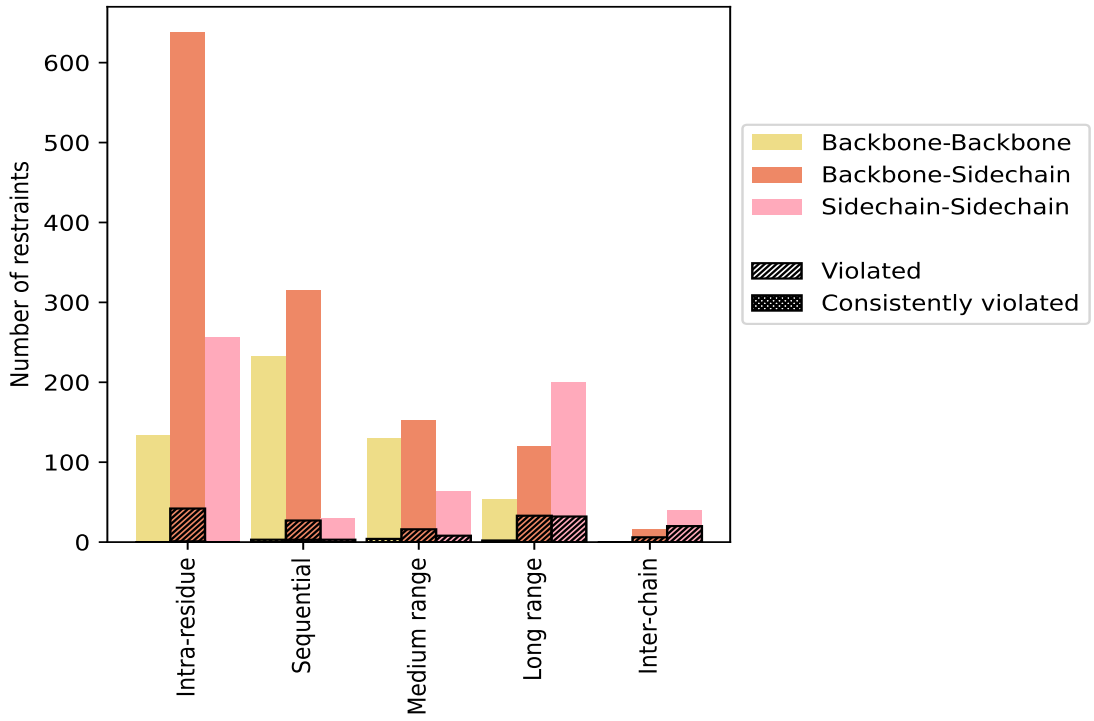
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	1028	43.2	42	4.1	1.8	1	0.1	0.0
Backbone-Backbone	134	5.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	638	26.8	42	6.6	1.8	1	0.2	0.0
Sidechain-Sidechain	256	10.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	577	24.2	33	5.7	1.4	3	0.5	0.1
Backbone-Backbone	232	9.7	3	1.3	0.1	0	0.0	0.0
Backbone-Sidechain	315	13.2	27	8.6	1.1	3	1.0	0.1
Sidechain-Sidechain	30	1.3	3	10.0	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	346	14.5	28	8.1	1.2	0	0.0	0.0
Backbone-Backbone	130	5.5	4	3.1	0.2	0	0.0	0.0
Backbone-Sidechain	152	6.4	16	10.5	0.7	0	0.0	0.0
Sidechain-Sidechain	64	2.7	8	12.5	0.3	0	0.0	0.0
Long range (|i-j|≥5)	374	15.7	67	17.9	2.8	0	0.0	0.0
Backbone-Backbone	54	2.3	2	3.7	0.1	0	0.0	0.0
Backbone-Sidechain	120	5.0	33	27.5	1.4	0	0.0	0.0
Sidechain-Sidechain	200	8.4	32	16.0	1.3	0	0.0	0.0
Inter-chain	56	2.4	26	46.4	1.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	16	0.7	6	37.5	0.3	0	0.0	0.0
Sidechain-Sidechain	40	1.7	20	50.0	0.8	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2381	100.0	196	8.2	8.2	4	0.2	0.2
Backbone-Backbone	550	23.1	9	1.6	0.4	0	0.0	0.0
Backbone-Sidechain	1241	52.1	124	10.0	5.2	4	0.3	0.2
Sidechain-Sidechain	590	24.8	63	10.7	2.6	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

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[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	13	10	6	14	7	50	0.19	0.72	0.1	0.16
2	13	10	6	17	7	53	0.19	0.91	0.13	0.16
3	14	14	7	16	8	59	0.19	0.62	0.09	0.18
4	10	9	4	14	4	41	0.2	0.59	0.09	0.2
5	11	12	8	14	5	50	0.18	0.62	0.09	0.15
6	14	8	7	12	4	45	0.2	1.16	0.16	0.18
7	11	10	4	17	7	49	0.23	1.1	0.19	0.18
8	12	10	9	16	7	54	0.19	1.05	0.13	0.18
9	16	14	6	15	8	59	0.18	0.58	0.09	0.16
10	16	10	3	14	7	50	0.17	0.64	0.08	0.17
11	16	7	6	13	4	46	0.19	0.63	0.09	0.17

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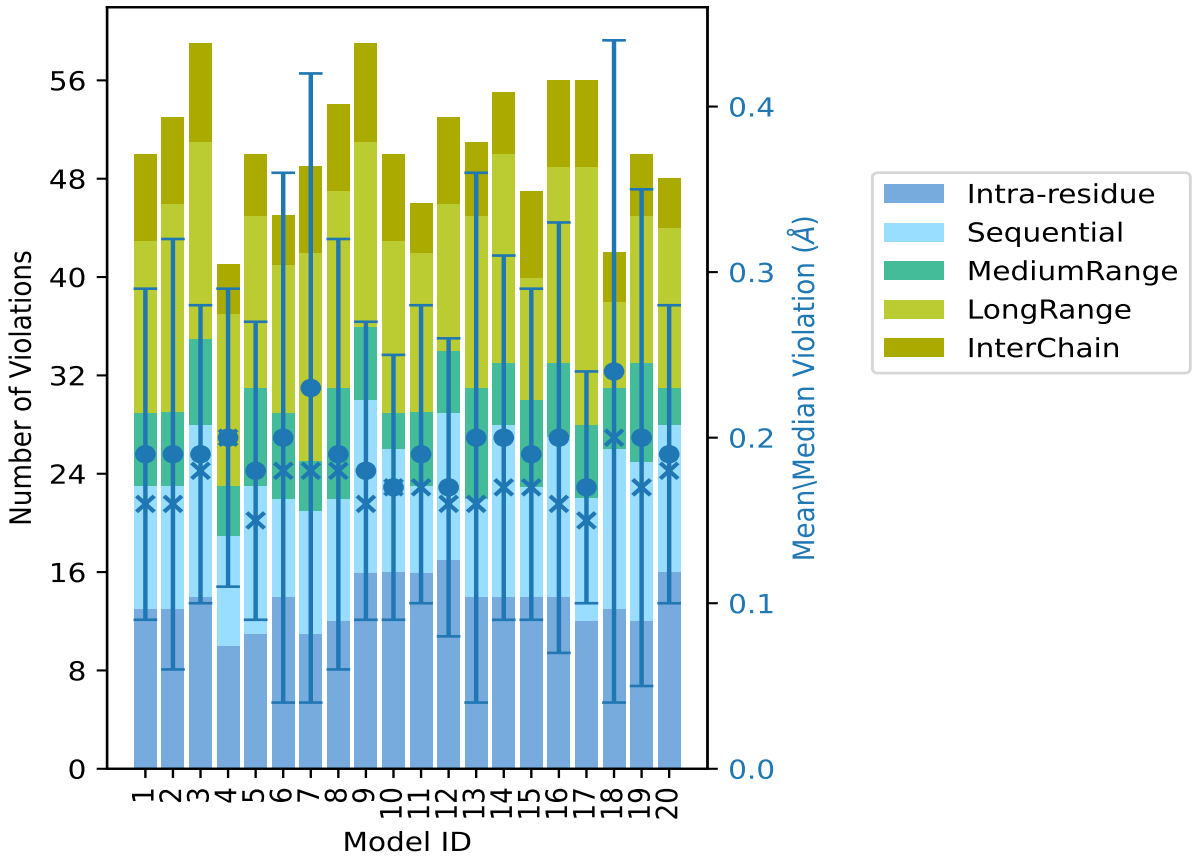
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	17	12	5	12	7	53	0.17	0.69	0.09	0.16
13	14	8	9	14	6	51	0.2	1.18	0.16	0.16
14	14	14	5	17	5	55	0.2	0.85	0.11	0.17
15	14	9	7	10	7	47	0.19	0.66	0.1	0.17
16	14	13	6	16	7	56	0.2	0.86	0.13	0.16
17	12	10	6	21	7	56	0.17	0.51	0.07	0.15
18	13	13	5	7	4	42	0.24	1.05	0.2	0.2
19	12	13	8	12	5	50	0.2	1.15	0.15	0.17
20	16	12	3	13	4	48	0.19	0.64	0.09	0.18

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



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

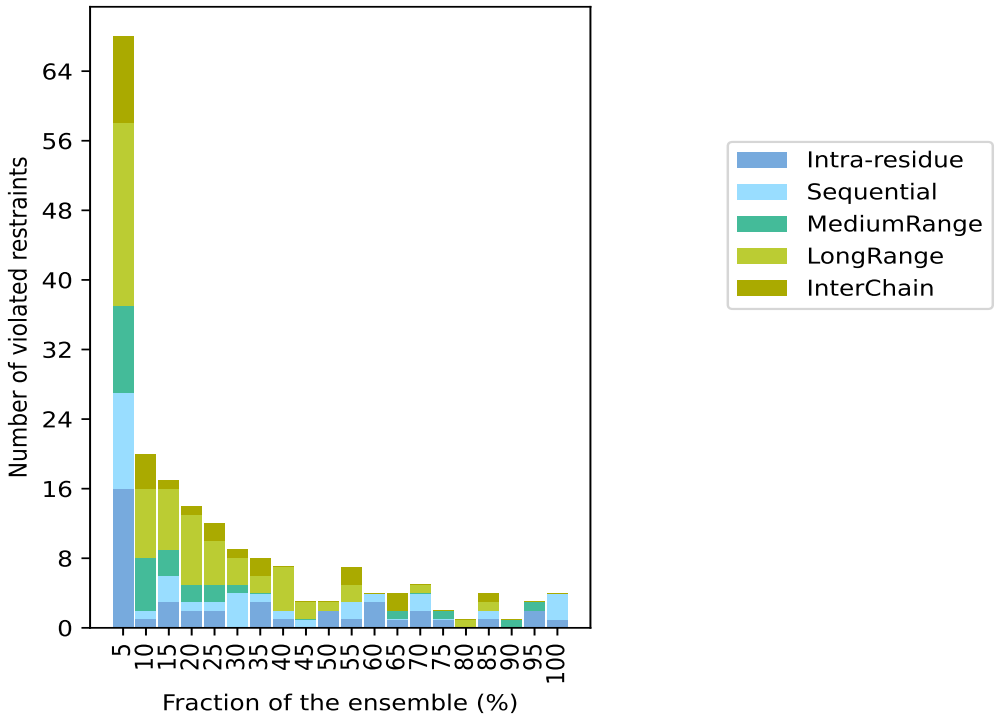
9.3 Distance violation statistics for the ensemble (i)

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, 2185(IR:986, SQ:544, MR:318, LR:307, IC:30) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
16	11	10	21	10	68	1	5.0
1	1	6	8	4	20	2	10.0
3	3	3	7	1	17	3	15.0
2	1	2	8	1	14	4	20.0
2	1	2	5	2	12	5	25.0
0	4	1	3	1	9	6	30.0
3	1	0	2	2	8	7	35.0
1	1	0	5	0	7	8	40.0
0	1	0	2	0	3	9	45.0
2	0	0	1	0	3	10	50.0
1	2	0	2	2	7	11	55.0
3	1	0	0	0	4	12	60.0
1	0	1	0	2	4	13	65.0
2	2	0	1	0	5	14	70.0
1	0	1	0	0	2	15	75.0
0	0	0	1	0	1	16	80.0
1	1	0	1	1	4	17	85.0
0	0	1	0	0	1	18	90.0
2	0	1	0	0	3	19	95.0
1	3	0	0	0	4	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

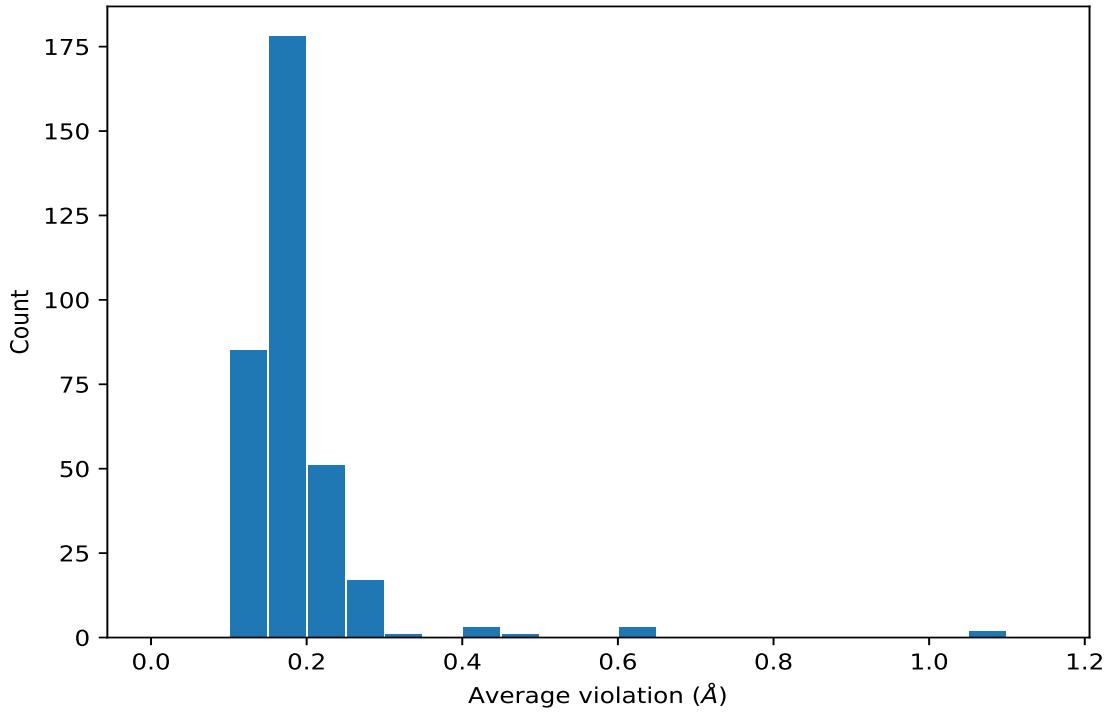
9.3.1 Bar graph : Distance violation statistics for the ensemble



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[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	20	0.3	0.1	0.34
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	20	0.28	0.11	0.3
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	20	0.2	0.02	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	20	0.2	0.02	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	20	0.2	0.02	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	20	0.2	0.01	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	20	0.2	0.01	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	20	0.2	0.01	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	19	0.2	0.01	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	19	0.2	0.01	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	19	0.2	0.01	0.2
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	19	0.19	0.03	0.2
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	19	0.18	0.04	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	19	0.18	0.04	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	19	0.18	0.04	0.18
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	18	0.18	0.03	0.19

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	17	0.62	0.09	0.63
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	17	0.62	0.09	0.63
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	17	0.62	0.09	0.63
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	17	0.2	0.05	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	17	0.2	0.02	0.2
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	17	0.2	0.02	0.2
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	17	0.2	0.02	0.2
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	17	0.16	0.05	0.15
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	17	0.16	0.05	0.15
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	17	0.16	0.05	0.15
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	16	0.18	0.06	0.18
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	15	0.2	0.04	0.21
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	15	0.2	0.04	0.21
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	15	0.12	0.02	0.11
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	14	0.19	0.05	0.2
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	14	0.19	0.05	0.2
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	14	0.19	0.05	0.2
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	14	0.18	0.04	0.18
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	14	0.18	0.04	0.18
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	14	0.18	0.04	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	14	0.17	0.03	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	14	0.17	0.03	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	14	0.17	0.03	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	14	0.17	0.03	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	14	0.17	0.03	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	14	0.17	0.03	0.18
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	14	0.16	0.03	0.16
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	14	0.16	0.03	0.16
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	14	0.16	0.03	0.16
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	14	0.12	0.01	0.12
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	13	0.18	0.05	0.19
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	13	0.18	0.05	0.19
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	13	0.18	0.05	0.19
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	13	0.18	0.05	0.19
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	13	0.18	0.05	0.19
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	13	0.18	0.05	0.19
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	13	0.18	0.05	0.19
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	13	0.18	0.05	0.19
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	13	0.18	0.05	0.19
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	13	0.18	0.05	0.19
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	13	0.18	0.05	0.19
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	13	0.18	0.05	0.19

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	13	0.18	0.05	0.19
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	13	0.18	0.05	0.19
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	13	0.18	0.05	0.19
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	13	0.18	0.05	0.19
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	13	0.18	0.05	0.19
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	13	0.18	0.05	0.19
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	13	0.18	0.03	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	13	0.18	0.03	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	13	0.18	0.03	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	13	0.18	0.03	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	13	0.18	0.03	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	13	0.18	0.03	0.18
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	13	0.18	0.04	0.17
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	13	0.18	0.04	0.17
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	12	0.28	0.09	0.29
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	12	0.28	0.09	0.29
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	12	0.28	0.09	0.29
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	12	0.21	0.01	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	12	0.21	0.01	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	12	0.21	0.01	0.21
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	12	0.13	0.02	0.12
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	12	0.12	0.01	0.11
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	11	0.47	0.34	0.35
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	11	0.26	0.02	0.27
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	11	0.21	0.05	0.21
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	11	0.21	0.05	0.21
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	11	0.18	0.01	0.18
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	11	0.16	0.02	0.17
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	11	0.16	0.02	0.17
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	11	0.16	0.02	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	11	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	11	0.16	0.04	0.16
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	11	0.16	0.04	0.16
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	11	0.16	0.06	0.14
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	11	0.16	0.06	0.14
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	11	0.16	0.06	0.14
(1,297)	1:243:B:ASP:H	1:243:B:ASP:HB3	10	0.26	0.01	0.26
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG21	10	0.21	0.01	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG22	10	0.21	0.01	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG23	10	0.21	0.01	0.21
(1,1918)	1:269:A:CYS:H	1:274:A:GLN:HG3	10	0.18	0.04	0.18
(1,547)	1:259:B:GLN:H	1:258:B:ILE:HB	9	0.19	0.02	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD11	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD12	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD13	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD21	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD22	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD23	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD11	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD12	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD13	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD21	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD22	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD23	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD11	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD12	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD13	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD21	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD22	9	0.15	0.04	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD23	9	0.15	0.04	0.16
(1,452)	1:253:B:TYR:HE1	1:247:B:VAL:HB	9	0.14	0.02	0.15
(1,452)	1:253:B:TYR:HE2	1:247:B:VAL:HB	9	0.14	0.02	0.15
(1,1352)	1:237:A:SER:H	1:236:A:ILE:HB	8	0.28	0.06	0.3
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB2	8	0.16	0.04	0.16
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB3	8	0.16	0.04	0.16
(1,1037)	1:294:B:TRP:HH2	1:228:B:ILE:HB	8	0.16	0.03	0.14
(1,1613)	1:253:A:TYR:HE1	1:247:A:VAL:HB	8	0.15	0.04	0.15
(1,1613)	1:253:A:TYR:HE2	1:247:A:VAL:HB	8	0.15	0.04	0.15
(1,1260)	1:232:A:PHE:HA	1:303:A:PRO:HD3	8	0.13	0.04	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,757)	1:269:B:CYS:H	1:274:B:GLN:HG3	8	0.13	0.03	0.12
(1,881)	1:285:B:PHE:HD1	1:285:B:PHE:HA	8	0.12	0.02	0.13
(1,881)	1:285:B:PHE:HD2	1:285:B:PHE:HA	8	0.12	0.02	0.13
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG2	7	1.06	0.12	1.1
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG3	7	1.06	0.12	1.1
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD11	7	0.28	0.04	0.28
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD12	7	0.28	0.04	0.28
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD13	7	0.28	0.04	0.28
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG21	7	0.2	0.04	0.19
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG22	7	0.2	0.04	0.19
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG23	7	0.2	0.04	0.19
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG21	7	0.2	0.04	0.19
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG22	7	0.2	0.04	0.19
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG23	7	0.2	0.04	0.19
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG21	7	0.2	0.04	0.19
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG22	7	0.2	0.04	0.19
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG23	7	0.2	0.04	0.19
(1,2365)	1:246:B:ILE:HD11	1:282:A:THR:HB	7	0.18	0.05	0.17
(1,2365)	1:246:B:ILE:HD12	1:282:A:THR:HB	7	0.18	0.05	0.17
(1,2365)	1:246:B:ILE:HD13	1:282:A:THR:HB	7	0.18	0.05	0.17
(1,608)	1:261:B:TRP:HE1	1:270:B:PRO:HB2	7	0.13	0.03	0.12
(1,749)	1:269:B:CYS:H	1:275:B:PRO:HB2	7	0.13	0.03	0.12
(1,2042)	1:285:A:PHE:HD1	1:285:A:PHE:HA	7	0.13	0.01	0.13
(1,2042)	1:285:A:PHE:HD2	1:285:A:PHE:HA	7	0.13	0.01	0.13
(1,1863)	1:266:A:HIS:H	1:266:A:HIS:HB3	7	0.12	0.02	0.13
(1,191)	1:237:B:SER:H	1:236:B:ILE:HB	6	0.24	0.07	0.28
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD11	6	0.2	0.07	0.18
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD12	6	0.2	0.07	0.18
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD13	6	0.2	0.07	0.18
(1,743)	1:269:B:CYS:H	1:268:B:THR:HB	6	0.19	0.03	0.19
(1,1904)	1:269:A:CYS:H	1:268:A:THR:HB	6	0.17	0.03	0.16
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG12	6	0.16	0.06	0.15
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG13	6	0.16	0.06	0.15
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG12	6	0.16	0.06	0.15
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG13	6	0.16	0.06	0.15
(1,393)	1:249:B:SER:H	1:251:B:GLN:HE21	6	0.15	0.04	0.14
(1,1769)	1:261:A:TRP:HE1	1:270:A:PRO:HB2	6	0.14	0.02	0.14
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG12	6	0.14	0.03	0.12
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG13	6	0.14	0.03	0.12
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG12	6	0.14	0.03	0.12
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG13	6	0.14	0.03	0.12
(1,2377)	1:285:B:PHE:HZ	1:250:A:GLY:HA3	6	0.14	0.03	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD21	5	0.44	0.21	0.35
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD22	5	0.44	0.21	0.35
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD23	5	0.44	0.21	0.35
(1,1910)	1:269:A:CYS:H	1:275:A:PRO:HB2	5	0.19	0.06	0.16
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG21	5	0.19	0.05	0.21
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG22	5	0.19	0.05	0.21
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG23	5	0.19	0.05	0.21
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG21	5	0.19	0.05	0.21
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG22	5	0.19	0.05	0.21
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG23	5	0.19	0.05	0.21
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG21	5	0.19	0.05	0.21
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG22	5	0.19	0.05	0.21
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG23	5	0.19	0.05	0.21
(1,1522)	1:246:A:ILE:HG12	1:284:A:ASN:HA	5	0.18	0.06	0.16
(1,1522)	1:246:A:ILE:HG13	1:284:A:ASN:HA	5	0.18	0.06	0.16
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD21	5	0.18	0.03	0.18
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD22	5	0.18	0.03	0.18
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD23	5	0.18	0.03	0.18
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD2	5	0.16	0.04	0.14
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD3	5	0.16	0.04	0.14
(1,259)	1:241:B:MET:H	1:241:B:MET:HB2	5	0.15	0.04	0.15
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD2	5	0.15	0.02	0.15
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD3	5	0.15	0.02	0.15
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB2	5	0.14	0.03	0.13
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB3	5	0.14	0.03	0.13
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG21	5	0.13	0.02	0.14
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG22	5	0.13	0.02	0.14
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG23	5	0.13	0.02	0.14
(1,702)	1:266:B:HIS:H	1:266:B:HIS:HB3	5	0.12	0.02	0.11
(1,2199)	1:294:A:TRP:HH2	1:228:A:ILE:HB	5	0.11	0.01	0.1
(1,198)	1:237:B:SER:H	1:234:B:CYS:HB2	4	0.25	0.05	0.26
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD11	4	0.22	0.06	0.21
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD12	4	0.22	0.06	0.21
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD13	4	0.22	0.06	0.21
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD11	4	0.22	0.06	0.21
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD12	4	0.22	0.06	0.21
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD13	4	0.22	0.06	0.21
(1,269)	1:241:B:MET:H	1:241:B:MET:HE1	4	0.19	0.07	0.18
(1,269)	1:241:B:MET:H	1:241:B:MET:HE2	4	0.19	0.07	0.18
(1,269)	1:241:B:MET:H	1:241:B:MET:HE3	4	0.19	0.07	0.18
(1,892)	1:285:B:PHE:HZ	1:250:B:GLY:HA2	4	0.18	0.04	0.2
(1,180)	1:236:B:ILE:H	1:253:B:TYR:HE1	4	0.16	0.04	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,180)	1:236:B:ILE:H	1:253:B:TYR:HE2	4	0.16	0.04	0.15
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG21	4	0.15	0.04	0.15
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG22	4	0.15	0.04	0.15
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG23	4	0.15	0.04	0.15
(1,1971)	1:273:A:GLN:H	1:268:A:THR:HB	4	0.15	0.03	0.15
(1,822)	1:274:B:GLN:H	1:272:B:THR:HA	4	0.15	0.05	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD21	4	0.14	0.02	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD22	4	0.14	0.02	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD23	4	0.14	0.02	0.13
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD11	4	0.14	0.03	0.13
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD12	4	0.14	0.03	0.13
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD13	4	0.14	0.03	0.13
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD11	4	0.13	0.02	0.14
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD12	4	0.13	0.02	0.14
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD13	4	0.13	0.02	0.14
(1,1122)	1:300:B:ILE:H	1:295:B:CYS:HB2	4	0.12	0.02	0.12
(1,1122)	1:300:B:ILE:H	1:295:B:CYS:HB3	4	0.12	0.02	0.12
(1,1124)	1:300:B:ILE:H	1:295:B:CYS:HB2	4	0.12	0.02	0.12
(1,1124)	1:300:B:ILE:H	1:295:B:CYS:HB3	4	0.12	0.02	0.12
(1,167)	1:236:B:ILE:H	1:236:B:ILE:HB	4	0.12	0.01	0.12
(1,2053)	1:285:A:PHE:HZ	1:250:A:GLY:HA2	3	0.18	0.04	0.18
(1,1420)	1:241:A:MET:H	1:241:A:MET:HB2	3	0.17	0.05	0.21
(1,361)	1:246:B:ILE:HG12	1:284:B:ASN:HA	3	0.16	0.02	0.17
(1,361)	1:246:B:ILE:HG13	1:284:B:ASN:HA	3	0.16	0.02	0.17
(1,99)	1:232:B:PHE:HA	1:303:B:PRO:HD3	3	0.15	0.0	0.15
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE1	3	0.15	0.03	0.17
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE2	3	0.15	0.03	0.17
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE3	3	0.15	0.03	0.17
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD11	3	0.14	0.02	0.14
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD12	3	0.14	0.02	0.14
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD13	3	0.14	0.02	0.14
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE1	3	0.13	0.03	0.11
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE2	3	0.13	0.03	0.11
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE3	3	0.13	0.03	0.11
(1,1521)	1:246:A:ILE:HA	1:252:A:THR:HB	3	0.13	0.02	0.12
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD11	3	0.13	0.01	0.13
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD12	3	0.13	0.01	0.13
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD13	3	0.13	0.01	0.13
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD11	3	0.13	0.01	0.13
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD12	3	0.13	0.01	0.13
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD13	3	0.13	0.01	0.13
(1,1102)	1:299:B:GLY:H	1:298:B:ASN:HD22	3	0.13	0.0	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1983)	1:274:A:GLN:H	1:272:A:THR:HA	3	0.13	0.02	0.11
(1,2264)	1:299:A:GLY:H	1:298:A:ASN:HD22	3	0.12	0.01	0.11
(1,2349)	1:285:A:PHE:HZ	1:250:B:GLY:HA3	3	0.12	0.01	0.12
(1,810)	1:273:B:GLN:H	1:268:B:THR:HB	3	0.12	0.01	0.11
(1,2022)	1:278:A:HIS:HD2	1:248:A:SER:H	3	0.11	0.01	0.11
(1,861)	1:278:B:HIS:HD2	1:248:B:SER:H	3	0.11	0.0	0.11
(1,950)	1:290:B:LEU:HD11	1:293:B:GLN:HB2	2	0.25	0.04	0.25
(1,950)	1:290:B:LEU:HD11	1:293:B:GLN:HB3	2	0.25	0.04	0.25
(1,950)	1:290:B:LEU:HD12	1:293:B:GLN:HB2	2	0.25	0.04	0.25
(1,950)	1:290:B:LEU:HD12	1:293:B:GLN:HB3	2	0.25	0.04	0.25
(1,950)	1:290:B:LEU:HD13	1:293:B:GLN:HB2	2	0.25	0.04	0.25
(1,950)	1:290:B:LEU:HD13	1:293:B:GLN:HB3	2	0.25	0.04	0.25
(1,2356)	1:231:B:GLU:HG2	1:290:A:LEU:HD11	2	0.22	0.08	0.22
(1,2356)	1:231:B:GLU:HG2	1:290:A:LEU:HD12	2	0.22	0.08	0.22
(1,2356)	1:231:B:GLU:HG2	1:290:A:LEU:HD13	2	0.22	0.08	0.22
(1,2356)	1:231:B:GLU:HG3	1:290:A:LEU:HD11	2	0.22	0.08	0.22
(1,2356)	1:231:B:GLU:HG3	1:290:A:LEU:HD12	2	0.22	0.08	0.22
(1,2356)	1:231:B:GLU:HG3	1:290:A:LEU:HD13	2	0.22	0.08	0.22
(1,304)	1:243:B:ASP:H	1:241:B:MET:HE1	2	0.21	0.03	0.21
(1,304)	1:243:B:ASP:H	1:241:B:MET:HE2	2	0.21	0.03	0.21
(1,304)	1:243:B:ASP:H	1:241:B:MET:HE3	2	0.21	0.03	0.21
(1,1559)	1:249:A:SER:HB2	1:269:A:CYS:HB2	2	0.19	0.02	0.19
(1,1559)	1:249:A:SER:HB2	1:269:A:CYS:HB3	2	0.19	0.02	0.19
(1,2112)	1:290:A:LEU:HD11	1:293:A:GLN:HB2	2	0.19	0.08	0.19
(1,2112)	1:290:A:LEU:HD11	1:293:A:GLN:HB3	2	0.19	0.08	0.19
(1,2112)	1:290:A:LEU:HD12	1:293:A:GLN:HB2	2	0.19	0.08	0.19
(1,2112)	1:290:A:LEU:HD12	1:293:A:GLN:HB3	2	0.19	0.08	0.19
(1,2112)	1:290:A:LEU:HD13	1:293:A:GLN:HB2	2	0.19	0.08	0.19
(1,2112)	1:290:A:LEU:HD13	1:293:A:GLN:HB3	2	0.19	0.08	0.19
(1,360)	1:246:B:ILE:HA	1:252:B:THR:HB	2	0.18	0.03	0.18
(1,2363)	1:246:B:ILE:HG21	1:282:A:THR:HG21	2	0.17	0.0	0.17
(1,2363)	1:246:B:ILE:HG21	1:282:A:THR:HG22	2	0.17	0.0	0.17
(1,2363)	1:246:B:ILE:HG21	1:282:A:THR:HG23	2	0.17	0.0	0.17
(1,2363)	1:246:B:ILE:HG22	1:282:A:THR:HG21	2	0.17	0.0	0.17
(1,2363)	1:246:B:ILE:HG22	1:282:A:THR:HG22	2	0.17	0.0	0.17
(1,2363)	1:246:B:ILE:HG22	1:282:A:THR:HG23	2	0.17	0.0	0.17
(1,2363)	1:246:B:ILE:HG23	1:282:A:THR:HG21	2	0.17	0.0	0.17
(1,2363)	1:246:B:ILE:HG23	1:282:A:THR:HG22	2	0.17	0.0	0.17
(1,2363)	1:246:B:ILE:HG23	1:282:A:THR:HG23	2	0.17	0.0	0.17
(1,2362)	1:246:B:ILE:HG21	1:282:A:THR:HB	2	0.16	0.05	0.16
(1,2362)	1:246:B:ILE:HG22	1:282:A:THR:HB	2	0.16	0.05	0.16
(1,2362)	1:246:B:ILE:HG23	1:282:A:THR:HB	2	0.16	0.05	0.16

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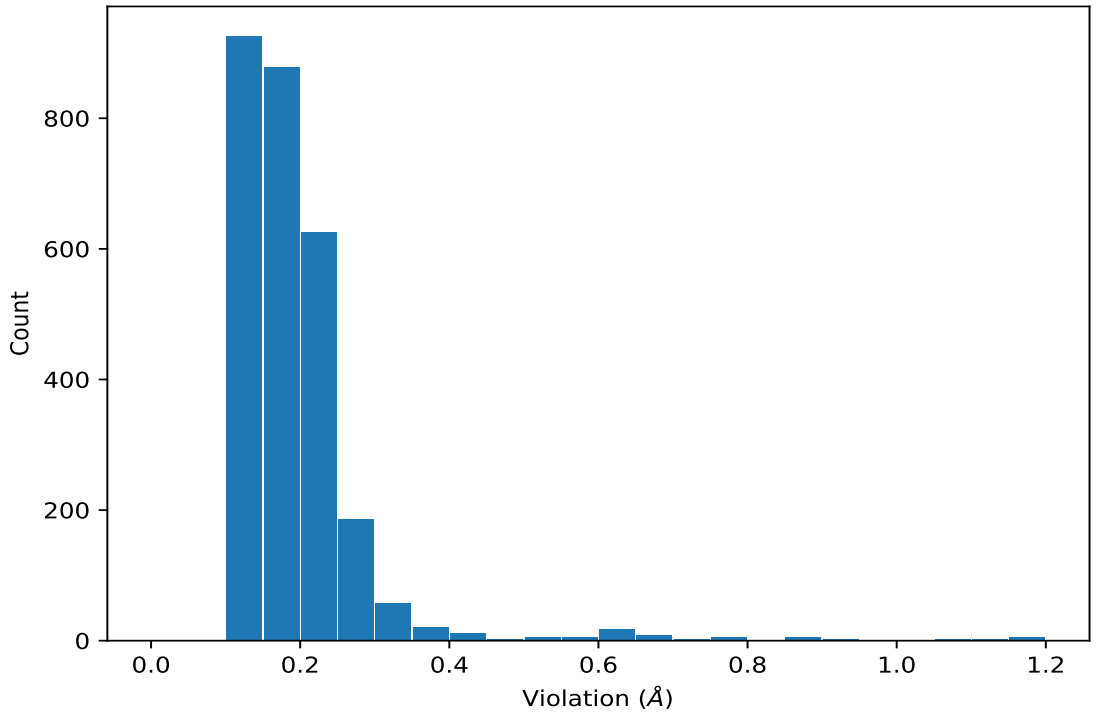
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,345)	1:245:B:VAL:HG11	1:283:B:PRO:HG2	2	0.16	0.01	0.16
(1,345)	1:245:B:VAL:HG11	1:283:B:PRO:HG3	2	0.16	0.01	0.16
(1,345)	1:245:B:VAL:HG12	1:283:B:PRO:HG2	2	0.16	0.01	0.16
(1,345)	1:245:B:VAL:HG12	1:283:B:PRO:HG3	2	0.16	0.01	0.16
(1,345)	1:245:B:VAL:HG13	1:283:B:PRO:HG2	2	0.16	0.01	0.16
(1,345)	1:245:B:VAL:HG13	1:283:B:PRO:HG3	2	0.16	0.01	0.16
(1,1341)	1:236:A:ILE:H	1:253:A:TYR:HE1	2	0.16	0.05	0.16
(1,1341)	1:236:A:ILE:H	1:253:A:TYR:HE2	2	0.16	0.05	0.16
(1,1554)	1:249:A:SER:H	1:251:A:GLN:HE21	2	0.14	0.01	0.14
(1,1028)	1:294:B:TRP:HD1	1:232:B:PHE:HE1	2	0.12	0.02	0.12
(1,1028)	1:294:B:TRP:HD1	1:232:B:PHE:HE2	2	0.12	0.02	0.12
(1,1328)	1:236:A:ILE:H	1:236:A:ILE:HB	2	0.12	0.01	0.12
(1,2330)	1:232:A:PHE:HE1	1:290:B:LEU:HD11	2	0.12	0.02	0.12
(1,2330)	1:232:A:PHE:HE1	1:290:B:LEU:HD12	2	0.12	0.02	0.12
(1,2330)	1:232:A:PHE:HE1	1:290:B:LEU:HD13	2	0.12	0.02	0.12
(1,2330)	1:232:A:PHE:HE2	1:290:B:LEU:HD11	2	0.12	0.02	0.12
(1,2330)	1:232:A:PHE:HE2	1:290:B:LEU:HD12	2	0.12	0.02	0.12
(1,2330)	1:232:A:PHE:HE2	1:290:B:LEU:HD13	2	0.12	0.02	0.12
(1,2190)	1:294:A:TRP:HD1	1:232:A:PHE:HE1	2	0.12	0.01	0.12
(1,2190)	1:294:A:TRP:HD1	1:232:A:PHE:HE2	2	0.12	0.01	0.12
(1,890)	1:285:B:PHE:HB2	1:283:B:PRO:HG2	2	0.11	0.01	0.11
(1,890)	1:285:B:PHE:HB2	1:283:B:PRO:HG3	2	0.11	0.01	0.11
(1,1374)	1:238:A:LEU:H	1:237:A:SER:HB2	2	0.11	0.0	0.11
(1,1374)	1:238:A:LEU:H	1:237:A:SER:HB3	2	0.11	0.0	0.11
(1,811)	1:273:B:GLN:H	1:269:B:CYS:HB2	2	0.11	0.0	0.11
(1,811)	1:273:B:GLN:H	1:269:B:CYS:HB3	2	0.11	0.0	0.11
(1,1917)	1:269:A:CYS:HB2	1:274:A:GLN:HE21	2	0.11	0.0	0.11
(1,1917)	1:269:A:CYS:HB3	1:274:A:GLN:HE21	2	0.11	0.0	0.11
(1,1931)	1:270:A:PRO:HD3	1:258:A:ILE:HD11	2	0.11	0.0	0.11
(1,1931)	1:270:A:PRO:HD3	1:258:A:ILE:HD12	2	0.11	0.0	0.11
(1,1931)	1:270:A:PRO:HD3	1:258:A:ILE:HD13	2	0.11	0.0	0.11

[1]Number of violated models, [2]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)
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG2	13	1.18
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG3	13	1.18
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG2	6	1.16
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG3	6	1.16
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG2	19	1.15
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG3	19	1.15
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG2	7	1.1
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG3	7	1.1
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG2	18	1.05
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG3	18	1.05
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	8	1.05
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	18	1.02
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	7	0.96
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG2	2	0.91
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG3	2	0.91
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG2	16	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1966)	1:273:A:GLN:H	1:273:A:GLN:HG3	16	0.86
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD21	14	0.85
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD22	14	0.85
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD23	14	0.85
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	7	0.75
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	7	0.75
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	7	0.75
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	16	0.75
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	16	0.75
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	16	0.75
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	1	0.72
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	1	0.72
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	1	0.72
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	12	0.69
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	12	0.69
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	12	0.69
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	15	0.66
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	15	0.66
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	15	0.66
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	13	0.65
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	13	0.65
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	13	0.65
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	10	0.64
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	10	0.64
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	10	0.64
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	20	0.64
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	20	0.64
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	20	0.64
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	11	0.63
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	11	0.63
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	11	0.63
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	18	0.63
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	18	0.63
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	18	0.63
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	3	0.62
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	3	0.62
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	3	0.62
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	5	0.62
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	5	0.62
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	5	0.62
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	4	0.59
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	4	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	4	0.59
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	9	0.58
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	9	0.58
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	9	0.58
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	2	0.54
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	2	0.54
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	2	0.54
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	17	0.51
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	17	0.51
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	17	0.51
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	11	0.46
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	7	0.46
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD21	1	0.42
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD22	1	0.42
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD23	1	0.42
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	14	0.42
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	20	0.42
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	20	0.42
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	20	0.42
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	3	0.41
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	9	0.41
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	9	0.41
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	9	0.41
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	4	0.4
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	5	0.39
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	9	0.39
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	13	0.39
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	15	0.39
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	1	0.38
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	15	0.38
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	17	0.38
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	20	0.38
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD11	14	0.37
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD12	14	0.37
(1,2332)	1:232:A:PHE:HZ	1:290:B:LEU:HD13	14	0.37
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	12	0.37
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	16	0.37
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	19	0.37
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	3	0.36
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD21	13	0.35
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD22	13	0.35
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD23	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	3	0.35
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	6	0.35
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	16	0.35
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	2	0.34
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	4	0.34
(1,1352)	1:237:A:SER:H	1:236:A:ILE:HB	3	0.33
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	18	0.33
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	19	0.33
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	5	0.33
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	5	0.33
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	5	0.33
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	8	0.33
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	8	0.33
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	8	0.33
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	18	0.33
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	18	0.33
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	18	0.33
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	2	0.32
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD11	9	0.32
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD12	9	0.32
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD13	9	0.32
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD11	19	0.32
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD12	19	0.32
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD13	19	0.32
(1,1352)	1:237:A:SER:H	1:236:A:ILE:HB	14	0.32
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD11	9	0.32
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD12	9	0.32
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD13	9	0.32
(1,2356)	1:231:B:GLU:HG2	1:290:A:LEU:HD11	14	0.31
(1,2356)	1:231:B:GLU:HG2	1:290:A:LEU:HD12	14	0.31
(1,2356)	1:231:B:GLU:HG2	1:290:A:LEU:HD13	14	0.31
(1,2356)	1:231:B:GLU:HG3	1:290:A:LEU:HD11	14	0.31
(1,2356)	1:231:B:GLU:HG3	1:290:A:LEU:HD12	14	0.31
(1,2356)	1:231:B:GLU:HG3	1:290:A:LEU:HD13	14	0.31
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	12	0.31
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	12	0.31
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	12	0.31
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	18	0.31
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD11	5	0.31
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD12	5	0.31
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD13	5	0.31
(1,1352)	1:237:A:SER:H	1:236:A:ILE:HB	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1352)	1:237:A:SER:H	1:236:A:ILE:HB	19	0.31
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	1	0.31
(1,198)	1:237:B:SER:H	1:234:B:CYS:HB2	19	0.31
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD21	2	0.3
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD22	2	0.3
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD23	2	0.3
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	11	0.3
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	11	0.3
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	11	0.3
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD11	8	0.3
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD12	8	0.3
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD13	8	0.3
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD11	8	0.3
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD12	8	0.3
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD13	8	0.3
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	7	0.3
(1,191)	1:237:B:SER:H	1:236:B:ILE:HB	3	0.3
(1,191)	1:237:B:SER:H	1:236:B:ILE:HB	16	0.3
(1,191)	1:237:B:SER:H	1:236:B:ILE:HB	18	0.3
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	14	0.29
(1,1459)	1:243:A:ASP:H	1:243:A:ASP:HB2	14	0.29
(1,1352)	1:237:A:SER:H	1:236:A:ILE:HB	8	0.29
(1,1352)	1:237:A:SER:H	1:236:A:ILE:HB	16	0.29
(1,950)	1:290:B:LEU:HD11	1:293:B:GLN:HB2	15	0.29
(1,950)	1:290:B:LEU:HD11	1:293:B:GLN:HB3	15	0.29
(1,950)	1:290:B:LEU:HD12	1:293:B:GLN:HB2	15	0.29
(1,950)	1:290:B:LEU:HD12	1:293:B:GLN:HB3	15	0.29
(1,950)	1:290:B:LEU:HD13	1:293:B:GLN:HB2	15	0.29
(1,950)	1:290:B:LEU:HD13	1:293:B:GLN:HB3	15	0.29
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	18	0.29
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	18	0.29
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	18	0.29
(1,269)	1:241:B:MET:H	1:241:B:MET:HE1	3	0.29
(1,269)	1:241:B:MET:H	1:241:B:MET:HE2	3	0.29
(1,269)	1:241:B:MET:H	1:241:B:MET:HE3	3	0.29
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	2	0.29
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	2	0.29
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	2	0.29
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	19	0.29
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	19	0.29
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	19	0.29
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	15	0.28
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	11	0.28
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	6	0.28
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	6	0.28
(1,1522)	1:246:A:ILE:HG12	1:284:A:ASN:HA	7	0.28
(1,1522)	1:246:A:ILE:HG13	1:284:A:ASN:HA	7	0.28
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	3	0.28
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	18	0.28
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD11	1	0.28
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD12	1	0.28
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD13	1	0.28
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD11	15	0.28
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD12	15	0.28
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD13	15	0.28
(1,297)	1:243:B:ASP:H	1:243:B:ASP:HB3	9	0.28
(1,297)	1:243:B:ASP:H	1:243:B:ASP:HB3	13	0.28
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	6	0.27
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	6	0.27
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	6	0.27
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	6	0.27
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	6	0.27
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	6	0.27
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	6	0.27
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	6	0.27
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	6	0.27
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD21	10	0.27
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD22	10	0.27
(1,2361)	1:232:B:PHE:HZ	1:290:A:LEU:HD23	10	0.27
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	7	0.27
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	7	0.27
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	6	0.27
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	6	0.27
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	6	0.27
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	6	0.27
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	6	0.27
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	6	0.27
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	6	0.27
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	6	0.27
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	6	0.27
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG21	3	0.27
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG22	3	0.27
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG23	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG21	3	0.27
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG22	3	0.27
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG23	3	0.27
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG21	3	0.27
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG22	3	0.27
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG23	3	0.27
(1,2112)	1:290:A:LEU:HD11	1:293:A:GLN:HB2	19	0.27
(1,2112)	1:290:A:LEU:HD11	1:293:A:GLN:HB3	19	0.27
(1,2112)	1:290:A:LEU:HD12	1:293:A:GLN:HB2	19	0.27
(1,2112)	1:290:A:LEU:HD12	1:293:A:GLN:HB3	19	0.27
(1,2112)	1:290:A:LEU:HD13	1:293:A:GLN:HB2	19	0.27
(1,2112)	1:290:A:LEU:HD13	1:293:A:GLN:HB3	19	0.27
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	19	0.27
(1,1910)	1:269:A:CYS:H	1:275:A:PRO:HB2	17	0.27
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	1	0.27
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	4	0.27
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	8	0.27
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	9	0.27
(1,1352)	1:237:A:SER:H	1:236:A:ILE:HB	1	0.27
(1,297)	1:243:B:ASP:H	1:243:B:ASP:HB3	6	0.27
(1,297)	1:243:B:ASP:H	1:243:B:ASP:HB3	8	0.27
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	14	0.27
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	14	0.27
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	14	0.27
(1,198)	1:237:B:SER:H	1:234:B:CYS:HB2	14	0.27
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG12	13	0.27
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG13	13	0.27
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG12	13	0.27
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG13	13	0.27
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	10	0.26
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	10	0.26
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	16	0.26
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	16	0.26
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	16	0.26
(1,1918)	1:269:A:CYS:H	1:274:A:GLN:HG3	8	0.26
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	7	0.26
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	15	0.26
(1,297)	1:243:B:ASP:H	1:243:B:ASP:HB3	2	0.26
(1,297)	1:243:B:ASP:H	1:243:B:ASP:HB3	10	0.26
(1,297)	1:243:B:ASP:H	1:243:B:ASP:HB3	20	0.26
(1,191)	1:237:B:SER:H	1:236:B:ILE:HB	17	0.26
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	4	0.25
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	4	0.25
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	4	0.25
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	4	0.25
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	4	0.25
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	4	0.25
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	4	0.25
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	4	0.25
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	18	0.25
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	18	0.25
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	18	0.25
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	18	0.25
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	18	0.25
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	18	0.25
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	18	0.25
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	18	0.25
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	18	0.25
(1,2365)	1:246:B:ILE:HD11	1:282:A:THR:HB	16	0.25
(1,2365)	1:246:B:ILE:HD12	1:282:A:THR:HB	16	0.25
(1,2365)	1:246:B:ILE:HD13	1:282:A:THR:HB	16	0.25
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	4	0.25
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	4	0.25
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	4	0.25
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	4	0.25
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	4	0.25
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	4	0.25
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	4	0.25
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	4	0.25
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	4	0.25
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	18	0.25
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	18	0.25
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	18	0.25
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	18	0.25
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	18	0.25
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	18	0.25
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	18	0.25
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	18	0.25
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	18	0.25
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	14	0.25
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	15	0.25
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	15	0.25
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	15	0.25
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	15	0.25
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	15	0.25
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	15	0.25
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	15	0.25
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	15	0.25
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	15	0.25
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	15	0.25
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	15	0.25
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	15	0.25
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	15	0.25
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	15	0.25
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	15	0.25
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	15	0.25
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	15	0.25
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	20	0.25
(1,1910)	1:269:A:CYS:H	1:275:A:PRO:HB2	18	0.25
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	1	0.25
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	1	0.25
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	1	0.25
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	2	0.25
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	2	0.25
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	2	0.25
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	4	0.25
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	8	0.25
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	10	0.25
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	16	0.25
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	16	0.25
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	16	0.25
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	2	0.25
(1,297)	1:243:B:ASP:H	1:243:B:ASP:HB3	11	0.25
(1,297)	1:243:B:ASP:H	1:243:B:ASP:HB3	14	0.25
(1,297)	1:243:B:ASP:H	1:243:B:ASP:HB3	19	0.25
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	17	0.25
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	17	0.25
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	17	0.25
(1,198)	1:237:B:SER:H	1:234:B:CYS:HB2	4	0.25
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG21	3	0.24
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG22	3	0.24
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG23	3	0.24
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG21	3	0.24
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG22	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG23	3	0.24
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG21	3	0.24
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG22	3	0.24
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG23	3	0.24
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	12	0.24
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	12	0.24
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	20	0.24
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	20	0.24
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	15	0.24
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	15	0.24
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	15	0.24
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	15	0.24
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	15	0.24
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	15	0.24
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	9	0.24
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	9	0.24
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	9	0.24
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	9	0.24
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	4	0.24
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	4	0.24
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	18	0.24
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	18	0.24
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	20	0.24
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD11	3	0.24
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD12	3	0.24
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD13	3	0.24
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	9	0.24
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	9	0.24
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	9	0.24
(1,907)	1:287:B:LEU:HA	1:290:B:LEU:HD21	5	0.24
(1,907)	1:287:B:LEU:HA	1:290:B:LEU:HD22	5	0.24
(1,907)	1:287:B:LEU:HA	1:290:B:LEU:HD23	5	0.24
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	6	0.24
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	6	0.24
(1,304)	1:243:B:ASP:H	1:241:B:MET:HE1	13	0.24
(1,304)	1:243:B:ASP:H	1:241:B:MET:HE2	13	0.24
(1,304)	1:243:B:ASP:H	1:241:B:MET:HE3	13	0.24
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	16	0.23
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	16	0.23
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	16	0.23
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	6	0.23
(1,2053)	1:285:A:PHE:HZ	1:250:A:GLY:HA2	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	9	0.23
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	3	0.23
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	3	0.23
(1,1918)	1:269:A:CYS:H	1:274:A:GLN:HG3	14	0.23
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	4	0.23
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	4	0.23
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	4	0.23
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	6	0.23
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	6	0.23
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	6	0.23
(1,1522)	1:246:A:ILE:HG12	1:284:A:ASN:HA	3	0.23
(1,1522)	1:246:A:ILE:HG13	1:284:A:ASN:HA	3	0.23
(1,1505)	1:245:A:VAL:HG11	1:255:A:ARG:HB2	11	0.23
(1,1505)	1:245:A:VAL:HG11	1:255:A:ARG:HB3	11	0.23
(1,1505)	1:245:A:VAL:HG12	1:255:A:ARG:HB2	11	0.23
(1,1505)	1:245:A:VAL:HG12	1:255:A:ARG:HB3	11	0.23
(1,1505)	1:245:A:VAL:HG13	1:255:A:ARG:HB2	11	0.23
(1,1505)	1:245:A:VAL:HG13	1:255:A:ARG:HB3	11	0.23
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	10	0.23
(1,1458)	1:243:A:ASP:H	1:243:A:ASP:HB3	16	0.23
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG21	13	0.23
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG22	13	0.23
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG23	13	0.23
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD2	14	0.23
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD3	14	0.23
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD11	20	0.23
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD12	20	0.23
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD13	20	0.23
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	12	0.23
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	12	0.23
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	12	0.23
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	20	0.23
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	20	0.23
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	20	0.23
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	4	0.23
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	13	0.23
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	1	0.23
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	1	0.23
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	1	0.23
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	13	0.23
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	13	0.23
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	18	0.23
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	18	0.23
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	18	0.23
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	5	0.23
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	7	0.23
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	9	0.23
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	18	0.23
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	18	0.23
(1,822)	1:274:B:GLN:H	1:272:B:THR:HA	13	0.23
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	4	0.23
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	4	0.23
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	4	0.23
(1,743)	1:269:B:CYS:H	1:268:B:THR:HB	14	0.23
(1,2365)	1:246:B:ILE:HD11	1:282:A:THR:HB	20	0.22
(1,2365)	1:246:B:ILE:HD12	1:282:A:THR:HB	20	0.22
(1,2365)	1:246:B:ILE:HD13	1:282:A:THR:HB	20	0.22
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG21	8	0.22
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG22	8	0.22
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG23	8	0.22
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG21	8	0.22
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG22	8	0.22
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG23	8	0.22
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG21	8	0.22
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG22	8	0.22
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG23	8	0.22
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG21	2	0.22
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG22	2	0.22
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG23	2	0.22
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG21	2	0.22
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG22	2	0.22
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG23	2	0.22
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG21	2	0.22
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG22	2	0.22
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG23	2	0.22
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD11	6	0.22
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD12	6	0.22
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD13	6	0.22
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD11	6	0.22
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD12	6	0.22
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD13	6	0.22
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	2	0.22
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	4	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	4	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	4	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	16	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	16	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	16	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	18	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	18	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	18	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	19	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	19	0.22
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	19	0.22
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	5	0.22
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	5	0.22
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	5	0.22
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	8	0.22
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	13	0.22
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	13	0.22
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	15	0.22
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	15	0.22
(1,1904)	1:269:A:CYS:H	1:268:A:THR:HB	7	0.22
(1,1613)	1:253:A:TYR:HE1	1:247:A:VAL:HB	14	0.22
(1,1613)	1:253:A:TYR:HE2	1:247:A:VAL:HB	14	0.22
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	2	0.22
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	2	0.22
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	2	0.22
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	3	0.22
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	3	0.22
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	3	0.22
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD21	7	0.22
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD22	7	0.22
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD23	7	0.22
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG21	9	0.22
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG22	9	0.22
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG23	9	0.22
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG21	20	0.22
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG22	20	0.22
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG23	20	0.22
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	7	0.22
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	7	0.22
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	7	0.22
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	7	0.22
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	7	0.22
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	7	0.22
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	14	0.22
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	14	0.22
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	14	0.22
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	1	0.22
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	1	0.22
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	1	0.22
(1,892)	1:285:B:PHE:HZ	1:250:B:GLY:HA2	20	0.22
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	2	0.22
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	6	0.22
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	19	0.22
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	19	0.22
(1,815)	1:274:B:GLN:H	1:274:B:GLN:HB2	10	0.22
(1,815)	1:274:B:GLN:H	1:274:B:GLN:HB3	10	0.22
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	5	0.22
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	11	0.22
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	2	0.22
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	2	0.22
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	2	0.22
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	5	0.22
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	5	0.22
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	5	0.22
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	6	0.22
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	6	0.22
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	6	0.22
(1,743)	1:269:B:CYS:H	1:268:B:THR:HB	20	0.22
(1,547)	1:259:B:GLN:H	1:258:B:ILE:HB	8	0.22
(1,393)	1:249:B:SER:H	1:251:B:GLN:HE21	18	0.22
(1,180)	1:236:B:ILE:H	1:253:B:TYR:HE1	4	0.22
(1,180)	1:236:B:ILE:H	1:253:B:TYR:HE2	4	0.22
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	1	0.22
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	1	0.22
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	1	0.22
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	4	0.22
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	4	0.22
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	4	0.22
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	5	0.22
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	5	0.22
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	5	0.22
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	12	0.22
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	12	0.22
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	8	0.21
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	8	0.21
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	8	0.21
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	8	0.21
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	8	0.21
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	8	0.21
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	8	0.21
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	8	0.21
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	8	0.21
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG21	7	0.21
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG22	7	0.21
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG23	7	0.21
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG21	7	0.21
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG22	7	0.21
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG23	7	0.21
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG21	7	0.21
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG22	7	0.21
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG23	7	0.21
(1,2362)	1:246:B:ILE:HG21	1:282:A:THR:HB	9	0.21
(1,2362)	1:246:B:ILE:HG22	1:282:A:THR:HB	9	0.21
(1,2362)	1:246:B:ILE:HG23	1:282:A:THR:HB	9	0.21
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	11	0.21
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	11	0.21
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	8	0.21
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	8	0.21
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	8	0.21
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	8	0.21
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	8	0.21
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	8	0.21
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	8	0.21
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	8	0.21
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	8	0.21
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	7	0.21
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	7	0.21
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	7	0.21
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	18	0.21
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	1	0.21
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	1	0.21
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	1	0.21
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	5	0.21
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	5	0.21
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	13	0.21
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	13	0.21
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	13	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	3	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	3	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	3	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	8	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	8	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	8	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	13	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	13	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	13	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	15	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	15	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	15	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	16	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	16	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	16	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	18	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	18	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	18	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	19	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	19	0.21
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	19	0.21
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	11	0.21
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	11	0.21
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	16	0.21
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	16	0.21
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	16	0.21
(1,1918)	1:269:A:CYS:H	1:274:A:GLN:HG3	15	0.21
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	5	0.21
(1,1559)	1:249:A:SER:HB2	1:269:A:CYS:HB2	9	0.21
(1,1559)	1:249:A:SER:HB2	1:269:A:CYS:HB3	9	0.21
(1,1420)	1:241:A:MET:H	1:241:A:MET:HB2	6	0.21
(1,1420)	1:241:A:MET:H	1:241:A:MET:HB2	19	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG21	6	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG22	6	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG23	6	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG21	7	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG22	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG23	7	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG21	10	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG22	10	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG23	10	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG21	11	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG22	11	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG23	11	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG21	15	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG22	15	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG23	15	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG21	17	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG22	17	0.21
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG23	17	0.21
(1,1260)	1:232:A:PHE:HA	1:303:A:PRO:HD3	11	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	4	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	4	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	4	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	4	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	4	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	4	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	5	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	5	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	5	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	5	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	5	0.21
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	5	0.21
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	17	0.21
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	17	0.21
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	17	0.21
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	3	0.21
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	5	0.21
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	5	0.21
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	5	0.21
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	5	0.21
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	17	0.21
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	17	0.21
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	17	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	3	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	3	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	3	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	4	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	4	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	5	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	5	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	5	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	7	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	7	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	7	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	9	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	9	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	9	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	18	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	18	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	18	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	19	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	19	0.21
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	19	0.21
(1,950)	1:290:B:LEU:HD11	1:293:B:GLN:HB2	5	0.21
(1,950)	1:290:B:LEU:HD11	1:293:B:GLN:HB3	5	0.21
(1,950)	1:290:B:LEU:HD12	1:293:B:GLN:HB2	5	0.21
(1,950)	1:290:B:LEU:HD12	1:293:B:GLN:HB3	5	0.21
(1,950)	1:290:B:LEU:HD13	1:293:B:GLN:HB2	5	0.21
(1,950)	1:290:B:LEU:HD13	1:293:B:GLN:HB3	5	0.21
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	15	0.21
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	15	0.21
(1,757)	1:269:B:CYS:H	1:274:B:GLN:HG3	7	0.21
(1,749)	1:269:B:CYS:H	1:275:B:PRO:HB2	11	0.21
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	1	0.21
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	1	0.21
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	1	0.21
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	14	0.21
(1,547)	1:259:B:GLN:H	1:258:B:ILE:HB	16	0.21
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	8	0.21
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	8	0.21
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	8	0.21
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB2	7	0.21
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB3	7	0.21
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB2	9	0.21
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB3	9	0.21
(1,360)	1:246:B:ILE:HA	1:252:B:THR:HB	17	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	6	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	6	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	8	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	8	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	8	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	10	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	10	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	10	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	11	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	11	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	11	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	13	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	13	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	13	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	15	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	15	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	15	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	19	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	19	0.21
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	19	0.21
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	1	0.2
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	1	0.2
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	1	0.2
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	1	0.2
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	1	0.2
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	1	0.2
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	1	0.2
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	1	0.2
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	1	0.2
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	1	0.2
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	1	0.2
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	1	0.2
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	1	0.2
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	1	0.2
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	1	0.2
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	1	0.2
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	1	0.2
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	1	0.2
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG21	9	0.2
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG22	9	0.2
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG23	9	0.2
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG21	9	0.2
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG22	9	0.2
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG23	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG21	9	0.2
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG22	9	0.2
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG23	9	0.2
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD11	19	0.2
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD12	19	0.2
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD13	19	0.2
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD11	19	0.2
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD12	19	0.2
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD13	19	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	3	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	3	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	3	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	3	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	3	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	3	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	13	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	13	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	13	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	13	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	13	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	13	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	18	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	18	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	18	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	18	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	18	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	18	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	19	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	19	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	19	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	19	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	19	0.2
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	19	0.2
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	4	0.2
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	4	0.2
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	4	0.2
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	5	0.2
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	5	0.2
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	5	0.2
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	1	0.2
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	4	0.2
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	19	0.2
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	3	0.2
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	3	0.2
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	3	0.2
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	7	0.2
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	7	0.2
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	7	0.2
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	12	0.2
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	12	0.2
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	12	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	4	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	4	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	4	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	7	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	7	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	7	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	9	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	9	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	9	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	10	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	10	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	10	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	11	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	11	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	11	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	12	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	12	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	12	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	20	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	20	0.2
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	20	0.2
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	17	0.2
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	8	0.2
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	8	0.2
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	8	0.2
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	20	0.2
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	20	0.2
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	20	0.2
(1,1904)	1:269:A:CYS:H	1:268:A:THR:HB	12	0.2
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	1	0.2
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	16	0.2
(1,1341)	1:236:A:ILE:H	1:253:A:TYR:HE1	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1341)	1:236:A:ILE:H	1:253:A:TYR:HE2	3	0.2
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG21	12	0.2
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG22	12	0.2
(1,1331)	1:236:A:ILE:H	1:236:A:ILE:HG23	12	0.2
(1,1275)	1:232:A:PHE:HZ	1:290:A:LEU:HD21	14	0.2
(1,1275)	1:232:A:PHE:HZ	1:290:A:LEU:HD22	14	0.2
(1,1275)	1:232:A:PHE:HZ	1:290:A:LEU:HD23	14	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	2	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	2	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	2	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	2	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	2	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	2	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	3	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	3	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	3	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	3	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	3	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	3	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	10	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	10	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	10	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	10	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	10	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	10	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	14	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	14	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	14	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	14	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	14	0.2
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	14	0.2
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	8	0.2
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	8	0.2
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	8	0.2
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	2	0.2
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	12	0.2
(1,1037)	1:294:B:TRP:HH2	1:228:B:ILE:HB	1	0.2
(1,1037)	1:294:B:TRP:HH2	1:228:B:ILE:HB	19	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	3	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	3	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	3	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	4	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	4	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	8	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	8	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	8	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	10	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	10	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	10	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	11	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	11	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	11	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	19	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	19	0.2
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	19	0.2
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD11	4	0.2
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD12	4	0.2
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD13	4	0.2
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD21	4	0.2
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD22	4	0.2
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD23	4	0.2
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD11	4	0.2
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD12	4	0.2
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD13	4	0.2
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD21	4	0.2
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD22	4	0.2
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD23	4	0.2
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD11	4	0.2
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD12	4	0.2
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD13	4	0.2
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD21	4	0.2
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD22	4	0.2
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD23	4	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	2	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	2	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	2	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	6	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	6	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	6	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	11	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	11	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	11	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	12	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	12	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	13	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	13	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	13	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	14	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	14	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	14	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	17	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	17	0.2
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	17	0.2
(1,892)	1:285:B:PHE:HZ	1:250:B:GLY:HA2	3	0.2
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	11	0.2
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	16	0.2
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	16	0.2
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	18	0.2
(1,743)	1:269:B:CYS:H	1:268:B:THR:HB	15	0.2
(1,547)	1:259:B:GLN:H	1:258:B:ILE:HB	9	0.2
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG21	7	0.2
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG22	7	0.2
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG23	7	0.2
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB2	20	0.2
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB3	20	0.2
(1,259)	1:241:B:MET:H	1:241:B:MET:HB2	1	0.2
(1,259)	1:241:B:MET:H	1:241:B:MET:HB2	20	0.2
(1,215)	1:238:B:LEU:H	1:233:B:ARG:HA	11	0.2
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG21	20	0.2
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG22	20	0.2
(1,170)	1:236:B:ILE:H	1:236:B:ILE:HG23	20	0.2
(1,29)	1:228:B:ILE:H	1:228:B:ILE:HD11	16	0.2
(1,29)	1:228:B:ILE:H	1:228:B:ILE:HD12	16	0.2
(1,29)	1:228:B:ILE:H	1:228:B:ILE:HD13	16	0.2
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	10	0.19
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	10	0.19
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	10	0.19
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	10	0.19
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	10	0.19
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	10	0.19
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	10	0.19
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	10	0.19
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	10	0.19
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	12	0.19
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	12	0.19
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	12	0.19
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	12	0.19
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	12	0.19
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	12	0.19
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	12	0.19
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	12	0.19
(1,2365)	1:246:B:ILE:HD11	1:282:A:THR:HB	7	0.19
(1,2365)	1:246:B:ILE:HD12	1:282:A:THR:HB	7	0.19
(1,2365)	1:246:B:ILE:HD13	1:282:A:THR:HB	7	0.19
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	9	0.19
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	9	0.19
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	10	0.19
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	10	0.19
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	10	0.19
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	10	0.19
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	10	0.19
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	10	0.19
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	10	0.19
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	10	0.19
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	10	0.19
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	12	0.19
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	12	0.19
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	12	0.19
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	12	0.19
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	12	0.19
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	12	0.19
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	12	0.19
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	12	0.19
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	12	0.19
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	8	0.19
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	8	0.19
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	8	0.19
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG21	14	0.19
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG22	14	0.19
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG23	14	0.19
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG21	14	0.19
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG22	14	0.19
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG23	14	0.19
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG21	14	0.19
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG22	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG23	14	0.19
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG21	19	0.19
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG22	19	0.19
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG23	19	0.19
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG21	19	0.19
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG22	19	0.19
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG23	19	0.19
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG21	19	0.19
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG22	19	0.19
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG23	19	0.19
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	2	0.19
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	2	0.19
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	2	0.19
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	2	0.19
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	2	0.19
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	2	0.19
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	8	0.19
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	6	0.19
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	6	0.19
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	6	0.19
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	20	0.19
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	20	0.19
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	20	0.19
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	3	0.19
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	3	0.19
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	3	0.19
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	3	0.19
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	3	0.19
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	3	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	3	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	3	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	3	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	3	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	3	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	3	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	3	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	3	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	3	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	3	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	3	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	3	0.19
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	16	0.19
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	16	0.19
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	16	0.19
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	16	0.19
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	16	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	16	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	16	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	16	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	16	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	16	0.19
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	16	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	16	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	16	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	16	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	16	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	16	0.19
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	16	0.19
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	1	0.19
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	1	0.19
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	1	0.19
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	6	0.19
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	6	0.19
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	6	0.19
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	3	0.19
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	13	0.19
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	7	0.19
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	7	0.19
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	8	0.19
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	8	0.19
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	12	0.19
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	12	0.19
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	20	0.19
(1,1971)	1:273:A:GLN:H	1:268:A:THR:HB	14	0.19
(1,1918)	1:269:A:CYS:H	1:274:A:GLN:HG3	6	0.19
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	15	0.19
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	15	0.19
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	15	0.19
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD21	18	0.19
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD22	18	0.19
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD23	18	0.19
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD11	14	0.19
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD12	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1392)	1:239:A:GLU:H	1:238:A:LEU:HD13	14	0.19
(1,1259)	1:232:A:PHE:HB2	1:291:A:ILE:HG21	17	0.19
(1,1259)	1:232:A:PHE:HB2	1:291:A:ILE:HG22	17	0.19
(1,1259)	1:232:A:PHE:HB2	1:291:A:ILE:HG23	17	0.19
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD11	2	0.19
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD12	2	0.19
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD13	2	0.19
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	1	0.19
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	1	0.19
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	1	0.19
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	1	0.19
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	16	0.19
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	20	0.19
(1,1037)	1:294:B:TRP:HH2	1:228:B:ILE:HB	10	0.19
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	6	0.19
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	6	0.19
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	6	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD11	3	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD12	3	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD13	3	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD21	3	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD22	3	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD23	3	0.19
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD11	3	0.19
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD12	3	0.19
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD13	3	0.19
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD21	3	0.19
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD22	3	0.19
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD23	3	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD11	3	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD12	3	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD13	3	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD21	3	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD22	3	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD23	3	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD11	14	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD12	14	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD13	14	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD21	14	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD22	14	0.19
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD23	14	0.19
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD11	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD12	14	0.19
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD13	14	0.19
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD21	14	0.19
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD22	14	0.19
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD23	14	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD11	14	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD12	14	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD13	14	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD21	14	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD22	14	0.19
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD23	14	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	10	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	10	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	10	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	15	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	15	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	15	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	16	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	16	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	16	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	20	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	20	0.19
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	20	0.19
(1,892)	1:285:B:PHE:HZ	1:250:B:GLY:HA2	17	0.19
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	12	0.19
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	8	0.19
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	20	0.19
(1,547)	1:259:B:GLN:H	1:258:B:ILE:HB	3	0.19
(1,547)	1:259:B:GLN:H	1:258:B:ILE:HB	17	0.19
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG21	9	0.19
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG22	9	0.19
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG23	9	0.19
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	6	0.19
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	6	0.19
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	6	0.19
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB2	3	0.19
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB3	3	0.19
(1,361)	1:246:B:ILE:HG12	1:284:B:ASN:HA	13	0.19
(1,361)	1:246:B:ILE:HG13	1:284:B:ASN:HA	13	0.19
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG12	17	0.19
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG13	17	0.19
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG12	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG13	17	0.19
(1,2377)	1:285:B:PHE:HZ	1:250:A:GLY:HA3	3	0.18
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	15	0.18
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	15	0.18
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	15	0.18
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	15	0.18
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	15	0.18
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	15	0.18
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	15	0.18
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	15	0.18
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	15	0.18
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	5	0.18
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	5	0.18
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	13	0.18
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	13	0.18
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	15	0.18
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	15	0.18
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	15	0.18
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	15	0.18
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	15	0.18
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	15	0.18
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	15	0.18
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	15	0.18
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	15	0.18
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG21	16	0.18
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG22	16	0.18
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG23	16	0.18
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG21	16	0.18
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG22	16	0.18
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG23	16	0.18
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG21	16	0.18
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG22	16	0.18
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG23	16	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	8	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	8	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	8	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	8	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	8	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	8	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	11	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	11	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	11	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	11	0.18
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	11	0.18
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	8	0.18
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	8	0.18
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	8	0.18
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	10	0.18
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	15	0.18
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	17	0.18
(1,2196)	1:294:A:TRP:HZ3	1:300:A:ILE:HD11	2	0.18
(1,2196)	1:294:A:TRP:HZ3	1:300:A:ILE:HD12	2	0.18
(1,2196)	1:294:A:TRP:HZ3	1:300:A:ILE:HD13	2	0.18
(1,2053)	1:285:A:PHE:HZ	1:250:A:GLY:HA2	17	0.18
(1,1918)	1:269:A:CYS:H	1:274:A:GLN:HG3	4	0.18
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	5	0.18
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	5	0.18
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	5	0.18
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	17	0.18
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	17	0.18
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	17	0.18
(1,1769)	1:261:A:TRP:HE1	1:270:A:PRO:HB2	4	0.18
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	4	0.18
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	12	0.18
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	14	0.18
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	19	0.18
(1,1613)	1:253:A:TYR:HE1	1:247:A:VAL:HB	7	0.18
(1,1613)	1:253:A:TYR:HE2	1:247:A:VAL:HB	7	0.18
(1,1613)	1:253:A:TYR:HE1	1:247:A:VAL:HB	11	0.18
(1,1613)	1:253:A:TYR:HE2	1:247:A:VAL:HB	11	0.18
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	5	0.18
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	5	0.18
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	5	0.18
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	13	0.18
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	13	0.18
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	13	0.18
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB2	6	0.18
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB3	6	0.18
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE1	3	0.18
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE2	3	0.18
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE3	3	0.18
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD21	20	0.18
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD22	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD23	20	0.18
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG12	4	0.18
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG13	4	0.18
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG12	4	0.18
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG13	4	0.18
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG12	9	0.18
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG13	9	0.18
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG12	9	0.18
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG13	9	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	13	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	13	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	13	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	13	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	13	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	13	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	16	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	16	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	16	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	16	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	16	0.18
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	16	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	2	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	2	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	2	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	10	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	10	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	10	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	14	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	14	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	14	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	16	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	16	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	16	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	18	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	18	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	18	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	19	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	19	0.18
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	19	0.18
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	6	0.18
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	12	0.18
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	12	0.18
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	15	0.18
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	15	0.18
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	15	0.18
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	16	0.18
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	16	0.18
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	16	0.18
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG21	8	0.18
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG22	8	0.18
(1,954)	1:291:B:ILE:H	1:291:B:ILE:HG23	8	0.18
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	3	0.18
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	3	0.18
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	10	0.18
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	15	0.18
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	12	0.18
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	12	0.18
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	12	0.18
(1,743)	1:269:B:CYS:H	1:268:B:THR:HB	11	0.18
(1,608)	1:261:B:TRP:HE1	1:270:B:PRO:HB2	13	0.18
(1,547)	1:259:B:GLN:H	1:258:B:ILE:HB	2	0.18
(1,547)	1:259:B:GLN:H	1:258:B:ILE:HB	12	0.18
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	5	0.18
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	5	0.18
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	5	0.18
(1,304)	1:243:B:ASP:H	1:241:B:MET:HE1	8	0.18
(1,304)	1:243:B:ASP:H	1:241:B:MET:HE2	8	0.18
(1,304)	1:243:B:ASP:H	1:241:B:MET:HE3	8	0.18
(1,269)	1:241:B:MET:H	1:241:B:MET:HE1	8	0.18
(1,269)	1:241:B:MET:H	1:241:B:MET:HE2	8	0.18
(1,269)	1:241:B:MET:H	1:241:B:MET:HE3	8	0.18
(1,198)	1:237:B:SER:H	1:234:B:CYS:HB2	9	0.18
(1,2365)	1:246:B:ILE:HD11	1:282:A:THR:HB	11	0.17
(1,2365)	1:246:B:ILE:HD12	1:282:A:THR:HB	11	0.17
(1,2365)	1:246:B:ILE:HD13	1:282:A:THR:HB	11	0.17
(1,2365)	1:246:B:ILE:HD11	1:282:A:THR:HB	17	0.17
(1,2365)	1:246:B:ILE:HD12	1:282:A:THR:HB	17	0.17
(1,2365)	1:246:B:ILE:HD13	1:282:A:THR:HB	17	0.17
(1,2363)	1:246:B:ILE:HG21	1:282:A:THR:HG21	12	0.17
(1,2363)	1:246:B:ILE:HG21	1:282:A:THR:HG22	12	0.17
(1,2363)	1:246:B:ILE:HG21	1:282:A:THR:HG23	12	0.17
(1,2363)	1:246:B:ILE:HG22	1:282:A:THR:HG21	12	0.17
(1,2363)	1:246:B:ILE:HG22	1:282:A:THR:HG22	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2363)	1:246:B:ILE:HG22	1:282:A:THR:HG23	12	0.17
(1,2363)	1:246:B:ILE:HG23	1:282:A:THR:HG21	12	0.17
(1,2363)	1:246:B:ILE:HG23	1:282:A:THR:HG22	12	0.17
(1,2363)	1:246:B:ILE:HG23	1:282:A:THR:HG23	12	0.17
(1,2363)	1:246:B:ILE:HG21	1:282:A:THR:HG21	15	0.17
(1,2363)	1:246:B:ILE:HG21	1:282:A:THR:HG22	15	0.17
(1,2363)	1:246:B:ILE:HG21	1:282:A:THR:HG23	15	0.17
(1,2363)	1:246:B:ILE:HG22	1:282:A:THR:HG21	15	0.17
(1,2363)	1:246:B:ILE:HG22	1:282:A:THR:HG22	15	0.17
(1,2363)	1:246:B:ILE:HG22	1:282:A:THR:HG23	15	0.17
(1,2363)	1:246:B:ILE:HG23	1:282:A:THR:HG21	15	0.17
(1,2363)	1:246:B:ILE:HG23	1:282:A:THR:HG22	15	0.17
(1,2363)	1:246:B:ILE:HG23	1:282:A:THR:HG23	15	0.17
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	2	0.17
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	2	0.17
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	10	0.17
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	10	0.17
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	10	0.17
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	10	0.17
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	10	0.17
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	10	0.17
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	9	0.17
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	9	0.17
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	9	0.17
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	3	0.17
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	7	0.17
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	8	0.17
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	8	0.17
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	8	0.17
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	10	0.17
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	10	0.17
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	10	0.17
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	11	0.17
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	11	0.17
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	11	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	10	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	10	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	10	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	10	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	10	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	10	0.17
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	10	0.17
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	10	0.17
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	10	0.17
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	10	0.17
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	10	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	10	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	10	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	10	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	10	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	10	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	10	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	12	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	12	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	12	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	12	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	12	0.17
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	12	0.17
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	12	0.17
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	12	0.17
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	12	0.17
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	12	0.17
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	12	0.17
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	12	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	12	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	12	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	12	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	12	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	12	0.17
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	12	0.17
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	14	0.17
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	14	0.17
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	14	0.17
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	2	0.17
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	2	0.17
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	10	0.17
(1,1971)	1:273:A:GLN:H	1:268:A:THR:HB	12	0.17
(1,1918)	1:269:A:CYS:H	1:274:A:GLN:HG3	11	0.17
(1,1918)	1:269:A:CYS:H	1:274:A:GLN:HG3	16	0.17
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	11	0.17
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	11	0.17
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	11	0.17
(1,1904)	1:269:A:CYS:H	1:268:A:THR:HB	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	3	0.17
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	17	0.17
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	20	0.17
(1,1613)	1:253:A:TYR:HE1	1:247:A:VAL:HB	20	0.17
(1,1613)	1:253:A:TYR:HE2	1:247:A:VAL:HB	20	0.17
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	6	0.17
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	6	0.17
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	6	0.17
(1,1559)	1:249:A:SER:HB2	1:269:A:CYS:HB2	10	0.17
(1,1559)	1:249:A:SER:HB2	1:269:A:CYS:HB3	10	0.17
(1,1544)	1:248:A:SER:H	1:276:A:LEU:HD21	12	0.17
(1,1544)	1:248:A:SER:H	1:276:A:LEU:HD22	12	0.17
(1,1544)	1:248:A:SER:H	1:276:A:LEU:HD23	12	0.17
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE1	17	0.17
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE2	17	0.17
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE3	17	0.17
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE1	20	0.17
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE2	20	0.17
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE3	20	0.17
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD11	18	0.17
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD12	18	0.17
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD13	18	0.17
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	15	0.17
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	15	0.17
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	15	0.17
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	11	0.17
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	15	0.17
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	17	0.17
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD11	19	0.17
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD12	19	0.17
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD13	19	0.17
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	9	0.17
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	9	0.17
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	9	0.17
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG21	20	0.17
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG22	20	0.17
(1,991)	1:292:B:SER:H	1:291:B:ILE:HG23	20	0.17
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD11	1	0.17
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD12	1	0.17
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD13	1	0.17
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD21	1	0.17
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD22	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD23	1	0.17
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD11	1	0.17
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD12	1	0.17
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD13	1	0.17
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD21	1	0.17
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD22	1	0.17
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD23	1	0.17
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD11	1	0.17
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD12	1	0.17
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD13	1	0.17
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD21	1	0.17
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD22	1	0.17
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD23	1	0.17
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	12	0.17
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	12	0.17
(1,871)	1:284:B:ASN:H	1:246:B:ILE:H	17	0.17
(1,608)	1:261:B:TRP:HE1	1:270:B:PRO:HB2	1	0.17
(1,547)	1:259:B:GLN:H	1:258:B:ILE:HB	18	0.17
(1,452)	1:253:B:TYR:HE1	1:247:B:VAL:HB	5	0.17
(1,452)	1:253:B:TYR:HE2	1:247:B:VAL:HB	5	0.17
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	2	0.17
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	2	0.17
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	2	0.17
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	16	0.17
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	16	0.17
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	16	0.17
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	19	0.17
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	19	0.17
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	19	0.17
(1,393)	1:249:B:SER:H	1:251:B:GLN:HE21	12	0.17
(1,361)	1:246:B:ILE:HG12	1:284:B:ASN:HA	10	0.17
(1,361)	1:246:B:ILE:HG13	1:284:B:ASN:HA	10	0.17
(1,269)	1:241:B:MET:H	1:241:B:MET:HE1	14	0.17
(1,269)	1:241:B:MET:H	1:241:B:MET:HE2	14	0.17
(1,269)	1:241:B:MET:H	1:241:B:MET:HE3	14	0.17
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD21	1	0.17
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD22	1	0.17
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD23	1	0.17
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	6	0.17
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	6	0.17
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	6	0.17
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD2	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD3	11	0.17
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD2	19	0.17
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD3	19	0.17
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG12	10	0.17
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG13	10	0.17
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG12	10	0.17
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG13	10	0.17
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD11	18	0.17
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD12	18	0.17
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD13	18	0.17
(1,2377)	1:285:B:PHE:HZ	1:250:A:GLY:HA3	1	0.16
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	19	0.16
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	19	0.16
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	19	0.16
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	19	0.16
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	19	0.16
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	19	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	19	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	19	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	19	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	19	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	19	0.16
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	19	0.16
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	19	0.16
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	19	0.16
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	19	0.16
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	19	0.16
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	19	0.16
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	19	0.16
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG21	2	0.16
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG22	2	0.16
(1,2116)	1:291:A:ILE:H	1:291:A:ILE:HG23	2	0.16
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	2	0.16
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	16	0.16
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	14	0.16
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	14	0.16
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	17	0.16
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	17	0.16
(1,1983)	1:274:A:GLN:H	1:272:A:THR:HA	1	0.16
(1,1918)	1:269:A:CYS:H	1:274:A:GLN:HG3	2	0.16
(1,1910)	1:269:A:CYS:H	1:275:A:PRO:HB2	7	0.16
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	2	0.16
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	2	0.16
(1,1904)	1:269:A:CYS:H	1:268:A:THR:HB	13	0.16
(1,1708)	1:259:A:GLN:H	1:258:A:ILE:HB	13	0.16
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	8	0.16
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	8	0.16
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	8	0.16
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	15	0.16
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	15	0.16
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	15	0.16
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB2	16	0.16
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB3	16	0.16
(1,1522)	1:246:A:ILE:HG12	1:284:A:ASN:HA	16	0.16
(1,1522)	1:246:A:ILE:HG13	1:284:A:ASN:HA	16	0.16
(1,1521)	1:246:A:ILE:HA	1:252:A:THR:HB	14	0.16
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD21	10	0.16
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD22	10	0.16
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD23	10	0.16
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD2	13	0.16
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD3	13	0.16
(1,1260)	1:232:A:PHE:HA	1:303:A:PRO:HD3	3	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	1	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	1	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	1	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	1	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	1	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	1	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	9	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	9	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	9	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	9	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	9	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	9	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	15	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	15	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	15	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	15	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	15	0.16
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	15	0.16
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	5	0.16
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	5	0.16
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	13	0.16
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	13	0.16
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	13	0.16
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	9	0.16
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD11	17	0.16
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD12	17	0.16
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD13	17	0.16
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD21	17	0.16
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD22	17	0.16
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD23	17	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD11	17	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD12	17	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD13	17	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD21	17	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD22	17	0.16
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD23	17	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD11	17	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD12	17	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD13	17	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD21	17	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD22	17	0.16
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD23	17	0.16
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	1	0.16
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	14	0.16
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	7	0.16
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	7	0.16
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	13	0.16
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	13	0.16
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	12	0.16
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	3	0.16
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	3	0.16
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	3	0.16
(1,743)	1:269:B:CYS:H	1:268:B:THR:HB	8	0.16
(1,608)	1:261:B:TRP:HE1	1:270:B:PRO:HB2	17	0.16
(1,547)	1:259:B:GLN:H	1:258:B:ILE:HB	20	0.16
(1,452)	1:253:B:TYR:HE1	1:247:B:VAL:HB	16	0.16
(1,452)	1:253:B:TYR:HE2	1:247:B:VAL:HB	16	0.16
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	9	0.16
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	9	0.16
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	9	0.16
(1,345)	1:245:B:VAL:HG11	1:283:B:PRO:HG2	9	0.16
(1,345)	1:245:B:VAL:HG11	1:283:B:PRO:HG3	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,345)	1:245:B:VAL:HG12	1:283:B:PRO:HG2	9	0.16
(1,345)	1:245:B:VAL:HG12	1:283:B:PRO:HG3	9	0.16
(1,345)	1:245:B:VAL:HG13	1:283:B:PRO:HG2	9	0.16
(1,345)	1:245:B:VAL:HG13	1:283:B:PRO:HG3	9	0.16
(1,191)	1:237:B:SER:H	1:236:B:ILE:HB	9	0.16
(1,99)	1:232:B:PHE:HA	1:303:B:PRO:HD3	11	0.16
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	20	0.16
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG21	5	0.15
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG22	5	0.15
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG23	5	0.15
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG21	5	0.15
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG22	5	0.15
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG23	5	0.15
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG21	5	0.15
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG22	5	0.15
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG23	5	0.15
(1,2359)	1:232:B:PHE:HE1	1:290:A:LEU:HD21	12	0.15
(1,2359)	1:232:B:PHE:HE1	1:290:A:LEU:HD22	12	0.15
(1,2359)	1:232:B:PHE:HE1	1:290:A:LEU:HD23	12	0.15
(1,2359)	1:232:B:PHE:HE2	1:290:A:LEU:HD21	12	0.15
(1,2359)	1:232:B:PHE:HE2	1:290:A:LEU:HD22	12	0.15
(1,2359)	1:232:B:PHE:HE2	1:290:A:LEU:HD23	12	0.15
(1,2347)	1:282:A:THR:HG21	1:250:B:GLY:HA2	9	0.15
(1,2347)	1:282:A:THR:HG22	1:250:B:GLY:HA2	9	0.15
(1,2347)	1:282:A:THR:HG23	1:250:B:GLY:HA2	9	0.15
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	10	0.15
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	10	0.15
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	10	0.15
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	19	0.15
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	19	0.15
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	19	0.15
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	5	0.15
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	5	0.15
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	5	0.15
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	5	0.15
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	5	0.15
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	5	0.15
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	14	0.15
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	14	0.15
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	14	0.15
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	14	0.15
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	14	0.15
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	13	0.15
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	13	0.15
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	13	0.15
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	17	0.15
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	17	0.15
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	17	0.15
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	20	0.15
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	5	0.15
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	12	0.15
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG21	15	0.15
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG22	15	0.15
(1,2153)	1:292:A:SER:H	1:291:A:ILE:HG23	15	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	9	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	9	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	9	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	9	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	9	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	9	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	9	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	9	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	9	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	9	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	9	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	9	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	9	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	9	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	9	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	9	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	9	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	9	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	13	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	13	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	13	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	13	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	13	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	13	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	13	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	13	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	13	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	13	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	13	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	13	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	13	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	13	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	13	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	13	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	13	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	17	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	17	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	17	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	17	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	17	0.15
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	17	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	17	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	17	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	17	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	17	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	17	0.15
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	17	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	17	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	17	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	17	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	17	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	17	0.15
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	17	0.15
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	1	0.15
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	8	0.15
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	9	0.15
(1,1910)	1:269:A:CYS:H	1:275:A:PRO:HB2	10	0.15
(1,1904)	1:269:A:CYS:H	1:268:A:THR:HB	19	0.15
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD11	7	0.15
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD12	7	0.15
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD13	7	0.15
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG21	14	0.15
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG22	14	0.15
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG23	14	0.15
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG21	20	0.15
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG22	20	0.15
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG23	20	0.15
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	18	0.15
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	18	0.15
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1522)	1:246:A:ILE:HG12	1:284:A:ASN:HA	19	0.15
(1,1522)	1:246:A:ILE:HG13	1:284:A:ASN:HA	19	0.15
(1,1359)	1:237:A:SER:H	1:234:A:CYS:HB2	9	0.15
(1,1278)	1:233:A:ARG:H	1:233:A:ARG:HB2	15	0.15
(1,1278)	1:233:A:ARG:H	1:233:A:ARG:HB3	15	0.15
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	9	0.15
(1,1124)	1:300:B:ILE:H	1:295:B:CYS:HB2	7	0.15
(1,1124)	1:300:B:ILE:H	1:295:B:CYS:HB3	7	0.15
(1,1122)	1:300:B:ILE:H	1:295:B:CYS:HB2	7	0.15
(1,1122)	1:300:B:ILE:H	1:295:B:CYS:HB3	7	0.15
(1,1084)	1:298:B:ASN:H	1:298:B:ASN:HB2	12	0.15
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	18	0.15
(1,1028)	1:294:B:TRP:HD1	1:232:B:PHE:HE1	17	0.15
(1,1028)	1:294:B:TRP:HD1	1:232:B:PHE:HE2	17	0.15
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD11	14	0.15
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD12	14	0.15
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD13	14	0.15
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	17	0.15
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	20	0.15
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	1	0.15
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	1	0.15
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	8	0.15
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	8	0.15
(1,881)	1:285:B:PHE:HD1	1:285:B:PHE:HA	20	0.15
(1,881)	1:285:B:PHE:HD2	1:285:B:PHE:HA	20	0.15
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD11	4	0.15
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD12	4	0.15
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD13	4	0.15
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	7	0.15
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	7	0.15
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	7	0.15
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	13	0.15
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	13	0.15
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	13	0.15
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	17	0.15
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	17	0.15
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	17	0.15
(1,702)	1:266:B:HIS:H	1:266:B:HIS:HB3	17	0.15
(1,681)	1:264:B:SER:H	1:262:B:LEU:HB2	3	0.15
(1,452)	1:253:B:TYR:HE1	1:247:B:VAL:HB	3	0.15
(1,452)	1:253:B:TYR:HE2	1:247:B:VAL:HB	3	0.15
(1,452)	1:253:B:TYR:HE1	1:247:B:VAL:HB	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:253:B:TYR:HE2	1:247:B:VAL:HB	7	0.15
(1,452)	1:253:B:TYR:HE1	1:247:B:VAL:HB	12	0.15
(1,452)	1:253:B:TYR:HE2	1:247:B:VAL:HB	12	0.15
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	10	0.15
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	10	0.15
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	10	0.15
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	17	0.15
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	17	0.15
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	17	0.15
(1,393)	1:249:B:SER:H	1:251:B:GLN:HE21	1	0.15
(1,360)	1:246:B:ILE:HA	1:252:B:THR:HB	7	0.15
(1,345)	1:245:B:VAL:HG11	1:283:B:PRO:HG2	10	0.15
(1,345)	1:245:B:VAL:HG11	1:283:B:PRO:HG3	10	0.15
(1,345)	1:245:B:VAL:HG12	1:283:B:PRO:HG2	10	0.15
(1,345)	1:245:B:VAL:HG12	1:283:B:PRO:HG3	10	0.15
(1,345)	1:245:B:VAL:HG13	1:283:B:PRO:HG2	10	0.15
(1,345)	1:245:B:VAL:HG13	1:283:B:PRO:HG3	10	0.15
(1,259)	1:241:B:MET:H	1:241:B:MET:HB2	14	0.15
(1,180)	1:236:B:ILE:H	1:253:B:TYR:HE1	8	0.15
(1,180)	1:236:B:ILE:H	1:253:B:TYR:HE2	8	0.15
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD2	15	0.15
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD3	15	0.15
(1,99)	1:232:B:PHE:HA	1:303:B:PRO:HD3	13	0.15
(1,99)	1:232:B:PHE:HA	1:303:B:PRO:HD3	14	0.15
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	4	0.15
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	7	0.15
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	9	0.15
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	15	0.15
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	17	0.14
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	17	0.14
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	17	0.14
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	17	0.14
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	17	0.14
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	17	0.14
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	17	0.14
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	17	0.14
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	17	0.14
(1,2356)	1:231:B:GLU:HG2	1:290:A:LEU:HD11	1	0.14
(1,2356)	1:231:B:GLU:HG2	1:290:A:LEU:HD12	1	0.14
(1,2356)	1:231:B:GLU:HG2	1:290:A:LEU:HD13	1	0.14
(1,2356)	1:231:B:GLU:HG3	1:290:A:LEU:HD11	1	0.14
(1,2356)	1:231:B:GLU:HG3	1:290:A:LEU:HD12	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2356)	1:231:B:GLU:HG3	1:290:A:LEU:HD13	1	0.14
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	17	0.14
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	17	0.14
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	17	0.14
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	17	0.14
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	17	0.14
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	17	0.14
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	17	0.14
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	17	0.14
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	17	0.14
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	2	0.14
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	2	0.14
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	2	0.14
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	17	0.14
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	17	0.14
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	17	0.14
(1,2331)	1:232:A:PHE:HE1	1:290:B:LEU:HD21	14	0.14
(1,2331)	1:232:A:PHE:HE1	1:290:B:LEU:HD22	14	0.14
(1,2331)	1:232:A:PHE:HE1	1:290:B:LEU:HD23	14	0.14
(1,2331)	1:232:A:PHE:HE2	1:290:B:LEU:HD21	14	0.14
(1,2331)	1:232:A:PHE:HE2	1:290:B:LEU:HD22	14	0.14
(1,2331)	1:232:A:PHE:HE2	1:290:B:LEU:HD23	14	0.14
(1,2330)	1:232:A:PHE:HE1	1:290:B:LEU:HD11	6	0.14
(1,2330)	1:232:A:PHE:HE1	1:290:B:LEU:HD12	6	0.14
(1,2330)	1:232:A:PHE:HE1	1:290:B:LEU:HD13	6	0.14
(1,2330)	1:232:A:PHE:HE2	1:290:B:LEU:HD11	6	0.14
(1,2330)	1:232:A:PHE:HE2	1:290:B:LEU:HD12	6	0.14
(1,2330)	1:232:A:PHE:HE2	1:290:B:LEU:HD13	6	0.14
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD11	15	0.14
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD12	15	0.14
(1,2328)	1:231:A:GLU:HG2	1:290:B:LEU:HD13	15	0.14
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD11	15	0.14
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD12	15	0.14
(1,2328)	1:231:A:GLU:HG3	1:290:B:LEU:HD13	15	0.14
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	9	0.14
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	9	0.14
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	9	0.14
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	9	0.14
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	9	0.14
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	9	0.14
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	1	0.14
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	1	0.14
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	11	0.14
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	11	0.14
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	11	0.14
(1,2264)	1:299:A:GLY:H	1:298:A:ASN:HD22	12	0.14
(1,2053)	1:285:A:PHE:HZ	1:250:A:GLY:HA2	12	0.14
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	4	0.14
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	19	0.14
(1,2042)	1:285:A:PHE:HD1	1:285:A:PHE:HA	11	0.14
(1,2042)	1:285:A:PHE:HD2	1:285:A:PHE:HA	11	0.14
(1,2035)	1:284:A:ASN:HA	1:246:A:ILE:HB	18	0.14
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	7	0.14
(1,1918)	1:269:A:CYS:H	1:274:A:GLN:HG3	9	0.14
(1,1918)	1:269:A:CYS:H	1:274:A:GLN:HG3	12	0.14
(1,1863)	1:266:A:HIS:H	1:266:A:HIS:HB3	16	0.14
(1,1783)	1:261:A:TRP:HD1	1:262:A:LEU:HD11	14	0.14
(1,1783)	1:261:A:TRP:HD1	1:262:A:LEU:HD12	14	0.14
(1,1783)	1:261:A:TRP:HD1	1:262:A:LEU:HD13	14	0.14
(1,1783)	1:261:A:TRP:HD1	1:262:A:LEU:HD21	14	0.14
(1,1783)	1:261:A:TRP:HD1	1:262:A:LEU:HD22	14	0.14
(1,1783)	1:261:A:TRP:HD1	1:262:A:LEU:HD23	14	0.14
(1,1769)	1:261:A:TRP:HE1	1:270:A:PRO:HB2	2	0.14
(1,1769)	1:261:A:TRP:HE1	1:270:A:PRO:HB2	9	0.14
(1,1769)	1:261:A:TRP:HE1	1:270:A:PRO:HB2	19	0.14
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG21	4	0.14
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG22	4	0.14
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG23	4	0.14
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	7	0.14
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	7	0.14
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	7	0.14
(1,1554)	1:249:A:SER:H	1:251:A:GLN:HE21	11	0.14
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD21	6	0.14
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD22	6	0.14
(1,1393)	1:239:A:GLU:H	1:238:A:LEU:HD23	6	0.14
(1,1294)	1:233:A:ARG:HA	1:239:A:GLU:HG2	17	0.14
(1,1294)	1:233:A:ARG:HA	1:239:A:GLU:HG3	17	0.14
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD2	17	0.14
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD3	17	0.14
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD2	19	0.14
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD3	19	0.14
(1,1260)	1:232:A:PHE:HA	1:303:A:PRO:HD3	1	0.14
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD11	5	0.14
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD12	5	0.14
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD13	5	0.14
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	6	0.14
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	6	0.14
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	6	0.14
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	6	0.14
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	6	0.14
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	6	0.14
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	7	0.14
(1,1037)	1:294:B:TRP:HH2	1:228:B:ILE:HB	13	0.14
(1,1037)	1:294:B:TRP:HH2	1:228:B:ILE:HB	14	0.14
(1,1035)	1:294:B:TRP:HD1	1:229:B:PRO:HG2	14	0.14
(1,1035)	1:294:B:TRP:HD1	1:229:B:PRO:HG3	14	0.14
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD11	6	0.14
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD12	6	0.14
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD13	6	0.14
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD21	6	0.14
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD22	6	0.14
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD23	6	0.14
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD11	6	0.14
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD12	6	0.14
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD13	6	0.14
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD21	6	0.14
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD22	6	0.14
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD23	6	0.14
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD11	6	0.14
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD12	6	0.14
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD13	6	0.14
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD21	6	0.14
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD22	6	0.14
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD23	6	0.14
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	3	0.14
(1,881)	1:285:B:PHE:HD1	1:285:B:PHE:HA	3	0.14
(1,881)	1:285:B:PHE:HD2	1:285:B:PHE:HA	3	0.14
(1,881)	1:285:B:PHE:HD1	1:285:B:PHE:HA	11	0.14
(1,881)	1:285:B:PHE:HD2	1:285:B:PHE:HA	11	0.14
(1,849)	1:276:B:LEU:H	1:275:B:PRO:HB2	5	0.14
(1,822)	1:274:B:GLN:H	1:272:B:THR:HA	16	0.14
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD11	13	0.14
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD12	13	0.14
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD13	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD11	16	0.14
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD12	16	0.14
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD13	16	0.14
(1,749)	1:269:B:CYS:H	1:275:B:PRO:HB2	14	0.14
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	10	0.14
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	10	0.14
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	10	0.14
(1,743)	1:269:B:CYS:H	1:268:B:THR:HB	9	0.14
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD11	8	0.14
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD12	8	0.14
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD13	8	0.14
(1,452)	1:253:B:TYR:HE1	1:247:B:VAL:HB	14	0.14
(1,452)	1:253:B:TYR:HE2	1:247:B:VAL:HB	14	0.14
(1,255)	1:240:B:LEU:HB2	1:228:B:ILE:HD11	9	0.14
(1,255)	1:240:B:LEU:HB2	1:228:B:ILE:HD12	9	0.14
(1,255)	1:240:B:LEU:HB2	1:228:B:ILE:HD13	9	0.14
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	11	0.14
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	11	0.14
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	11	0.14
(1,191)	1:237:B:SER:H	1:236:B:ILE:HB	14	0.14
(1,180)	1:236:B:ILE:H	1:253:B:TYR:HE1	16	0.14
(1,180)	1:236:B:ILE:H	1:253:B:TYR:HE2	16	0.14
(1,117)	1:233:B:ARG:H	1:233:B:ARG:HB2	2	0.14
(1,117)	1:233:B:ARG:H	1:233:B:ARG:HB3	2	0.14
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD2	16	0.14
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD3	16	0.14
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD11	15	0.14
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD12	15	0.14
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD13	15	0.14
(1,2377)	1:285:B:PHE:HZ	1:250:A:GLY:HA3	17	0.13
(1,2369)	1:246:B:ILE:HG21	1:246:A:ILE:HD11	9	0.13
(1,2369)	1:246:B:ILE:HG21	1:246:A:ILE:HD12	9	0.13
(1,2369)	1:246:B:ILE:HG21	1:246:A:ILE:HD13	9	0.13
(1,2369)	1:246:B:ILE:HG22	1:246:A:ILE:HD11	9	0.13
(1,2369)	1:246:B:ILE:HG22	1:246:A:ILE:HD12	9	0.13
(1,2369)	1:246:B:ILE:HG22	1:246:A:ILE:HD13	9	0.13
(1,2369)	1:246:B:ILE:HG23	1:246:A:ILE:HD11	9	0.13
(1,2369)	1:246:B:ILE:HG23	1:246:A:ILE:HD12	9	0.13
(1,2369)	1:246:B:ILE:HG23	1:246:A:ILE:HD13	9	0.13
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	3	0.13
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	3	0.13
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	3	0.13
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	3	0.13
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	3	0.13
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	3	0.13
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	3	0.13
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	3	0.13
(1,2365)	1:246:B:ILE:HD11	1:282:A:THR:HB	13	0.13
(1,2365)	1:246:B:ILE:HD12	1:282:A:THR:HB	13	0.13
(1,2365)	1:246:B:ILE:HD13	1:282:A:THR:HB	13	0.13
(1,2349)	1:285:A:PHE:HZ	1:250:B:GLY:HA3	7	0.13
(1,2345)	1:252:A:THR:HB	1:286:B:VAL:HG11	13	0.13
(1,2345)	1:252:A:THR:HB	1:286:B:VAL:HG12	13	0.13
(1,2345)	1:252:A:THR:HB	1:286:B:VAL:HG13	13	0.13
(1,2345)	1:252:A:THR:HB	1:286:B:VAL:HG21	13	0.13
(1,2345)	1:252:A:THR:HB	1:286:B:VAL:HG22	13	0.13
(1,2345)	1:252:A:THR:HB	1:286:B:VAL:HG23	13	0.13
(1,2340)	1:246:A:ILE:HD11	1:246:B:ILE:HG21	9	0.13
(1,2340)	1:246:A:ILE:HD11	1:246:B:ILE:HG22	9	0.13
(1,2340)	1:246:A:ILE:HD11	1:246:B:ILE:HG23	9	0.13
(1,2340)	1:246:A:ILE:HD12	1:246:B:ILE:HG21	9	0.13
(1,2340)	1:246:A:ILE:HD12	1:246:B:ILE:HG22	9	0.13
(1,2340)	1:246:A:ILE:HD12	1:246:B:ILE:HG23	9	0.13
(1,2340)	1:246:A:ILE:HD13	1:246:B:ILE:HG21	9	0.13
(1,2340)	1:246:A:ILE:HD13	1:246:B:ILE:HG22	9	0.13
(1,2340)	1:246:A:ILE:HD13	1:246:B:ILE:HG23	9	0.13
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	3	0.13
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	3	0.13
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	3	0.13
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	3	0.13
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	3	0.13
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	3	0.13
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	3	0.13
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	3	0.13
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	3	0.13
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	7	0.13
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	7	0.13
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	7	0.13
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	5	0.13
(1,2190)	1:294:A:TRP:HD1	1:232:A:PHE:HE1	5	0.13
(1,2190)	1:294:A:TRP:HD1	1:232:A:PHE:HE2	5	0.13
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD2	5	0.13
(1,2050)	1:285:A:PHE:H	1:283:A:PRO:HD3	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2042)	1:285:A:PHE:HD1	1:285:A:PHE:HA	1	0.13
(1,2042)	1:285:A:PHE:HD2	1:285:A:PHE:HA	1	0.13
(1,2042)	1:285:A:PHE:HD1	1:285:A:PHE:HA	3	0.13
(1,2042)	1:285:A:PHE:HD2	1:285:A:PHE:HA	3	0.13
(1,2042)	1:285:A:PHE:HD1	1:285:A:PHE:HA	5	0.13
(1,2042)	1:285:A:PHE:HD2	1:285:A:PHE:HA	5	0.13
(1,2042)	1:285:A:PHE:HD1	1:285:A:PHE:HA	17	0.13
(1,2042)	1:285:A:PHE:HD2	1:285:A:PHE:HA	17	0.13
(1,2022)	1:278:A:HIS:HD2	1:248:A:SER:H	18	0.13
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	6	0.13
(1,1910)	1:269:A:CYS:H	1:275:A:PRO:HB2	3	0.13
(1,1863)	1:266:A:HIS:H	1:266:A:HIS:HB3	2	0.13
(1,1863)	1:266:A:HIS:H	1:266:A:HIS:HB3	10	0.13
(1,1863)	1:266:A:HIS:H	1:266:A:HIS:HB3	13	0.13
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD11	2	0.13
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD12	2	0.13
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD13	2	0.13
(1,1754)	1:261:A:TRP:HE3	1:261:A:TRP:HA	18	0.13
(1,1613)	1:253:A:TYR:HE1	1:247:A:VAL:HB	16	0.13
(1,1613)	1:253:A:TYR:HE2	1:247:A:VAL:HB	16	0.13
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	17	0.13
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	17	0.13
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	17	0.13
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	19	0.13
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	19	0.13
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	19	0.13
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	20	0.13
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	20	0.13
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	20	0.13
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB2	7	0.13
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB3	7	0.13
(1,1554)	1:249:A:SER:H	1:251:A:GLN:HE21	8	0.13
(1,1328)	1:236:A:ILE:H	1:236:A:ILE:HB	18	0.13
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	11	0.13
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	15	0.13
(1,1102)	1:299:B:GLY:H	1:298:B:ASN:HD22	3	0.13
(1,1102)	1:299:B:GLY:H	1:298:B:ASN:HD22	16	0.13
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	8	0.13
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	16	0.13
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	19	0.13
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	10	0.13
(1,1037)	1:294:B:TRP:HH2	1:228:B:ILE:HB	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,881)	1:285:B:PHE:HD1	1:285:B:PHE:HA	1	0.13
(1,881)	1:285:B:PHE:HD2	1:285:B:PHE:HA	1	0.13
(1,881)	1:285:B:PHE:HD1	1:285:B:PHE:HA	13	0.13
(1,881)	1:285:B:PHE:HD2	1:285:B:PHE:HA	13	0.13
(1,813)	1:273:B:GLN:H	1:274:B:GLN:HE21	17	0.13
(1,810)	1:273:B:GLN:H	1:268:B:THR:HB	20	0.13
(1,800)	1:272:B:THR:HG21	1:271:B:LYS:HE2	10	0.13
(1,800)	1:272:B:THR:HG21	1:271:B:LYS:HE3	10	0.13
(1,800)	1:272:B:THR:HG22	1:271:B:LYS:HE2	10	0.13
(1,800)	1:272:B:THR:HG22	1:271:B:LYS:HE3	10	0.13
(1,800)	1:272:B:THR:HG23	1:271:B:LYS:HE2	10	0.13
(1,800)	1:272:B:THR:HG23	1:271:B:LYS:HE3	10	0.13
(1,757)	1:269:B:CYS:H	1:274:B:GLN:HG3	6	0.13
(1,651)	1:262:B:LEU:HA	1:258:B:ILE:HD11	8	0.13
(1,651)	1:262:B:LEU:HA	1:258:B:ILE:HD12	8	0.13
(1,651)	1:262:B:LEU:HA	1:258:B:ILE:HD13	8	0.13
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD11	16	0.13
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD12	16	0.13
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD13	16	0.13
(1,452)	1:253:B:TYR:HE1	1:247:B:VAL:HB	1	0.13
(1,452)	1:253:B:TYR:HE2	1:247:B:VAL:HB	1	0.13
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	3	0.13
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	3	0.13
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	3	0.13
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB2	6	0.13
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB3	6	0.13
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB2	17	0.13
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB3	17	0.13
(1,393)	1:249:B:SER:H	1:251:B:GLN:HE21	3	0.13
(1,393)	1:249:B:SER:H	1:251:B:GLN:HE21	6	0.13
(1,361)	1:246:B:ILE:HG12	1:284:B:ASN:HA	16	0.13
(1,361)	1:246:B:ILE:HG13	1:284:B:ASN:HA	16	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD21	7	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD22	7	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD23	7	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD21	10	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD22	10	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD23	10	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD21	16	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD22	16	0.13
(1,232)	1:239:B:GLU:H	1:238:B:LEU:HD23	16	0.13
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD11	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD12	7	0.13
(1,231)	1:239:B:GLU:H	1:238:B:LEU:HD13	7	0.13
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG12	2	0.13
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG13	2	0.13
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG12	2	0.13
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG13	2	0.13
(1,2377)	1:285:B:PHE:HZ	1:250:A:GLY:HA3	2	0.12
(1,2377)	1:285:B:PHE:HZ	1:250:A:GLY:HA3	20	0.12
(1,2373)	1:252:B:THR:HB	1:286:A:VAL:HG11	3	0.12
(1,2373)	1:252:B:THR:HB	1:286:A:VAL:HG12	3	0.12
(1,2373)	1:252:B:THR:HB	1:286:A:VAL:HG13	3	0.12
(1,2373)	1:252:B:THR:HB	1:286:A:VAL:HG21	3	0.12
(1,2373)	1:252:B:THR:HB	1:286:A:VAL:HG22	3	0.12
(1,2373)	1:252:B:THR:HB	1:286:A:VAL:HG23	3	0.12
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	5	0.12
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	5	0.12
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	5	0.12
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	5	0.12
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	5	0.12
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	5	0.12
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	5	0.12
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	5	0.12
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	5	0.12
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	16	0.12
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	16	0.12
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	16	0.12
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	16	0.12
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	16	0.12
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	16	0.12
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	16	0.12
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	16	0.12
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	16	0.12
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG21	13	0.12
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG22	13	0.12
(1,2364)	1:246:B:ILE:HD11	1:282:A:THR:HG23	13	0.12
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG21	13	0.12
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG22	13	0.12
(1,2364)	1:246:B:ILE:HD12	1:282:A:THR:HG23	13	0.12
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG21	13	0.12
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG22	13	0.12
(1,2364)	1:246:B:ILE:HD13	1:282:A:THR:HG23	13	0.12
(1,2353)	1:231:B:GLU:HA	1:289:A:SER:HB2	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2353)	1:231:B:GLU:HA	1:289:A:SER:HB3	2	0.12
(1,2349)	1:285:A:PHE:HZ	1:250:B:GLY:HA3	17	0.12
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	5	0.12
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	5	0.12
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	5	0.12
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	5	0.12
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	5	0.12
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	5	0.12
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	5	0.12
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	5	0.12
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	5	0.12
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	16	0.12
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	16	0.12
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	16	0.12
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	16	0.12
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	16	0.12
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	16	0.12
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	16	0.12
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	16	0.12
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	16	0.12
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG21	10	0.12
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG22	10	0.12
(1,2336)	1:246:A:ILE:HD11	1:282:B:THR:HG23	10	0.12
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG21	10	0.12
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG22	10	0.12
(1,2336)	1:246:A:ILE:HD12	1:282:B:THR:HG23	10	0.12
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG21	10	0.12
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG22	10	0.12
(1,2336)	1:246:A:ILE:HD13	1:282:B:THR:HG23	10	0.12
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	18	0.12
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	18	0.12
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	18	0.12
(1,2271)	1:300:A:ILE:H	1:300:A:ILE:HB	12	0.12
(1,2270)	1:300:A:ILE:H	1:300:A:ILE:HB	12	0.12
(1,2246)	1:298:A:ASN:H	1:298:A:ASN:HB2	6	0.12
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	4	0.12
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	11	0.12
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	14	0.12
(1,2199)	1:294:A:TRP:HH2	1:228:A:ILE:HB	5	0.12
(1,2197)	1:294:A:TRP:HD1	1:229:A:PRO:HG2	9	0.12
(1,2197)	1:294:A:TRP:HD1	1:229:A:PRO:HG3	9	0.12
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2042)	1:285:A:PHE:HD1	1:285:A:PHE:HA	10	0.12
(1,2042)	1:285:A:PHE:HD2	1:285:A:PHE:HA	10	0.12
(1,2042)	1:285:A:PHE:HD1	1:285:A:PHE:HA	20	0.12
(1,2042)	1:285:A:PHE:HD2	1:285:A:PHE:HA	20	0.12
(1,1971)	1:273:A:GLN:H	1:268:A:THR:HB	13	0.12
(1,1971)	1:273:A:GLN:H	1:268:A:THR:HB	19	0.12
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	9	0.12
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	9	0.12
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	9	0.12
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	18	0.12
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	18	0.12
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	18	0.12
(1,1904)	1:269:A:CYS:H	1:268:A:THR:HB	14	0.12
(1,1831)	1:263:A:ASP:H	1:259:A:GLN:HE22	6	0.12
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD11	9	0.12
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD12	9	0.12
(1,1812)	1:262:A:LEU:HA	1:258:A:ILE:HD13	9	0.12
(1,1769)	1:261:A:TRP:HE1	1:270:A:PRO:HB2	13	0.12
(1,1613)	1:253:A:TYR:HE1	1:247:A:VAL:HB	3	0.12
(1,1613)	1:253:A:TYR:HE2	1:247:A:VAL:HB	3	0.12
(1,1613)	1:253:A:TYR:HE1	1:247:A:VAL:HB	10	0.12
(1,1613)	1:253:A:TYR:HE2	1:247:A:VAL:HB	10	0.12
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG21	2	0.12
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG22	2	0.12
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG23	2	0.12
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB2	4	0.12
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB3	4	0.12
(1,1521)	1:246:A:ILE:HA	1:252:A:THR:HB	1	0.12
(1,1521)	1:246:A:ILE:HA	1:252:A:THR:HB	3	0.12
(1,1483)	1:245:A:VAL:H	1:245:A:VAL:HG21	11	0.12
(1,1483)	1:245:A:VAL:H	1:245:A:VAL:HG22	11	0.12
(1,1483)	1:245:A:VAL:H	1:245:A:VAL:HG23	11	0.12
(1,1417)	1:240:A:LEU:HD21	1:303:A:PRO:HB2	17	0.12
(1,1417)	1:240:A:LEU:HD21	1:303:A:PRO:HB3	17	0.12
(1,1417)	1:240:A:LEU:HD22	1:303:A:PRO:HB2	17	0.12
(1,1417)	1:240:A:LEU:HD22	1:303:A:PRO:HB3	17	0.12
(1,1417)	1:240:A:LEU:HD23	1:303:A:PRO:HB2	17	0.12
(1,1417)	1:240:A:LEU:HD23	1:303:A:PRO:HB3	17	0.12
(1,1416)	1:240:A:LEU:HB2	1:228:A:ILE:HD11	8	0.12
(1,1416)	1:240:A:LEU:HB2	1:228:A:ILE:HD12	8	0.12
(1,1416)	1:240:A:LEU:HB2	1:228:A:ILE:HD13	8	0.12
(1,1397)	1:240:A:LEU:H	1:240:A:LEU:HB3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1352)	1:237:A:SER:H	1:236:A:ILE:HB	5	0.12
(1,1328)	1:236:A:ILE:H	1:236:A:ILE:HB	5	0.12
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG12	2	0.12
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG13	2	0.12
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG12	2	0.12
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG13	2	0.12
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG12	8	0.12
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG13	8	0.12
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG12	8	0.12
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG13	8	0.12
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG12	16	0.12
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG13	16	0.12
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG12	16	0.12
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG13	16	0.12
(1,1260)	1:232:A:PHE:HA	1:303:A:PRO:HD3	2	0.12
(1,1260)	1:232:A:PHE:HA	1:303:A:PRO:HD3	15	0.12
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	18	0.12
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	19	0.12
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD11	14	0.12
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD12	14	0.12
(1,1201)	1:228:A:ILE:H	1:227:A:ILE:HD13	14	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	12	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	12	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	12	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	12	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	12	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	12	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD11	18	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD12	18	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD13	18	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD21	18	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD22	18	0.12
(1,1141)	1:302:B:LEU:H	1:302:B:LEU:HD23	18	0.12
(1,1124)	1:300:B:ILE:H	1:295:B:CYS:HB2	8	0.12
(1,1124)	1:300:B:ILE:H	1:295:B:CYS:HB3	8	0.12
(1,1122)	1:300:B:ILE:H	1:295:B:CYS:HB2	8	0.12
(1,1122)	1:300:B:ILE:H	1:295:B:CYS:HB3	8	0.12
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	4	0.12
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	4	0.12
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	4	0.12
(1,1102)	1:299:B:GLY:H	1:298:B:ASN:HD22	9	0.12
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	3	0.12
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	10	0.12
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	15	0.12
(1,1037)	1:294:B:TRP:HH2	1:228:B:ILE:HB	2	0.12
(1,1037)	1:294:B:TRP:HH2	1:228:B:ILE:HB	8	0.12
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD11	5	0.12
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD12	5	0.12
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD13	5	0.12
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD21	5	0.12
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD22	5	0.12
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD23	5	0.12
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD11	5	0.12
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD12	5	0.12
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD13	5	0.12
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD21	5	0.12
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD22	5	0.12
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD23	5	0.12
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD11	5	0.12
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD12	5	0.12
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD13	5	0.12
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD21	5	0.12
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD22	5	0.12
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD23	5	0.12
(1,890)	1:285:B:PHE:HB2	1:283:B:PRO:HG2	1	0.12
(1,890)	1:285:B:PHE:HB2	1:283:B:PRO:HG3	1	0.12
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	2	0.12
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	2	0.12
(1,822)	1:274:B:GLN:H	1:272:B:THR:HA	8	0.12
(1,757)	1:269:B:CYS:H	1:274:B:GLN:HG3	1	0.12
(1,757)	1:269:B:CYS:H	1:274:B:GLN:HG3	8	0.12
(1,749)	1:269:B:CYS:H	1:275:B:PRO:HB2	12	0.12
(1,749)	1:269:B:CYS:H	1:275:B:PRO:HB2	20	0.12
(1,702)	1:266:B:HIS:H	1:266:B:HIS:HB3	8	0.12
(1,622)	1:261:B:TRP:HD1	1:262:B:LEU:HD11	19	0.12
(1,622)	1:261:B:TRP:HD1	1:262:B:LEU:HD12	19	0.12
(1,622)	1:261:B:TRP:HD1	1:262:B:LEU:HD13	19	0.12
(1,622)	1:261:B:TRP:HD1	1:262:B:LEU:HD21	19	0.12
(1,622)	1:261:B:TRP:HD1	1:262:B:LEU:HD22	19	0.12
(1,622)	1:261:B:TRP:HD1	1:262:B:LEU:HD23	19	0.12
(1,608)	1:261:B:TRP:HE1	1:270:B:PRO:HB2	18	0.12
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD11	3	0.12
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD12	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:258:B:ILE:H	1:258:B:ILE:HD13	3	0.12
(1,452)	1:253:B:TYR:HE1	1:247:B:VAL:HB	6	0.12
(1,452)	1:253:B:TYR:HE2	1:247:B:VAL:HB	6	0.12
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG21	14	0.12
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG22	14	0.12
(1,405)	1:250:B:GLY:H	1:282:B:THR:HG23	14	0.12
(1,213)	1:238:B:LEU:H	1:237:B:SER:HB2	12	0.12
(1,213)	1:238:B:LEU:H	1:237:B:SER:HB3	12	0.12
(1,167)	1:236:B:ILE:H	1:236:B:ILE:HB	2	0.12
(1,167)	1:236:B:ILE:H	1:236:B:ILE:HB	9	0.12
(1,167)	1:236:B:ILE:H	1:236:B:ILE:HB	14	0.12
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD2	5	0.12
(1,115)	1:232:B:PHE:HZ	1:229:B:PRO:HD3	5	0.12
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG12	14	0.12
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG13	14	0.12
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG12	14	0.12
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG13	14	0.12
(1,91)	1:232:B:PHE:HB3	1:228:B:ILE:HB	5	0.12
(1,87)	1:232:B:PHE:H	1:231:B:GLU:HB2	17	0.12
(1,87)	1:232:B:PHE:H	1:231:B:GLU:HB3	17	0.12
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	5	0.12
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	11	0.12
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD11	12	0.12
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD12	12	0.12
(1,40)	1:228:B:ILE:H	1:227:B:ILE:HD13	12	0.12
(1,2375)	1:282:B:THR:HG21	1:250:A:GLY:HA2	7	0.11
(1,2375)	1:282:B:THR:HG22	1:250:A:GLY:HA2	7	0.11
(1,2375)	1:282:B:THR:HG23	1:250:A:GLY:HA2	7	0.11
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG21	19	0.11
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG22	19	0.11
(1,2367)	1:246:B:ILE:HG21	1:246:A:ILE:HG23	19	0.11
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG21	19	0.11
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG22	19	0.11
(1,2367)	1:246:B:ILE:HG22	1:246:A:ILE:HG23	19	0.11
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG21	19	0.11
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG22	19	0.11
(1,2367)	1:246:B:ILE:HG23	1:246:A:ILE:HG23	19	0.11
(1,2362)	1:246:B:ILE:HG21	1:282:A:THR:HB	4	0.11
(1,2362)	1:246:B:ILE:HG22	1:282:A:THR:HB	4	0.11
(1,2362)	1:246:B:ILE:HG23	1:282:A:THR:HB	4	0.11
(1,2349)	1:285:A:PHE:HZ	1:250:B:GLY:HA3	9	0.11
(1,2348)	1:285:A:PHE:HD1	1:250:B:GLY:HA2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2348)	1:285:A:PHE:HD2	1:250:B:GLY:HA2	3	0.11
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG21	19	0.11
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG22	19	0.11
(1,2339)	1:246:A:ILE:HG21	1:246:B:ILE:HG23	19	0.11
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG21	19	0.11
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG22	19	0.11
(1,2339)	1:246:A:ILE:HG22	1:246:B:ILE:HG23	19	0.11
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG21	19	0.11
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG22	19	0.11
(1,2339)	1:246:A:ILE:HG23	1:246:B:ILE:HG23	19	0.11
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	1	0.11
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	1	0.11
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	1	0.11
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	15	0.11
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	15	0.11
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	15	0.11
(1,2334)	1:246:A:ILE:HG21	1:282:B:THR:HB	12	0.11
(1,2334)	1:246:A:ILE:HG22	1:282:B:THR:HB	12	0.11
(1,2334)	1:246:A:ILE:HG23	1:282:B:THR:HB	12	0.11
(1,2330)	1:232:A:PHE:HE1	1:290:B:LEU:HD11	8	0.11
(1,2330)	1:232:A:PHE:HE1	1:290:B:LEU:HD12	8	0.11
(1,2330)	1:232:A:PHE:HE1	1:290:B:LEU:HD13	8	0.11
(1,2330)	1:232:A:PHE:HE2	1:290:B:LEU:HD11	8	0.11
(1,2330)	1:232:A:PHE:HE2	1:290:B:LEU:HD12	8	0.11
(1,2330)	1:232:A:PHE:HE2	1:290:B:LEU:HD13	8	0.11
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD11	12	0.11
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD12	12	0.11
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD13	12	0.11
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD21	12	0.11
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD22	12	0.11
(1,2303)	1:302:A:LEU:H	1:302:A:LEU:HD23	12	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	3	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	3	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	3	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	6	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	6	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	6	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	10	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	10	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	10	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	14	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	14	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD11	20	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD12	20	0.11
(1,2272)	1:300:A:ILE:H	1:300:A:ILE:HD13	20	0.11
(1,2264)	1:299:A:GLY:H	1:298:A:ASN:HD22	4	0.11
(1,2264)	1:299:A:GLY:H	1:298:A:ASN:HD22	10	0.11
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	2	0.11
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	7	0.11
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	9	0.11
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	12	0.11
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	16	0.11
(1,2199)	1:294:A:TRP:HH2	1:228:A:ILE:HB	16	0.11
(1,2190)	1:294:A:TRP:HD1	1:232:A:PHE:HE1	4	0.11
(1,2190)	1:294:A:TRP:HD1	1:232:A:PHE:HE2	4	0.11
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	5	0.11
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	5	0.11
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	5	0.11
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	5	0.11
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	5	0.11
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	5	0.11
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	5	0.11
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	5	0.11
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	5	0.11
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	5	0.11
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	5	0.11
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	5	0.11
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	5	0.11
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	5	0.11
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	5	0.11
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	5	0.11
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	5	0.11
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	5	0.11
(1,2112)	1:290:A:LEU:HD11	1:293:A:GLN:HB2	9	0.11
(1,2112)	1:290:A:LEU:HD11	1:293:A:GLN:HB3	9	0.11
(1,2112)	1:290:A:LEU:HD12	1:293:A:GLN:HB2	9	0.11
(1,2112)	1:290:A:LEU:HD12	1:293:A:GLN:HB3	9	0.11
(1,2112)	1:290:A:LEU:HD13	1:293:A:GLN:HB2	9	0.11
(1,2112)	1:290:A:LEU:HD13	1:293:A:GLN:HB3	9	0.11
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	5	0.11
(1,2052)	1:285:A:PHE:HZ	1:250:A:GLY:HA3	15	0.11
(1,2051)	1:285:A:PHE:HB2	1:283:A:PRO:HG2	20	0.11
(1,2051)	1:285:A:PHE:HB2	1:283:A:PRO:HG3	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2022)	1:278:A:HIS:HD2	1:248:A:SER:H	7	0.11
(1,1983)	1:274:A:GLN:H	1:272:A:THR:HA	13	0.11
(1,1983)	1:274:A:GLN:H	1:272:A:THR:HA	19	0.11
(1,1974)	1:273:A:GLN:H	1:274:A:GLN:HE21	13	0.11
(1,1931)	1:270:A:PRO:HD3	1:258:A:ILE:HD11	1	0.11
(1,1931)	1:270:A:PRO:HD3	1:258:A:ILE:HD12	1	0.11
(1,1931)	1:270:A:PRO:HD3	1:258:A:ILE:HD13	1	0.11
(1,1917)	1:269:A:CYS:HB2	1:274:A:GLN:HE21	12	0.11
(1,1917)	1:269:A:CYS:HB3	1:274:A:GLN:HE21	12	0.11
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	10	0.11
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	10	0.11
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	10	0.11
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG21	16	0.11
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG22	16	0.11
(1,1905)	1:269:A:CYS:H	1:268:A:THR:HG23	16	0.11
(1,1896)	1:268:A:THR:H	1:276:A:LEU:HD11	8	0.11
(1,1896)	1:268:A:THR:H	1:276:A:LEU:HD12	8	0.11
(1,1896)	1:268:A:THR:H	1:276:A:LEU:HD13	8	0.11
(1,1863)	1:266:A:HIS:H	1:266:A:HIS:HB3	9	0.11
(1,1810)	1:262:A:LEU:H	1:259:A:GLN:HE22	2	0.11
(1,1769)	1:261:A:TRP:HE1	1:270:A:PRO:HB2	11	0.11
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG21	16	0.11
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG22	16	0.11
(1,1587)	1:251:A:GLN:HA	1:272:A:THR:HG23	16	0.11
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	16	0.11
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	16	0.11
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	16	0.11
(1,1506)	1:245:A:VAL:HG11	1:283:A:PRO:HG2	1	0.11
(1,1506)	1:245:A:VAL:HG11	1:283:A:PRO:HG3	1	0.11
(1,1506)	1:245:A:VAL:HG12	1:283:A:PRO:HG2	1	0.11
(1,1506)	1:245:A:VAL:HG12	1:283:A:PRO:HG3	1	0.11
(1,1506)	1:245:A:VAL:HG13	1:283:A:PRO:HG2	1	0.11
(1,1506)	1:245:A:VAL:HG13	1:283:A:PRO:HG3	1	0.11
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE1	15	0.11
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE2	15	0.11
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE3	15	0.11
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE1	17	0.11
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE2	17	0.11
(1,1465)	1:243:A:ASP:H	1:241:A:MET:HE3	17	0.11
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE1	14	0.11
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE2	14	0.11
(1,1430)	1:241:A:MET:H	1:241:A:MET:HE3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1418)	1:240:A:LEU:HD21	1:303:A:PRO:HA	12	0.11
(1,1418)	1:240:A:LEU:HD22	1:303:A:PRO:HA	12	0.11
(1,1418)	1:240:A:LEU:HD23	1:303:A:PRO:HA	12	0.11
(1,1374)	1:238:A:LEU:H	1:237:A:SER:HB2	9	0.11
(1,1374)	1:238:A:LEU:H	1:237:A:SER:HB3	9	0.11
(1,1374)	1:238:A:LEU:H	1:237:A:SER:HB2	12	0.11
(1,1374)	1:238:A:LEU:H	1:237:A:SER:HB3	12	0.11
(1,1341)	1:236:A:ILE:H	1:253:A:TYR:HE1	14	0.11
(1,1341)	1:236:A:ILE:H	1:253:A:TYR:HE2	14	0.11
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD2	8	0.11
(1,1276)	1:232:A:PHE:HZ	1:229:A:PRO:HD3	8	0.11
(1,1252)	1:232:A:PHE:HB3	1:228:A:ILE:HB	6	0.11
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	1	0.11
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	12	0.11
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	13	0.11
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	14	0.11
(1,1190)	1:228:A:ILE:H	1:228:A:ILE:HD11	12	0.11
(1,1190)	1:228:A:ILE:H	1:228:A:ILE:HD12	12	0.11
(1,1190)	1:228:A:ILE:H	1:228:A:ILE:HD13	12	0.11
(1,1124)	1:300:B:ILE:H	1:295:B:CYS:HB2	20	0.11
(1,1124)	1:300:B:ILE:H	1:295:B:CYS:HB3	20	0.11
(1,1122)	1:300:B:ILE:H	1:295:B:CYS:HB2	20	0.11
(1,1122)	1:300:B:ILE:H	1:295:B:CYS:HB3	20	0.11
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	11	0.11
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	11	0.11
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	11	0.11
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	9	0.11
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	13	0.11
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	20	0.11
(1,1073)	1:297:B:ALA:H	1:299:B:GLY:H	19	0.11
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD11	1	0.11
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD12	1	0.11
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD13	1	0.11
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD11	2	0.11
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD12	2	0.11
(1,1023)	1:294:B:TRP:HE1	1:228:B:ILE:HD13	2	0.11
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD11	19	0.11
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD12	19	0.11
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD13	19	0.11
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD21	19	0.11
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD22	19	0.11
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD23	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD11	19	0.11
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD12	19	0.11
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD13	19	0.11
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD21	19	0.11
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD22	19	0.11
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD23	19	0.11
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD11	19	0.11
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD12	19	0.11
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD13	19	0.11
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD21	19	0.11
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD22	19	0.11
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD23	19	0.11
(1,892)	1:285:B:PHE:HZ	1:250:B:GLY:HA2	15	0.11
(1,891)	1:285:B:PHE:HZ	1:250:B:GLY:HA3	19	0.11
(1,881)	1:285:B:PHE:HD1	1:285:B:PHE:HA	16	0.11
(1,881)	1:285:B:PHE:HD2	1:285:B:PHE:HA	16	0.11
(1,861)	1:278:B:HIS:HD2	1:248:B:SER:H	12	0.11
(1,861)	1:278:B:HIS:HD2	1:248:B:SER:H	13	0.11
(1,861)	1:278:B:HIS:HD2	1:248:B:SER:H	17	0.11
(1,822)	1:274:B:GLN:H	1:272:B:THR:HA	20	0.11
(1,811)	1:273:B:GLN:H	1:269:B:CYS:HB2	10	0.11
(1,811)	1:273:B:GLN:H	1:269:B:CYS:HB3	10	0.11
(1,810)	1:273:B:GLN:H	1:268:B:THR:HB	8	0.11
(1,810)	1:273:B:GLN:H	1:268:B:THR:HB	15	0.11
(1,757)	1:269:B:CYS:H	1:274:B:GLN:HG3	4	0.11
(1,757)	1:269:B:CYS:H	1:274:B:GLN:HG3	15	0.11
(1,757)	1:269:B:CYS:H	1:274:B:GLN:HG3	16	0.11
(1,749)	1:269:B:CYS:H	1:275:B:PRO:HB2	9	0.11
(1,749)	1:269:B:CYS:H	1:275:B:PRO:HB2	15	0.11
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG21	19	0.11
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG22	19	0.11
(1,744)	1:269:B:CYS:H	1:268:B:THR:HG23	19	0.11
(1,717)	1:266:B:HIS:HD2	1:265:B:GLY:HA2	13	0.11
(1,702)	1:266:B:HIS:H	1:266:B:HIS:HB3	1	0.11
(1,702)	1:266:B:HIS:H	1:266:B:HIS:HB3	10	0.11
(1,702)	1:266:B:HIS:H	1:266:B:HIS:HB3	12	0.11
(1,670)	1:263:B:ASP:H	1:259:B:GLN:HE22	13	0.11
(1,623)	1:261:B:TRP:HZ2	1:268:B:THR:HB	17	0.11
(1,608)	1:261:B:TRP:HE1	1:270:B:PRO:HB2	12	0.11
(1,452)	1:253:B:TYR:HE1	1:247:B:VAL:HB	19	0.11
(1,452)	1:253:B:TYR:HE2	1:247:B:VAL:HB	19	0.11
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG21	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG22	5	0.11
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG23	5	0.11
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG21	11	0.11
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG22	11	0.11
(1,426)	1:251:B:GLN:HA	1:272:B:THR:HG23	11	0.11
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB2	11	0.11
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB3	11	0.11
(1,393)	1:249:B:SER:H	1:251:B:GLN:HE21	5	0.11
(1,343)	1:245:B:VAL:HG11	1:255:B:ARG:HA	20	0.11
(1,343)	1:245:B:VAL:HG12	1:255:B:ARG:HA	20	0.11
(1,343)	1:245:B:VAL:HG13	1:255:B:ARG:HA	20	0.11
(1,259)	1:241:B:MET:H	1:241:B:MET:HB2	15	0.11
(1,180)	1:236:B:ILE:H	1:253:B:TYR:HE1	1	0.11
(1,180)	1:236:B:ILE:H	1:253:B:TYR:HE2	1	0.11
(1,137)	1:233:B:ARG:HG2	1:240:B:LEU:HA	2	0.11
(1,137)	1:233:B:ARG:HG3	1:240:B:LEU:HA	2	0.11
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	3	0.11
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	17	0.11
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	19	0.11
(1,2377)	1:285:B:PHE:HZ	1:250:A:GLY:HA3	16	0.1
(1,2365)	1:246:B:ILE:HD11	1:282:A:THR:HB	8	0.1
(1,2365)	1:246:B:ILE:HD12	1:282:A:THR:HB	8	0.1
(1,2365)	1:246:B:ILE:HD13	1:282:A:THR:HB	8	0.1
(1,2337)	1:246:A:ILE:HD11	1:282:B:THR:HB	18	0.1
(1,2337)	1:246:A:ILE:HD12	1:282:B:THR:HB	18	0.1
(1,2337)	1:246:A:ILE:HD13	1:282:B:THR:HB	18	0.1
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	3	0.1
(1,2245)	1:298:A:ASN:H	1:298:A:ASN:HB3	17	0.1
(1,2235)	1:297:A:ALA:H	1:299:A:GLY:H	16	0.1
(1,2199)	1:294:A:TRP:HH2	1:228:A:ILE:HB	2	0.1
(1,2199)	1:294:A:TRP:HH2	1:228:A:ILE:HB	7	0.1
(1,2199)	1:294:A:TRP:HH2	1:228:A:ILE:HB	17	0.1
(1,2185)	1:294:A:TRP:HE1	1:228:A:ILE:HD11	6	0.1
(1,2185)	1:294:A:TRP:HE1	1:228:A:ILE:HD12	6	0.1
(1,2185)	1:294:A:TRP:HE1	1:228:A:ILE:HD13	6	0.1
(1,2161)	1:293:A:GLN:H	1:292:A:SER:HA	19	0.1
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD11	8	0.1
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD12	8	0.1
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD13	8	0.1
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD21	8	0.1
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD22	8	0.1
(1,2135)	1:291:A:ILE:HD11	1:302:A:LEU:HD23	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD11	8	0.1
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD12	8	0.1
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD13	8	0.1
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD21	8	0.1
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD22	8	0.1
(1,2135)	1:291:A:ILE:HD12	1:302:A:LEU:HD23	8	0.1
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD11	8	0.1
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD12	8	0.1
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD13	8	0.1
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD21	8	0.1
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD22	8	0.1
(1,2135)	1:291:A:ILE:HD13	1:302:A:LEU:HD23	8	0.1
(1,2022)	1:278:A:HIS:HD2	1:248:A:SER:H	3	0.1
(1,2010)	1:276:A:LEU:H	1:275:A:PRO:HB2	3	0.1
(1,1931)	1:270:A:PRO:HD3	1:258:A:ILE:HD11	5	0.1
(1,1931)	1:270:A:PRO:HD3	1:258:A:ILE:HD12	5	0.1
(1,1931)	1:270:A:PRO:HD3	1:258:A:ILE:HD13	5	0.1
(1,1917)	1:269:A:CYS:HB2	1:274:A:GLN:HE21	15	0.1
(1,1917)	1:269:A:CYS:HB3	1:274:A:GLN:HE21	15	0.1
(1,1863)	1:266:A:HIS:H	1:266:A:HIS:HB3	11	0.1
(1,1863)	1:266:A:HIS:H	1:266:A:HIS:HB3	15	0.1
(1,1678)	1:258:A:ILE:H	1:258:A:ILE:HD11	12	0.1
(1,1678)	1:258:A:ILE:H	1:258:A:ILE:HD12	12	0.1
(1,1678)	1:258:A:ILE:H	1:258:A:ILE:HD13	12	0.1
(1,1613)	1:253:A:TYR:HE1	1:247:A:VAL:HB	5	0.1
(1,1613)	1:253:A:TYR:HE2	1:247:A:VAL:HB	5	0.1
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG21	11	0.1
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG22	11	0.1
(1,1566)	1:250:A:GLY:H	1:282:A:THR:HG23	11	0.1
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB2	2	0.1
(1,1558)	1:249:A:SER:HB3	1:269:A:CYS:HB3	2	0.1
(1,1546)	1:249:A:SER:H	1:249:A:SER:HB3	17	0.1
(1,1522)	1:246:A:ILE:HG12	1:284:A:ASN:HA	20	0.1
(1,1522)	1:246:A:ILE:HG13	1:284:A:ASN:HA	20	0.1
(1,1420)	1:241:A:MET:H	1:241:A:MET:HB2	18	0.1
(1,1351)	1:237:A:SER:H	1:236:A:ILE:HA	9	0.1
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG12	5	0.1
(1,1265)	1:232:A:PHE:HD1	1:291:A:ILE:HG13	5	0.1
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG12	5	0.1
(1,1265)	1:232:A:PHE:HD2	1:291:A:ILE:HG13	5	0.1
(1,1260)	1:232:A:PHE:HA	1:303:A:PRO:HD3	6	0.1
(1,1260)	1:232:A:PHE:HA	1:303:A:PRO:HD3	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1260)	1:232:A:PHE:HA	1:303:A:PRO:HD3	18	0.1
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	2	0.1
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	3	0.1
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	10	0.1
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	17	0.1
(1,1235)	1:232:A:PHE:H	1:232:A:PHE:HB3	20	0.1
(1,1124)	1:300:B:ILE:H	1:295:B:CYS:HB2	10	0.1
(1,1124)	1:300:B:ILE:H	1:295:B:CYS:HB3	10	0.1
(1,1122)	1:300:B:ILE:H	1:295:B:CYS:HB2	10	0.1
(1,1122)	1:300:B:ILE:H	1:295:B:CYS:HB3	10	0.1
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD11	6	0.1
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD12	6	0.1
(1,1110)	1:300:B:ILE:H	1:300:B:ILE:HD13	6	0.1
(1,1085)	1:298:B:ASN:H	1:298:B:ASN:HD21	4	0.1
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	6	0.1
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	11	0.1
(1,1083)	1:298:B:ASN:H	1:298:B:ASN:HB3	18	0.1
(1,1028)	1:294:B:TRP:HD1	1:232:B:PHE:HE1	13	0.1
(1,1028)	1:294:B:TRP:HD1	1:232:B:PHE:HE2	13	0.1
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD11	13	0.1
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD12	13	0.1
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD13	13	0.1
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD21	13	0.1
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD22	13	0.1
(1,973)	1:291:B:ILE:HD11	1:302:B:LEU:HD23	13	0.1
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD11	13	0.1
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD12	13	0.1
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD13	13	0.1
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD21	13	0.1
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD22	13	0.1
(1,973)	1:291:B:ILE:HD12	1:302:B:LEU:HD23	13	0.1
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD11	13	0.1
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD12	13	0.1
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD13	13	0.1
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD21	13	0.1
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD22	13	0.1
(1,973)	1:291:B:ILE:HD13	1:302:B:LEU:HD23	13	0.1
(1,890)	1:285:B:PHE:HB2	1:283:B:PRO:HG2	8	0.1
(1,890)	1:285:B:PHE:HB2	1:283:B:PRO:HG3	8	0.1
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD2	11	0.1
(1,889)	1:285:B:PHE:H	1:283:B:PRO:HD3	11	0.1
(1,881)	1:285:B:PHE:HD1	1:285:B:PHE:HA	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,881)	1:285:B:PHE:HD2	1:285:B:PHE:HA	9	0.1
(1,881)	1:285:B:PHE:HD1	1:285:B:PHE:HA	19	0.1
(1,881)	1:285:B:PHE:HD2	1:285:B:PHE:HA	19	0.1
(1,811)	1:273:B:GLN:H	1:269:B:CYS:HB2	17	0.1
(1,811)	1:273:B:GLN:H	1:269:B:CYS:HB3	17	0.1
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD11	6	0.1
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD12	6	0.1
(1,770)	1:270:B:PRO:HD3	1:258:B:ILE:HD13	6	0.1
(1,757)	1:269:B:CYS:H	1:274:B:GLN:HG3	2	0.1
(1,749)	1:269:B:CYS:H	1:275:B:PRO:HB2	8	0.1
(1,608)	1:261:B:TRP:HE1	1:270:B:PRO:HB2	5	0.1
(1,608)	1:261:B:TRP:HE1	1:270:B:PRO:HB2	7	0.1
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB2	10	0.1
(1,397)	1:249:B:SER:HB3	1:269:B:CYS:HB3	10	0.1
(1,269)	1:241:B:MET:H	1:241:B:MET:HE1	1	0.1
(1,269)	1:241:B:MET:H	1:241:B:MET:HE2	1	0.1
(1,269)	1:241:B:MET:H	1:241:B:MET:HE3	1	0.1
(1,259)	1:241:B:MET:H	1:241:B:MET:HB2	6	0.1
(1,190)	1:237:B:SER:H	1:236:B:ILE:HA	4	0.1
(1,167)	1:236:B:ILE:H	1:236:B:ILE:HB	7	0.1
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG12	1	0.1
(1,104)	1:232:B:PHE:HD1	1:291:B:ILE:HG13	1	0.1
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG12	1	0.1
(1,104)	1:232:B:PHE:HD2	1:291:B:ILE:HG13	1	0.1
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	12	0.1
(1,74)	1:232:B:PHE:H	1:232:B:PHE:HB3	16	0.1
(1,41)	1:228:B:ILE:H	1:227:B:ILE:HG21	14	0.1
(1,41)	1:228:B:ILE:H	1:227:B:ILE:HG22	14	0.1
(1,41)	1:228:B:ILE:H	1:227:B:ILE:HG23	14	0.1

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found