



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 02:37 pm BST

PDB ID : 6FGS  
BMRB ID : 34233  
Title : Solution structure of p300Taz2-p73TA1  
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Deposited on : 2018-01-11

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Percentile statistics : 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) : 2.33

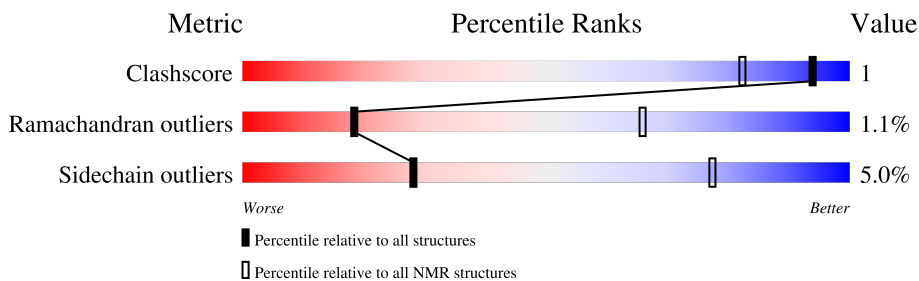
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 78%.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	130	

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 5 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:7-A:90, (103)	A:111-A:129 0.85	5

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 3 clusters and 5 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1915 atoms, of which 948 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone acetyltransferase p300,Tumor protein p73.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	130	1912	587	948	186	181	10	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	CYS	conflict	UNP Q09472
A	24	ALA	CYS	conflict	UNP Q09472
A	67	ALA	CYS	conflict	UNP Q09472
A	68	ALA	CYS	conflict	UNP Q09472
A	91	GLY	-	linker	UNP Q09472
A	92	GLY	-	linker	UNP Q09472
A	93	SER	-	linker	UNP Q09472
A	94	GLY	-	linker	UNP Q09472
A	95	GLY	-	linker	UNP Q09472
A	96	GLY	-	linker	UNP Q09472
A	97	THR	-	linker	UNP Q09472
A	98	GLY	-	linker	UNP Q09472
A	99	GLY	-	linker	UNP Q09472
A	100	GLY	-	linker	UNP Q09472
A	101	SER	-	linker	UNP Q09472
A	102	GLY	-	linker	UNP Q09472
A	103	THR	-	linker	UNP Q09472
A	104	ILE	-	linker	UNP Q09472
A	105	GLU	-	linker	UNP Q09472
A	106	GLY	-	linker	UNP Q09472
A	107	ARG	-	linker	UNP Q09472
A	108	GLY	-	linker	UNP Q09472

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

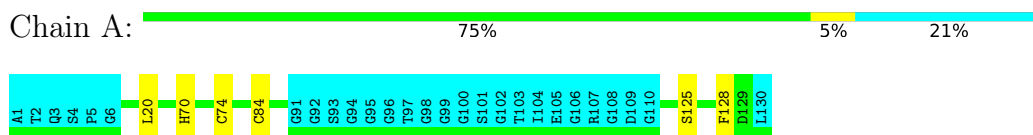
Mol	Chain	Residues	Atoms	
2	A	3	Total	Zn
			3	3

## 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: Histone acetyltransferase p300,Tumor protein p73

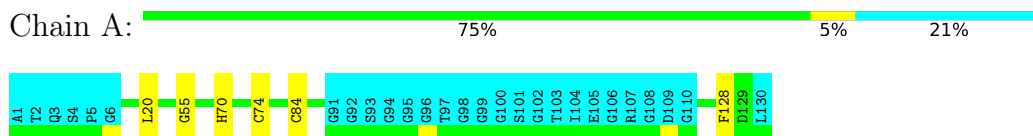


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

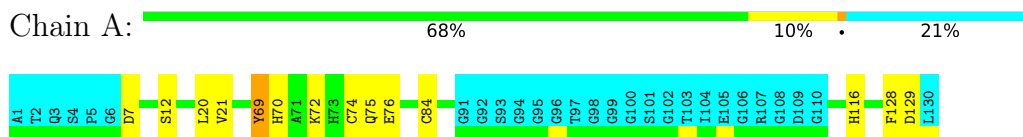
#### 4.2.1 Score per residue for model 1

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



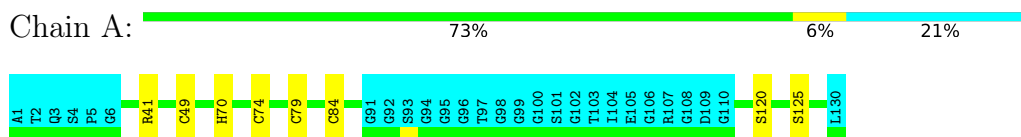
#### 4.2.2 Score per residue for model 2

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



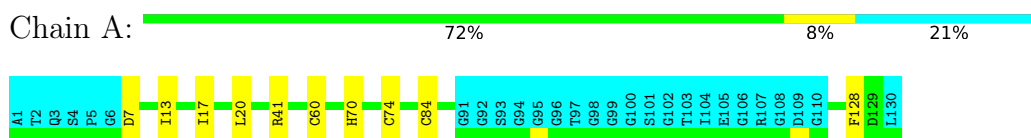
### 4.2.3 Score per residue for model 3

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



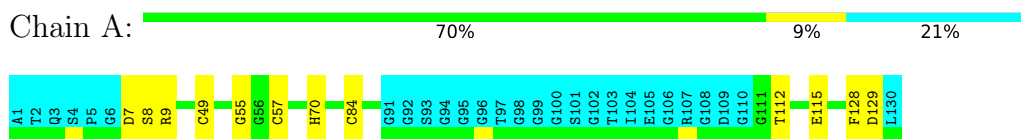
### 4.2.4 Score per residue for model 4

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



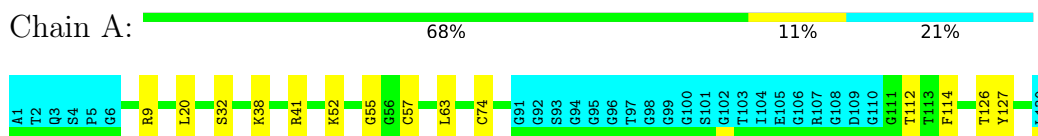
### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



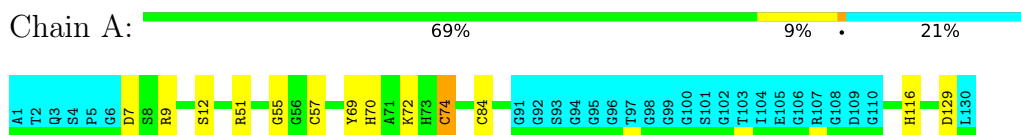
### 4.2.6 Score per residue for model 6

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



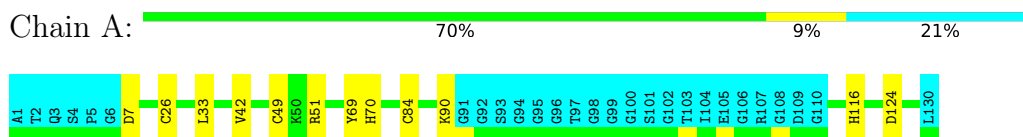
### 4.2.7 Score per residue for model 7

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



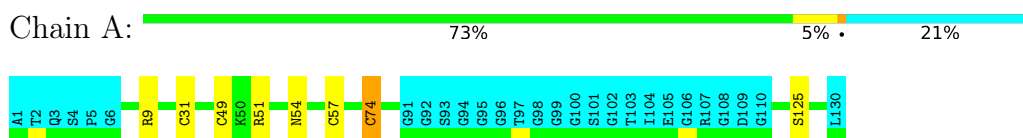
#### 4.2.8 Score per residue for model 8

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



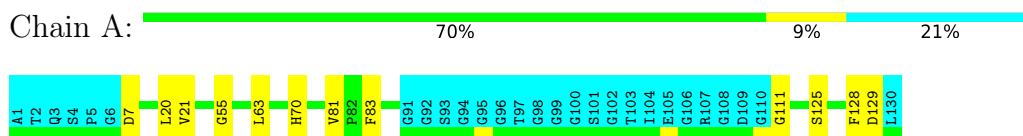
#### 4.2.9 Score per residue for model 9

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



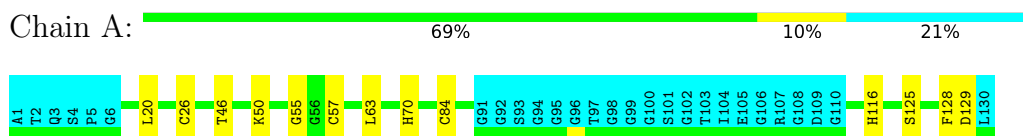
#### 4.2.10 Score per residue for model 10

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



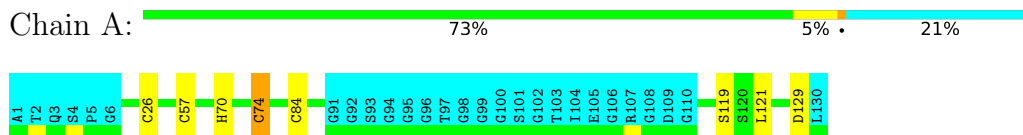
#### 4.2.11 Score per residue for model 11

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



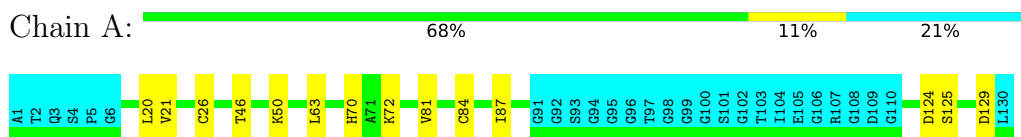
#### 4.2.12 Score per residue for model 12

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



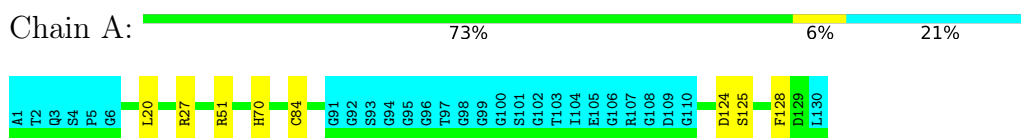
#### 4.2.13 Score per residue for model 13

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



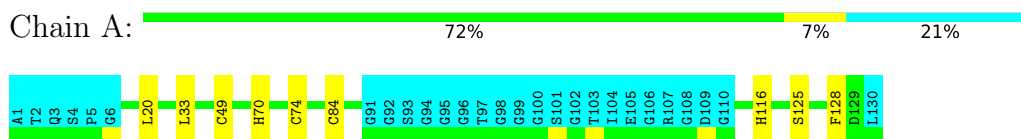
#### 4.2.14 Score per residue for model 14

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



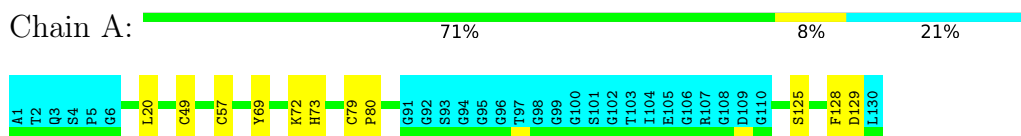
#### 4.2.15 Score per residue for model 15

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



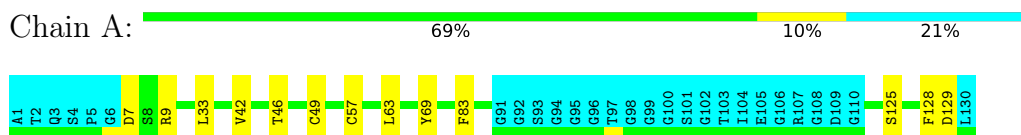
#### 4.2.16 Score per residue for model 16

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



#### 4.2.17 Score per residue for model 17

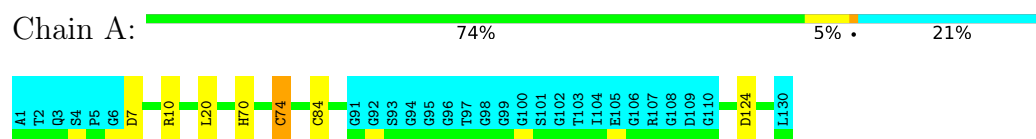
- Molecule 1: Histone acetyltransferase p300,Tumor protein p73





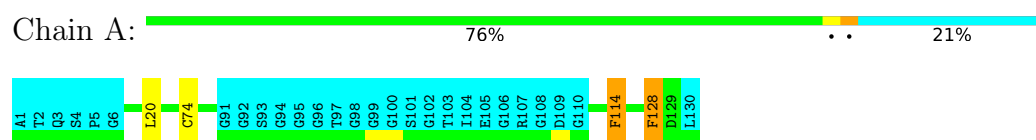
#### 4.2.18 Score per residue for model 18

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



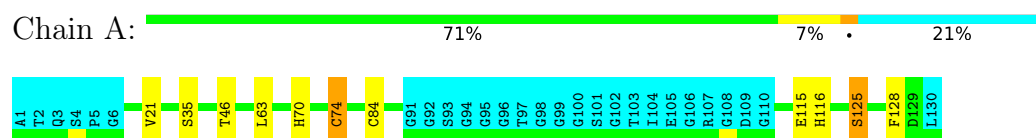
#### 4.2.19 Score per residue for model 19

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



#### 4.2.20 Score per residue for model 20

- Molecule 1: Histone acetyltransferase p300,Tumor protein p73



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	3.9
OPAL	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	1280
Number of shifts mapped to atoms	1280
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

## 6 Model quality i

### 6.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.54±0.01	0±0/825 ( 0.0± 0.0%)	0.97±0.02	1±1/1111 ( 0.0± 0.1%)
All	All	0.54	0/16500 ( 0.0%)	0.97	11/22220 ( 0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.4±1.2
All	All	0	29

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	51	ARG	NE-CZ-NH2	-6.55	117.03	120.30	7	4
1	A	69	TYR	CB-CG-CD2	-5.55	117.67	121.00	2	1
1	A	41	ARG	NE-CZ-NH2	-5.48	117.56	120.30	3	1
1	A	9	ARG	NE-CZ-NH2	-5.28	117.66	120.30	6	2
1	A	51	ARG	NE-CZ-NH1	5.15	122.88	120.30	7	1
1	A	74	CYS	CA-CB-SG	-5.03	104.95	114.00	9	1
1	A	10	ARG	NE-CZ-NH2	-5.02	117.79	120.30	18	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	129	ASP	Sidechain	8
1	A	69	TYR	Sidechain	5
1	A	7	ASP	Sidechain	4
1	A	9	ARG	Sidechain	3
1	A	115	GLU	Sidechain	2
1	A	50	LYS	Mainchain	2
1	A	76	GLU	Sidechain	1
1	A	54	ASN	Mainchain	1
1	A	124	ASP	Sidechain	1
1	A	114	PHE	Sidechain	1
1	A	128	PHE	Mainchain	1

## 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	808	808	808	2±1
All	All	16220	16160	16160	39

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:THR:HG21	1:A:63:LEU:HD22	0.69	1.61	17	4
1:A:21:VAL:HG21	1:A:70:HIS:CE1	0.57	2.34	10	2
1:A:20:LEU:HD11	1:A:63:LEU:CD1	0.55	2.32	6	1
1:A:70:HIS:CE1	1:A:74:CYS:SG	0.53	3.01	20	9
1:A:42:VAL:O	1:A:46:THR:HG23	0.52	2.05	17	1
1:A:70:HIS:CD2	1:A:84:CYS:SG	0.51	3.04	4	14
1:A:63:LEU:HD23	1:A:83:PHE:CD2	0.50	2.42	17	2
1:A:72:LYS:HZ3	1:A:73:HIS:CE1	0.49	2.25	16	1
1:A:13:ILE:HG22	1:A:17:ILE:CD1	0.43	2.43	4	1
1:A:21:VAL:HG23	1:A:81:VAL:HG21	0.41	1.91	10	2
1:A:79:CYS:SG	1:A:80:PRO:HD2	0.41	2.56	16	1
1:A:21:VAL:HG11	1:A:70:HIS:CG	0.40	2.51	2	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	103/130 (79%)	95±2 (92±2%)	7±3 (7±2%)	1±1 (1±1%)	18	66
All	All	2060/2600 (79%)	1897 (92%)	141 (7%)	22 (1%)	18	66

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	125	SER	8
1	A	55	GLY	6
1	A	26	CYS	4
1	A	7	ASP	1
1	A	75	GLN	1
1	A	111	GLY	1
1	A	49	CYS	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	91/104 (88%)	86±2 (95±2%)	5±2 (5±2%)	28	77
All	All	1820/2080 (88%)	1729 (95%)	91 (5%)	28	77

All 33 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	128	PHE	12
1	A	20	LEU	11
1	A	57	CYS	8

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Mol	Chain	Res	Type	Models (Total)
1	A	74	CYS	7
1	A	116	HIS	6
1	A	49	CYS	6
1	A	72	LYS	3
1	A	33	LEU	3
1	A	124	ASP	3
1	A	7	ASP	3
1	A	125	SER	3
1	A	12	SER	2
1	A	41	ARG	2
1	A	112	THR	2
1	A	114	PHE	2
1	A	79	CYS	1
1	A	120	SER	1
1	A	60	CYS	1
1	A	8	SER	1
1	A	32	SER	1
1	A	38	LYS	1
1	A	52	LYS	1
1	A	126	THR	1
1	A	127	TYR	1
1	A	42	VAL	1
1	A	90	LYS	1
1	A	31	CYS	1
1	A	129	ASP	1
1	A	119	SER	1
1	A	121	LEU	1
1	A	87	ILE	1
1	A	27	ARG	1
1	A	35	SER	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 77% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping i

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

Total number of shifts	1280
Number of shifts mapped to atoms	1280
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	130	$-0.34 \pm 0.09$	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	113	$0.18 \pm 0.08$	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	118	$-0.22 \pm 0.24$	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 78%, i.e. 1102 atoms were assigned a chemical shift out of a possible 1405. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	391/509 (77%)	193/205 (94%)	103/206 (50%)	95/98 (97%)
Sidechain	623/796 (78%)	415/514 (81%)	208/241 (86%)	0/41 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	88/100 (88%)	39/49 (80%)	38/40 (95%)	11/11 (100%)
Overall	1102/1405 (78%)	647/768 (84%)	349/487 (72%)	106/150 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1279 atoms were assigned a chemical shift out of a possible 1656. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	494/655 (75%)	246/271 (91%)	130/260 (50%)	118/124 (95%)
Sidechain	697/901 (77%)	463/582 (80%)	234/274 (85%)	0/45 (0%)
Aromatic	88/100 (88%)	39/49 (80%)	38/40 (95%)	11/11 (100%)
Overall	1279/1656 (77%)	748/902 (83%)	402/574 (70%)	129/180 (72%)

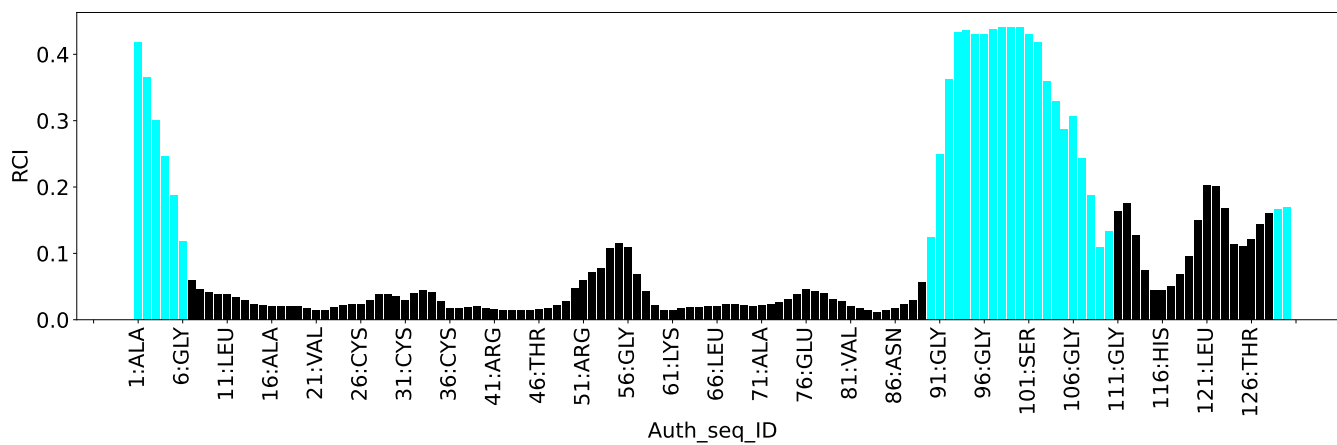
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1518
Intra-residue ( $ i-j =0$ )	354
Sequential ( $ i-j =1$ )	456
Medium range ( $ i-j >1$ and $ i-j <5$ )	373
Long range ( $ i-j \geq 5$ )	283
Inter-chain	0
Hydrogen bond restraints	52
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	11.7
Number of long range restraints per residue <sup>1</sup>	2.2

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	4.6	0.2
0.2-0.5 (Medium)	1.6	0.48
>0.5 (Large)	None	None

### 8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis

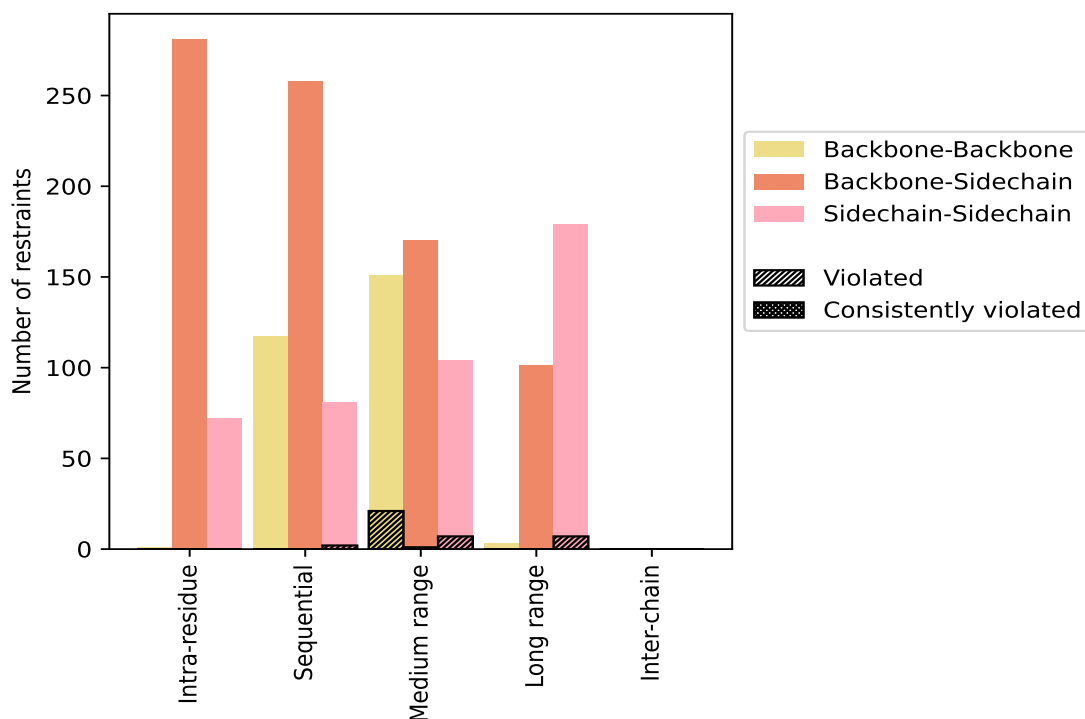
### 9.1 Summary of distance violations

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>354</b>	<b>23.3</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	281	18.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	72	4.7	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>456</b>	<b>30.0</b>	<b>2</b>	<b>0.4</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	117	7.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	258	17.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	81	5.3	2	2.5	0.1	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>373</b>	<b>24.6</b>	<b>8</b>	<b>2.1</b>	<b>0.5</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	99	6.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	170	11.2	1	0.6	0.1	0	0.0	0.0
Sidechain-Sidechain	104	6.9	7	6.7	0.5	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>283</b>	<b>18.6</b>	<b>7</b>	<b>2.5</b>	<b>0.5</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	101	6.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	179	11.8	7	3.9	0.5	0	0.0	0.0
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Hydrogen bond</b>	<b>52</b>	<b>3.4</b>	<b>21</b>	<b>40.4</b>	<b>1.4</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>1518</b>	<b>100.0</b>	<b>38</b>	<b>2.5</b>	<b>2.5</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	272	17.9	21	7.7	1.4	0	0.0	0.0
Backbone-Sidechain	810	53.4	1	0.1	0.1	0	0.0	0.0
Sidechain-Sidechain	436	28.7	16	3.7	1.1	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	0	0	3	0	0	3	0.19	0.25	0.06	0.2
2	0	1	1	0	0	2	0.12	0.12	0.0	0.12
3	0	1	7	2	0	10	0.18	0.44	0.1	0.13
4	0	1	2	1	0	4	0.12	0.14	0.01	0.12
5	0	1	5	1	0	7	0.19	0.35	0.09	0.19
6	0	1	5	1	0	7	0.18	0.3	0.06	0.19
7	0	0	6	1	0	7	0.21	0.41	0.13	0.12
8	0	1	5	1	0	7	0.19	0.39	0.1	0.13
9	0	0	6	1	0	7	0.13	0.17	0.02	0.12
10	0	1	0	1	0	2	0.12	0.12	0.0	0.12
11	0	0	4	1	0	5	0.17	0.28	0.07	0.12

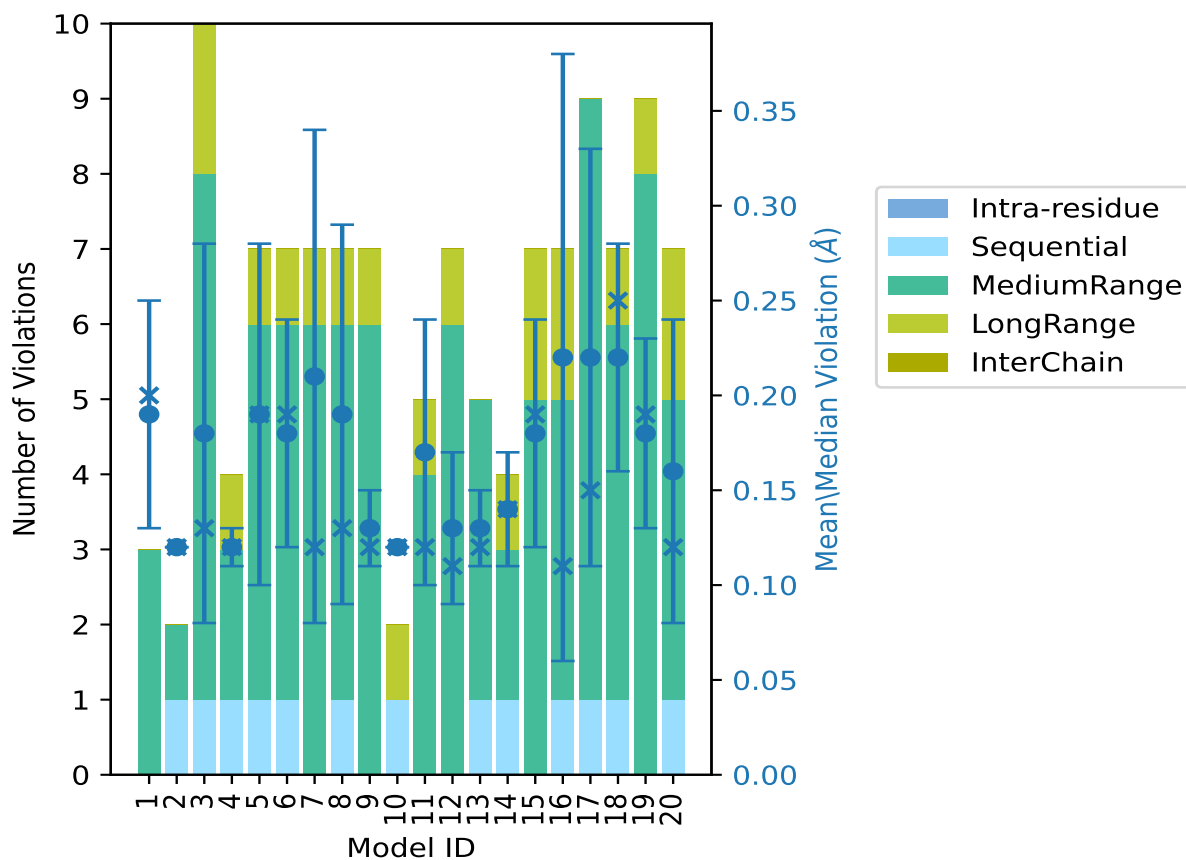
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>					
12	0	0	6	1	0	7	0.13	0.22	0.04	0.11
13	0	1	4	0	0	5	0.13	0.17	0.02	0.12
14	0	1	2	1	0	4	0.14	0.18	0.03	0.14
15	0	0	5	2	0	7	0.18	0.27	0.06	0.19
16	0	1	4	2	0	7	0.22	0.48	0.16	0.11
17	0	1	8	0	0	9	0.22	0.41	0.11	0.15
18	0	1	5	1	0	7	0.22	0.28	0.06	0.25
19	0	0	8	1	0	9	0.18	0.25	0.05	0.19
20	0	1	4	2	0	7	0.16	0.3	0.08	0.12

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

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



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

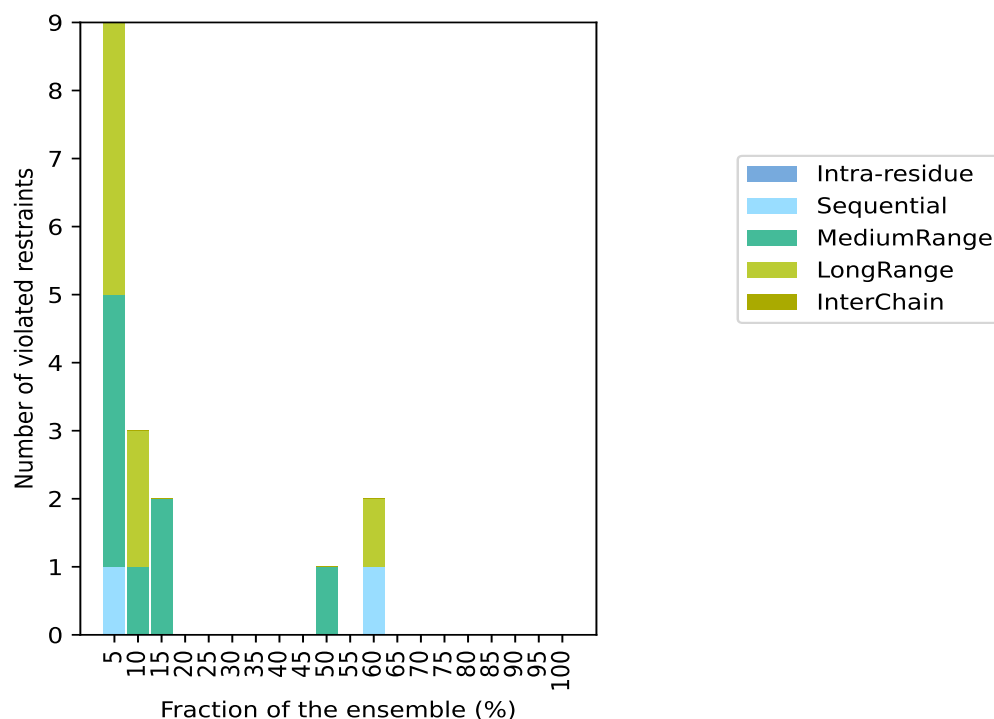
### 9.3 Distance violation statistics for the ensemble

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, 1449(IR:354, SQ:454, MR:365, LR:276, IC:0) restraints are not violated in the ensemble.

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

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

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

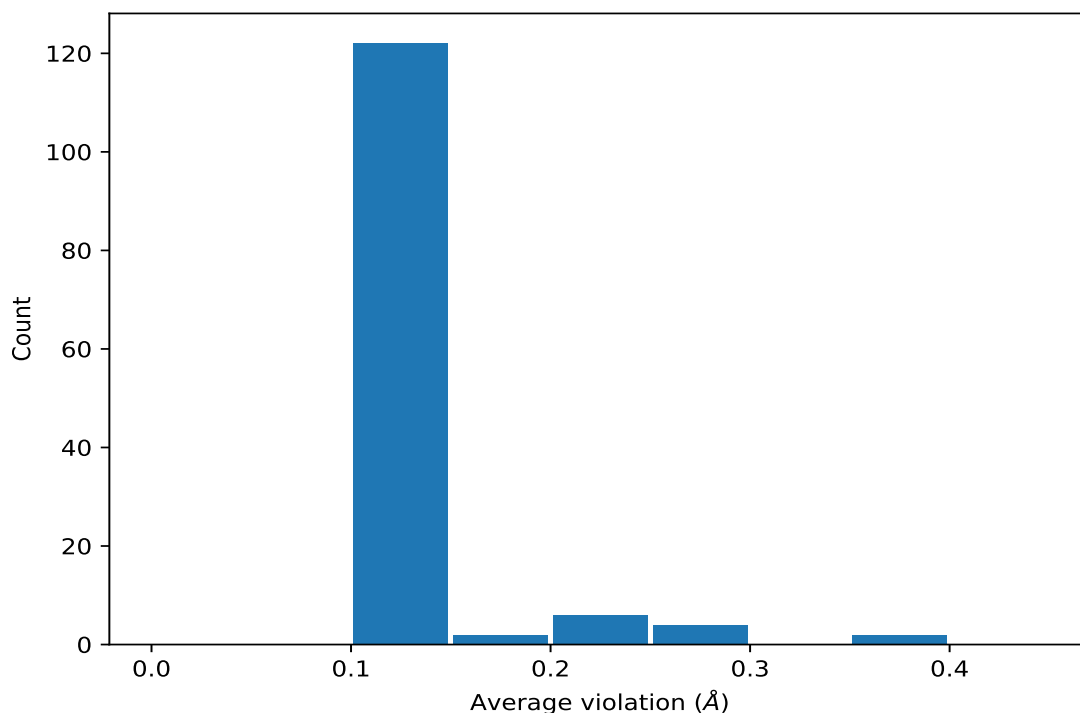


## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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





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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	12	0.25	0.09	0.24
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	12	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	12	0.12	0.01	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	12	0.12	0.01	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	12	0.12	0.01	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	12	0.12	0.01	0.11
(2,22)	1:A:18:GLN:O	1:A:22:HIS:N	10	0.21	0.08	0.2
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD11	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD12	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD13	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD21	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD22	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD23	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD11	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD12	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD13	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD21	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD22	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD23	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD11	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD12	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD13	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD21	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD22	10	0.12	0.01	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD23	10	0.12	0.01	0.12
(2,25)	1:A:20:LEU:O	1:A:24:ALA:H	9	0.24	0.1	0.2
(2,26)	1:A:20:LEU:O	1:A:24:ALA:N	4	0.2	0.05	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,15)	1:A:15:ARG:O	1:A:19:SER:H	4	0.16	0.03	0.16
(2,5)	1:A:10:ARG:O	1:A:14:GLN:H	4	0.15	0.04	0.14
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG11	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG12	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG13	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG21	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG22	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG23	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG11	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG12	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG13	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG21	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG22	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG23	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG11	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG12	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG13	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG21	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG22	3	0.12	0.0	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG23	3	0.12	0.0	0.12
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG21	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG22	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG23	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG21	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG22	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG23	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG21	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG22	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG23	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG21	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG22	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG23	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG21	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG22	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG23	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG21	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG22	3	0.11	0.0	0.11
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG23	3	0.11	0.0	0.11
(2,3)	1:A:9:ARG:O	1:A:13:ILE:H	2	0.39	0.09	0.39
(2,4)	1:A:9:ARG:O	1:A:13:ILE:N	2	0.36	0.09	0.36
(2,13)	1:A:14:GLN:O	1:A:18:GLN:H	2	0.28	0.01	0.28
(2,1)	1:A:8:SER:O	1:A:12:SER:H	2	0.26	0.15	0.26

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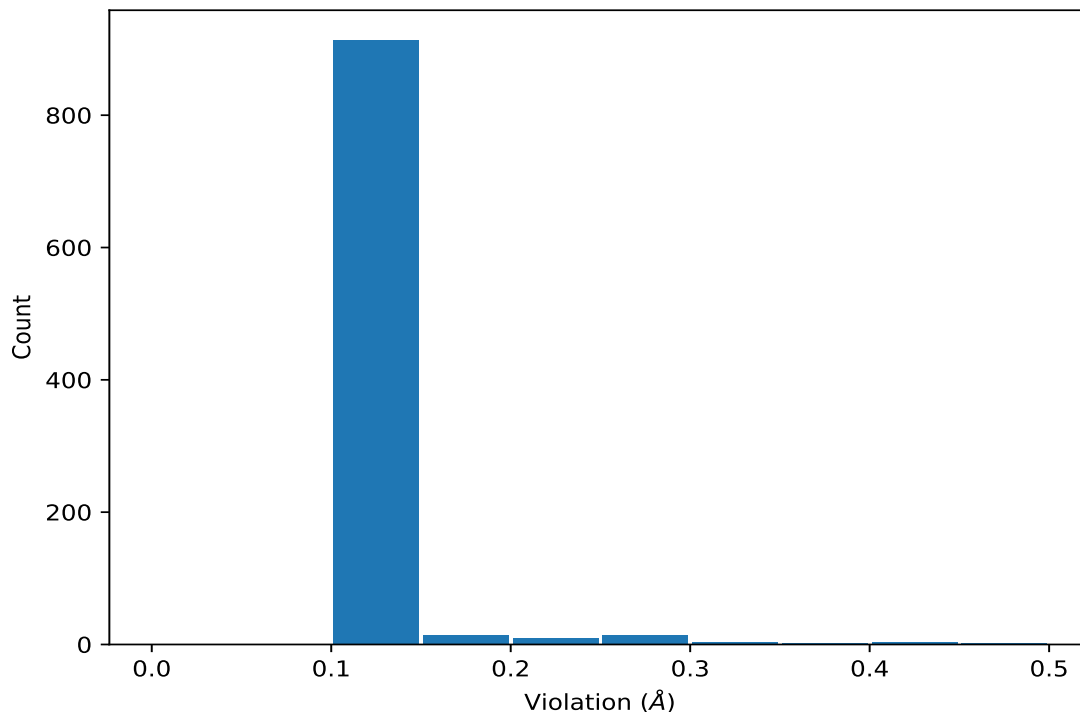
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,14)	1:A:14:GLN:O	1:A:18:GLN:N	2	0.26	0.01	0.26
(2,7)	1:A:11:LEU:O	1:A:15:ARG:H	2	0.2	0.06	0.2
(2,23)	1:A:19:SER:O	1:A:23:ALA:H	2	0.2	0.02	0.2
(2,24)	1:A:19:SER:O	1:A:23:ALA:N	2	0.2	0.01	0.2
(2,6)	1:A:10:ARG:O	1:A:14:GLN:N	2	0.16	0.05	0.16
(2,16)	1:A:15:ARG:O	1:A:19:SER:N	2	0.14	0.03	0.14
(1,190)	1:A:43:VAL:HG11	1:A:47:LYS:HE2	2	0.11	0.0	0.11
(1,190)	1:A:43:VAL:HG11	1:A:47:LYS:HE3	2	0.11	0.0	0.11
(1,190)	1:A:43:VAL:HG12	1:A:47:LYS:HE2	2	0.11	0.0	0.11
(1,190)	1:A:43:VAL:HG12	1:A:47:LYS:HE3	2	0.11	0.0	0.11
(1,190)	1:A:43:VAL:HG13	1:A:47:LYS:HE2	2	0.11	0.0	0.11
(1,190)	1:A:43:VAL:HG13	1:A:47:LYS:HE3	2	0.11	0.0	0.11
(1,190)	1:A:43:VAL:HG21	1:A:47:LYS:HE2	2	0.11	0.0	0.11
(1,190)	1:A:43:VAL:HG21	1:A:47:LYS:HE3	2	0.11	0.0	0.11
(1,190)	1:A:43:VAL:HG22	1:A:47:LYS:HE2	2	0.11	0.0	0.11
(1,190)	1:A:43:VAL:HG22	1:A:47:LYS:HE3	2	0.11	0.0	0.11
(1,190)	1:A:43:VAL:HG23	1:A:47:LYS:HE2	2	0.11	0.0	0.11
(1,190)	1:A:43:VAL:HG23	1:A:47:LYS:HE3	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD11	1:A:127:TYR:HD1	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD11	1:A:127:TYR:HD2	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD12	1:A:127:TYR:HD1	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD12	1:A:127:TYR:HD2	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD13	1:A:127:TYR:HD1	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD13	1:A:127:TYR:HD2	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD21	1:A:127:TYR:HD1	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD21	1:A:127:TYR:HD2	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD22	1:A:127:TYR:HD1	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD22	1:A:127:TYR:HD2	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD23	1:A:127:TYR:HD1	2	0.11	0.0	0.11
(1,1151)	1:A:121:LEU:HD23	1:A:127:TYR:HD2	2	0.11	0.0	0.11
(1,1283)	1:A:17:ILE:HG21	1:A:69:TYR:HD1	2	0.11	0.0	0.11
(1,1283)	1:A:17:ILE:HG21	1:A:69:TYR:HD2	2	0.11	0.0	0.11
(1,1283)	1:A:17:ILE:HG22	1:A:69:TYR:HD1	2	0.11	0.0	0.11
(1,1283)	1:A:17:ILE:HG22	1:A:69:TYR:HD2	2	0.11	0.0	0.11
(1,1283)	1:A:17:ILE:HG23	1:A:69:TYR:HD1	2	0.11	0.0	0.11
(1,1283)	1:A:17:ILE:HG23	1:A:69:TYR:HD2	2	0.11	0.0	0.11

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

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

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:A:9:ARG:O	1:A:13:ILE:H	16	0.48
(2,4)	1:A:9:ARG:O	1:A:13:ILE:N	16	0.45
(2,25)	1:A:20:LEU:O	1:A:24:ALA:H	3	0.44
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	17	0.41
(2,1)	1:A:8:SER:O	1:A:12:SER:H	7	0.41
(2,2)	1:A:8:SER:O	1:A:12:SER:N	7	0.4
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	8	0.39
(2,25)	1:A:20:LEU:O	1:A:24:ALA:H	17	0.36
(2,22)	1:A:18:GLN:O	1:A:22:HIS:N	17	0.35
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:A:18:GLN:O	1:A:22:HIS:N	8	0.32
(2,3)	1:A:9:ARG:O	1:A:13:ILE:H	20	0.3
(2,25)	1:A:20:LEU:O	1:A:24:ALA:H	6	0.3
(2,26)	1:A:20:LEU:O	1:A:24:ALA:N	3	0.29
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	11	0.28
(2,13)	1:A:14:GLN:O	1:A:18:GLN:H	18	0.28
(2,4)	1:A:9:ARG:O	1:A:13:ILE:N	20	0.27
(2,22)	1:A:18:GLN:O	1:A:22:HIS:N	5	0.27
(2,14)	1:A:14:GLN:O	1:A:18:GLN:N	18	0.27
(2,13)	1:A:14:GLN:O	1:A:18:GLN:H	15	0.27
(2,7)	1:A:11:LEU:O	1:A:15:ARG:H	18	0.26
(2,8)	1:A:11:LEU:O	1:A:15:ARG:N	18	0.25
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	1	0.25
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	19	0.25
(2,14)	1:A:14:GLN:O	1:A:18:GLN:N	15	0.25
(2,5)	1:A:10:ARG:O	1:A:14:GLN:H	6	0.22
(2,25)	1:A:20:LEU:O	1:A:24:ALA:H	19	0.22
(2,23)	1:A:19:SER:O	1:A:23:ALA:H	19	0.22
(2,22)	1:A:18:GLN:O	1:A:22:HIS:N	11	0.22
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	12	0.22
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	7	0.21
(2,6)	1:A:10:ARG:O	1:A:14:GLN:N	6	0.2
(2,25)	1:A:20:LEU:O	1:A:24:ALA:H	5	0.2
(2,24)	1:A:19:SER:O	1:A:23:ALA:N	19	0.2
(2,22)	1:A:18:GLN:O	1:A:22:HIS:N	1	0.2
(2,26)	1:A:20:LEU:O	1:A:24:ALA:N	6	0.19
(2,25)	1:A:20:LEU:O	1:A:24:ALA:H	18	0.19
(2,24)	1:A:19:SER:O	1:A:23:ALA:N	15	0.19
(2,23)	1:A:19:SER:O	1:A:23:ALA:H	15	0.19
(2,22)	1:A:18:GLN:O	1:A:22:HIS:N	19	0.19
(2,15)	1:A:15:ARG:O	1:A:19:SER:H	5	0.19
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	14	0.18
(2,15)	1:A:15:ARG:O	1:A:19:SER:H	3	0.18
(2,26)	1:A:20:LEU:O	1:A:24:ALA:N	17	0.17
(2,25)	1:A:20:LEU:O	1:A:24:ALA:H	13	0.17
(2,22)	1:A:18:GLN:O	1:A:22:HIS:N	14	0.17
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	9	0.17
(2,16)	1:A:15:ARG:O	1:A:19:SER:N	3	0.17
(2,26)	1:A:20:LEU:O	1:A:24:ALA:N	19	0.16
(2,9)	1:A:12:SER:O	1:A:16:ALA:H	8	0.15
(2,7)	1:A:11:LEU:O	1:A:15:ARG:H	17	0.15
(2,5)	1:A:10:ARG:O	1:A:14:GLN:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:A:18:GLN:O	1:A:22:HIS:N	12	0.15
(2,15)	1:A:15:ARG:O	1:A:19:SER:H	17	0.15
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	16	0.15
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	16	0.15
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	16	0.15
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	16	0.15
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	16	0.15
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	16	0.15
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	16	0.15
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	16	0.15
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	16	0.15
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	16	0.15
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	16	0.15
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	16	0.15
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	16	0.15
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	16	0.15
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	16	0.15
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	16	0.15
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	16	0.15
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	16	0.15
(2,25)	1:A:20:LEU:O	1:A:24:ALA:H	4	0.14
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	3	0.14
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	18	0.14
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	18	0.14
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	18	0.14
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	18	0.14
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	18	0.14
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	18	0.14
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	18	0.14
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	18	0.14
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	18	0.14
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	18	0.14
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	18	0.14
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	18	0.14
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	18	0.14
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	18	0.14
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	18	0.14
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	18	0.14
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	18	0.14
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	18	0.14
(2,5)	1:A:10:ARG:O	1:A:14:GLN:H	17	0.13
(2,10)	1:A:12:SER:O	1:A:16:ALA:N	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD11	6	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD12	6	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD13	6	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD21	6	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD22	6	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD23	6	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD11	6	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD12	6	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD13	6	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD21	6	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD22	6	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD23	6	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD11	6	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD12	6	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD13	6	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD21	6	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD22	6	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD23	6	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD11	8	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD12	8	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD13	8	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD21	8	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD22	8	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD23	8	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD11	8	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD12	8	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD13	8	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD21	8	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD22	8	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD23	8	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD11	8	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD12	8	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD13	8	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD21	8	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD22	8	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD23	8	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD11	13	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD12	13	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD13	13	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD21	13	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD22	13	0.13
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD23	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD11	13	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD12	13	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD13	13	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD21	13	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD22	13	0.13
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD23	13	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD11	13	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD12	13	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD13	13	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD21	13	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD22	13	0.13
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD23	13	0.13
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	18	0.13
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	18	0.13
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	18	0.13
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	18	0.13
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	18	0.13
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	18	0.13
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	18	0.13
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	18	0.13
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	18	0.13
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	18	0.13
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	18	0.13
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	18	0.13
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	18	0.13
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	18	0.13
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	18	0.13
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	18	0.13
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	18	0.13
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	18	0.13
(2,22)	1:A:18:GLN:O	1:A:22:HIS:N	9	0.12
(2,15)	1:A:15:ARG:O	1:A:19:SER:H	13	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD11	9	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD12	9	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD13	9	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD21	9	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD22	9	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD23	9	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD11	9	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD12	9	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD13	9	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD21	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD22	9	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD23	9	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD11	9	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD12	9	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD13	9	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD21	9	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD22	9	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD23	9	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD11	11	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD12	11	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD13	11	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD21	11	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD22	11	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD23	11	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD11	11	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD12	11	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD13	11	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD21	11	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD22	11	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD23	11	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD11	11	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD12	11	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD13	11	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD21	11	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD22	11	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD23	11	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD11	19	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD12	19	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD13	19	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD21	19	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD22	19	0.12
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD23	19	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD11	19	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD12	19	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD13	19	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD21	19	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD22	19	0.12
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD23	19	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD11	19	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD12	19	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD13	19	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD21	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD22	19	0.12
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD23	19	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	3	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	3	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	3	0.12
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	3	0.12
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	3	0.12
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	3	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	3	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	3	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	3	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	3	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	3	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	3	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	3	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	3	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	3	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	3	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	3	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	3	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	6	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	6	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	6	0.12
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	6	0.12
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	6	0.12
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	6	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	6	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	6	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	6	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	6	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	6	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	6	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	6	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	6	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	6	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	6	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	6	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	6	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	8	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	8	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	8	0.12
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	8	0.12
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	8	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	8	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	8	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	8	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	8	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	8	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	8	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	8	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	8	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	8	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	8	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	8	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	8	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	20	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	20	0.12
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	20	0.12
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	20	0.12
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	20	0.12
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	20	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	20	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	20	0.12
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	20	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	20	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	20	0.12
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	20	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	20	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	20	0.12
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	20	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	20	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	20	0.12
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	20	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	6	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	6	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	6	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	6	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	6	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	6	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	6	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	6	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	6	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	6	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	6	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	6	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	6	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	6	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	6	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	6	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	6	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	7	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	7	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	7	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	7	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	7	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	7	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	7	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	7	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	7	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	7	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	7	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	7	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	7	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	7	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	7	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	7	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	7	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	7	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	8	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	8	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	8	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	8	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	8	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	8	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	8	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	8	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	8	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	8	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	8	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	8	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	8	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	8	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	8	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	8	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	8	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	9	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	9	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	9	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	9	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	9	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	9	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	9	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	9	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	9	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	9	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	9	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	9	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	9	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	9	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	9	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	9	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	9	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	9	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	10	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	10	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	10	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	10	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	10	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	10	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	10	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	10	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	10	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	10	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	10	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	10	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	10	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	10	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	10	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	10	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	10	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	10	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	20	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	20	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	20	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	20	0.12
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	20	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	20	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	20	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	20	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	20	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	20	0.12
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	20	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	20	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	20	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	20	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	20	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	20	0.12
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	20	0.12
(1,164)	1:A:10:ARG:HD2	1:A:11:LEU:HD11	4	0.12
(1,164)	1:A:10:ARG:HD2	1:A:11:LEU:HD12	4	0.12
(1,164)	1:A:10:ARG:HD2	1:A:11:LEU:HD13	4	0.12
(1,164)	1:A:10:ARG:HD2	1:A:11:LEU:HD21	4	0.12
(1,164)	1:A:10:ARG:HD2	1:A:11:LEU:HD22	4	0.12
(1,164)	1:A:10:ARG:HD2	1:A:11:LEU:HD23	4	0.12
(1,164)	1:A:10:ARG:HD3	1:A:11:LEU:HD11	4	0.12
(1,164)	1:A:10:ARG:HD3	1:A:11:LEU:HD12	4	0.12
(1,164)	1:A:10:ARG:HD3	1:A:11:LEU:HD13	4	0.12
(1,164)	1:A:10:ARG:HD3	1:A:11:LEU:HD21	4	0.12
(1,164)	1:A:10:ARG:HD3	1:A:11:LEU:HD22	4	0.12
(1,164)	1:A:10:ARG:HD3	1:A:11:LEU:HD23	4	0.12
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG21	12	0.12
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG22	12	0.12
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG23	12	0.12
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG21	12	0.12
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG22	12	0.12
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG23	12	0.12
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG21	12	0.12
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG22	12	0.12
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG23	12	0.12
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG21	12	0.12
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG22	12	0.12
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG23	12	0.12
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG21	12	0.12
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG22	12	0.12
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG23	12	0.12
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG21	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG22	12	0.12
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG23	12	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG11	2	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG12	2	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG13	2	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG21	2	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG22	2	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG23	2	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG11	2	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG12	2	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG13	2	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG21	2	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG22	2	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG23	2	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG11	2	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG12	2	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG13	2	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG21	2	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG22	2	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG23	2	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG11	20	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG12	20	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG13	20	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG21	20	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG22	20	0.12
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG23	20	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG11	20	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG12	20	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG13	20	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG21	20	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG22	20	0.12
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG23	20	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG11	20	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG12	20	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG13	20	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG21	20	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG22	20	0.12
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG23	20	0.12
(2,6)	1:A:10:ARG:O	1:A:14:GLN:N	9	0.11
(2,5)	1:A:10:ARG:O	1:A:14:GLN:H	11	0.11
(2,25)	1:A:20:LEU:O	1:A:24:ALA:H	7	0.11
(2,22)	1:A:18:GLN:O	1:A:22:HIS:N	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:A:18:GLN:O	1:A:22:HIS:H	15	0.11
(2,17)	1:A:16:ALA:O	1:A:20:LEU:H	4	0.11
(2,16)	1:A:15:ARG:O	1:A:19:SER:N	13	0.11
(2,1)	1:A:8:SER:O	1:A:12:SER:H	3	0.11
(1,702)	1:A:21:VAL:HG11	1:A:25:GLN:H	12	0.11
(1,702)	1:A:21:VAL:HG12	1:A:25:GLN:H	12	0.11
(1,702)	1:A:21:VAL:HG13	1:A:25:GLN:H	12	0.11
(1,702)	1:A:21:VAL:HG21	1:A:25:GLN:H	12	0.11
(1,702)	1:A:21:VAL:HG22	1:A:25:GLN:H	12	0.11
(1,702)	1:A:21:VAL:HG23	1:A:25:GLN:H	12	0.11
(1,384)	1:A:23:ALA:HB1	1:A:43:VAL:HG11	20	0.11
(1,384)	1:A:23:ALA:HB1	1:A:43:VAL:HG12	20	0.11
(1,384)	1:A:23:ALA:HB1	1:A:43:VAL:HG13	20	0.11
(1,384)	1:A:23:ALA:HB1	1:A:43:VAL:HG21	20	0.11
(1,384)	1:A:23:ALA:HB1	1:A:43:VAL:HG22	20	0.11
(1,384)	1:A:23:ALA:HB1	1:A:43:VAL:HG23	20	0.11
(1,384)	1:A:23:ALA:HB2	1:A:43:VAL:HG11	20	0.11
(1,384)	1:A:23:ALA:HB2	1:A:43:VAL:HG12	20	0.11
(1,384)	1:A:23:ALA:HB2	1:A:43:VAL:HG13	20	0.11
(1,384)	1:A:23:ALA:HB2	1:A:43:VAL:HG21	20	0.11
(1,384)	1:A:23:ALA:HB2	1:A:43:VAL:HG22	20	0.11
(1,384)	1:A:23:ALA:HB2	1:A:43:VAL:HG23	20	0.11
(1,384)	1:A:23:ALA:HB3	1:A:43:VAL:HG11	20	0.11
(1,384)	1:A:23:ALA:HB3	1:A:43:VAL:HG12	20	0.11
(1,384)	1:A:23:ALA:HB3	1:A:43:VAL:HG13	20	0.11
(1,384)	1:A:23:ALA:HB3	1:A:43:VAL:HG21	20	0.11
(1,384)	1:A:23:ALA:HB3	1:A:43:VAL:HG22	20	0.11
(1,384)	1:A:23:ALA:HB3	1:A:43:VAL:HG23	20	0.11
(1,343)	1:A:7:ASP:HB2	1:A:11:LEU:HD11	1	0.11
(1,343)	1:A:7:ASP:HB2	1:A:11:LEU:HD12	1	0.11
(1,343)	1:A:7:ASP:HB2	1:A:11:LEU:HD13	1	0.11
(1,343)	1:A:7:ASP:HB2	1:A:11:LEU:HD21	1	0.11
(1,343)	1:A:7:ASP:HB2	1:A:11:LEU:HD22	1	0.11
(1,343)	1:A:7:ASP:HB2	1:A:11:LEU:HD23	1	0.11
(1,343)	1:A:7:ASP:HB3	1:A:11:LEU:HD11	1	0.11
(1,343)	1:A:7:ASP:HB3	1:A:11:LEU:HD12	1	0.11
(1,343)	1:A:7:ASP:HB3	1:A:11:LEU:HD13	1	0.11
(1,343)	1:A:7:ASP:HB3	1:A:11:LEU:HD21	1	0.11
(1,343)	1:A:7:ASP:HB3	1:A:11:LEU:HD22	1	0.11
(1,343)	1:A:7:ASP:HB3	1:A:11:LEU:HD23	1	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD11	5	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD12	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD13	5	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD21	5	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD22	5	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD23	5	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD11	5	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD12	5	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD13	5	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD21	5	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD22	5	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD23	5	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD11	5	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD12	5	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD13	5	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD21	5	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD22	5	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD23	5	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD11	16	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD12	16	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD13	16	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD21	16	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD22	16	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD23	16	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD11	16	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD12	16	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD13	16	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD21	16	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD22	16	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD23	16	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD11	16	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD12	16	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD13	16	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD21	16	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD22	16	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD23	16	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD11	17	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD12	17	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD13	17	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD21	17	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD22	17	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD23	17	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD11	17	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD12	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD13	17	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD21	17	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD22	17	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD23	17	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD11	17	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD12	17	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD13	17	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD21	17	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD22	17	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD23	17	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD11	20	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD12	20	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD13	20	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD21	20	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD22	20	0.11
(1,330)	1:A:59:ILE:HG21	1:A:63:LEU:HD23	20	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD11	20	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD12	20	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD13	20	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD21	20	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD22	20	0.11
(1,330)	1:A:59:ILE:HG22	1:A:63:LEU:HD23	20	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD11	20	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD12	20	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD13	20	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD21	20	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD22	20	0.11
(1,330)	1:A:59:ILE:HG23	1:A:63:LEU:HD23	20	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	2	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	2	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	2	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	2	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	2	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	2	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	2	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	2	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	2	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	2	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	2	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	2	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	2	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	2	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	2	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	2	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	2	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	5	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	5	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	5	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	5	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	5	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	5	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	5	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	5	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	5	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	5	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	5	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	5	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	5	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	5	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	5	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	5	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	5	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	5	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	10	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	10	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	10	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	10	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	10	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	10	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	10	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	10	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	10	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	10	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	10	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	10	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	10	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	10	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	10	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	10	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	10	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	10	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	13	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	13	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	13	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	13	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	13	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	13	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	13	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	13	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	13	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	13	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	13	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	13	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	13	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	13	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	13	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	13	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	13	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	14	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	14	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	14	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	14	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	14	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	14	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	14	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	14	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	14	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	14	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	14	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	14	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	14	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	14	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	14	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	14	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	14	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	14	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	16	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	16	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	16	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	16	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	16	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	16	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	16	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	16	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	16	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	16	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	16	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	16	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	16	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	16	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	16	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	16	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	16	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD11	17	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD12	17	0.11
(1,329)	1:A:63:LEU:HD11	1:A:64:ILE:HD13	17	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD11	17	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD12	17	0.11
(1,329)	1:A:63:LEU:HD12	1:A:64:ILE:HD13	17	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD11	17	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD12	17	0.11
(1,329)	1:A:63:LEU:HD13	1:A:64:ILE:HD13	17	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD11	17	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD12	17	0.11
(1,329)	1:A:63:LEU:HD21	1:A:64:ILE:HD13	17	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD11	17	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD12	17	0.11
(1,329)	1:A:63:LEU:HD22	1:A:64:ILE:HD13	17	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD11	17	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD12	17	0.11
(1,329)	1:A:63:LEU:HD23	1:A:64:ILE:HD13	17	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	4	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	4	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	4	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	4	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	4	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	4	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	4	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	4	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	4	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	4	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	4	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	4	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	4	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	4	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	4	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	4	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	4	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	5	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	5	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	5	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	5	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	5	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	5	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	5	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	5	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	5	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	5	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	5	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	5	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	5	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	5	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	5	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	5	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	5	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	5	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	15	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	15	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	15	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	15	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	15	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	15	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	15	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	15	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	15	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	15	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	15	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	15	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	15	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	15	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	15	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	15	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	15	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	15	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD11	19	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD12	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD13	19	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD21	19	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD22	19	0.11
(1,315)	1:A:24:ALA:HB1	1:A:63:LEU:HD23	19	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD11	19	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD12	19	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD13	19	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD21	19	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD22	19	0.11
(1,315)	1:A:24:ALA:HB2	1:A:63:LEU:HD23	19	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD11	19	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD12	19	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD13	19	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD21	19	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD22	19	0.11
(1,315)	1:A:24:ALA:HB3	1:A:63:LEU:HD23	19	0.11
(1,190)	1:A:43:VAL:HG11	1:A:47:LYS:HE2	7	0.11
(1,190)	1:A:43:VAL:HG11	1:A:47:LYS:HE3	7	0.11
(1,190)	1:A:43:VAL:HG12	1:A:47:LYS:HE2	7	0.11
(1,190)	1:A:43:VAL:HG12	1:A:47:LYS:HE3	7	0.11
(1,190)	1:A:43:VAL:HG13	1:A:47:LYS:HE2	7	0.11
(1,190)	1:A:43:VAL:HG13	1:A:47:LYS:HE3	7	0.11
(1,190)	1:A:43:VAL:HG21	1:A:47:LYS:HE2	7	0.11
(1,190)	1:A:43:VAL:HG21	1:A:47:LYS:HE3	7	0.11
(1,190)	1:A:43:VAL:HG22	1:A:47:LYS:HE2	7	0.11
(1,190)	1:A:43:VAL:HG22	1:A:47:LYS:HE3	7	0.11
(1,190)	1:A:43:VAL:HG23	1:A:47:LYS:HE2	7	0.11
(1,190)	1:A:43:VAL:HG23	1:A:47:LYS:HE3	7	0.11
(1,190)	1:A:43:VAL:HG11	1:A:47:LYS:HE2	9	0.11
(1,190)	1:A:43:VAL:HG11	1:A:47:LYS:HE3	9	0.11
(1,190)	1:A:43:VAL:HG12	1:A:47:LYS:HE2	9	0.11
(1,190)	1:A:43:VAL:HG12	1:A:47:LYS:HE3	9	0.11
(1,190)	1:A:43:VAL:HG13	1:A:47:LYS:HE2	9	0.11
(1,190)	1:A:43:VAL:HG13	1:A:47:LYS:HE3	9	0.11
(1,190)	1:A:43:VAL:HG21	1:A:47:LYS:HE2	9	0.11
(1,190)	1:A:43:VAL:HG21	1:A:47:LYS:HE3	9	0.11
(1,190)	1:A:43:VAL:HG22	1:A:47:LYS:HE2	9	0.11
(1,190)	1:A:43:VAL:HG22	1:A:47:LYS:HE3	9	0.11
(1,190)	1:A:43:VAL:HG23	1:A:47:LYS:HE2	9	0.11
(1,190)	1:A:43:VAL:HG23	1:A:47:LYS:HE3	9	0.11
(1,1455)	1:A:114:PHE:HD1	1:A:117:LEU:HD11	12	0.11
(1,1455)	1:A:114:PHE:HD1	1:A:117:LEU:HD12	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:A:114:PHE:HD1	1:A:117:LEU:HD13	12	0.11
(1,1455)	1:A:114:PHE:HD1	1:A:117:LEU:HD21	12	0.11
(1,1455)	1:A:114:PHE:HD1	1:A:117:LEU:HD22	12	0.11
(1,1455)	1:A:114:PHE:HD1	1:A:117:LEU:HD23	12	0.11
(1,1455)	1:A:114:PHE:HD2	1:A:117:LEU:HD11	12	0.11
(1,1455)	1:A:114:PHE:HD2	1:A:117:LEU:HD12	12	0.11
(1,1455)	1:A:114:PHE:HD2	1:A:117:LEU:HD13	12	0.11
(1,1455)	1:A:114:PHE:HD2	1:A:117:LEU:HD21	12	0.11
(1,1455)	1:A:114:PHE:HD2	1:A:117:LEU:HD22	12	0.11
(1,1455)	1:A:114:PHE:HD2	1:A:117:LEU:HD23	12	0.11
(1,1432)	1:A:80:PRO:HD2	1:A:85:LEU:HD11	3	0.11
(1,1432)	1:A:80:PRO:HD2	1:A:85:LEU:HD12	3	0.11
(1,1432)	1:A:80:PRO:HD2	1:A:85:LEU:HD13	3	0.11
(1,1432)	1:A:80:PRO:HD2	1:A:85:LEU:HD21	3	0.11
(1,1432)	1:A:80:PRO:HD2	1:A:85:LEU:HD22	3	0.11
(1,1432)	1:A:80:PRO:HD2	1:A:85:LEU:HD23	3	0.11
(1,1432)	1:A:80:PRO:HD3	1:A:85:LEU:HD11	3	0.11
(1,1432)	1:A:80:PRO:HD3	1:A:85:LEU:HD12	3	0.11
(1,1432)	1:A:80:PRO:HD3	1:A:85:LEU:HD13	3	0.11
(1,1432)	1:A:80:PRO:HD3	1:A:85:LEU:HD21	3	0.11
(1,1432)	1:A:80:PRO:HD3	1:A:85:LEU:HD22	3	0.11
(1,1432)	1:A:80:PRO:HD3	1:A:85:LEU:HD23	3	0.11
(1,1380)	1:A:42:VAL:HG11	1:A:128:PHE:HD1	3	0.11
(1,1380)	1:A:42:VAL:HG11	1:A:128:PHE:HD2	3	0.11
(1,1380)	1:A:42:VAL:HG12	1:A:128:PHE:HD1	3	0.11
(1,1380)	1:A:42:VAL:HG12	1:A:128:PHE:HD2	3	0.11
(1,1380)	1:A:42:VAL:HG13	1:A:128:PHE:HD1	3	0.11
(1,1380)	1:A:42:VAL:HG13	1:A:128:PHE:HD2	3	0.11
(1,1380)	1:A:42:VAL:HG21	1:A:128:PHE:HD1	3	0.11
(1,1380)	1:A:42:VAL:HG21	1:A:128:PHE:HD2	3	0.11
(1,1380)	1:A:42:VAL:HG22	1:A:128:PHE:HD1	3	0.11
(1,1380)	1:A:42:VAL:HG22	1:A:128:PHE:HD2	3	0.11
(1,1380)	1:A:42:VAL:HG23	1:A:128:PHE:HD1	3	0.11
(1,1380)	1:A:42:VAL:HG23	1:A:128:PHE:HD2	3	0.11
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG21	16	0.11
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG22	16	0.11
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG23	16	0.11
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG21	16	0.11
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG22	16	0.11
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG23	16	0.11
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG21	16	0.11
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG22	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG23	16	0.11
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG21	16	0.11
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG22	16	0.11
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG23	16	0.11
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG21	16	0.11
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG22	16	0.11
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG23	16	0.11
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG21	16	0.11
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG22	16	0.11
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG23	16	0.11
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG21	19	0.11
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG22	19	0.11
(1,1375)	1:A:42:VAL:HG11	1:A:46:THR:HG23	19	0.11
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG21	19	0.11
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG22	19	0.11
(1,1375)	1:A:42:VAL:HG12	1:A:46:THR:HG23	19	0.11
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG21	19	0.11
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG22	19	0.11
(1,1375)	1:A:42:VAL:HG13	1:A:46:THR:HG23	19	0.11
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG21	19	0.11
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG22	19	0.11
(1,1375)	1:A:42:VAL:HG21	1:A:46:THR:HG23	19	0.11
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG21	19	0.11
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG22	19	0.11
(1,1375)	1:A:42:VAL:HG22	1:A:46:THR:HG23	19	0.11
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG21	19	0.11
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG22	19	0.11
(1,1375)	1:A:42:VAL:HG23	1:A:46:THR:HG23	19	0.11
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG11	12	0.11
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG12	12	0.11
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG13	12	0.11
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG21	12	0.11
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG22	12	0.11
(1,1361)	1:A:39:MET:HE1	1:A:42:VAL:HG23	12	0.11
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG11	12	0.11
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG12	12	0.11
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG13	12	0.11
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG21	12	0.11
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG22	12	0.11
(1,1361)	1:A:39:MET:HE2	1:A:42:VAL:HG23	12	0.11
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG11	12	0.11
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG12	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG13	12	0.11
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG21	12	0.11
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG22	12	0.11
(1,1361)	1:A:39:MET:HE3	1:A:42:VAL:HG23	12	0.11
(1,1321)	1:A:20:LEU:HD11	1:A:24:ALA:HB1	3	0.11
(1,1321)	1:A:20:LEU:HD11	1:A:24:ALA:HB2	3	0.11
(1,1321)	1:A:20:LEU:HD11	1:A:24:ALA:HB3	3	0.11
(1,1321)	1:A:20:LEU:HD12	1:A:24:ALA:HB1	3	0.11
(1,1321)	1:A:20:LEU:HD12	1:A:24:ALA:HB2	3	0.11
(1,1321)	1:A:20:LEU:HD12	1:A:24:ALA:HB3	3	0.11
(1,1321)	1:A:20:LEU:HD13	1:A:24:ALA:HB1	3	0.11
(1,1321)	1:A:20:LEU:HD13	1:A:24:ALA:HB2	3	0.11
(1,1321)	1:A:20:LEU:HD13	1:A:24:ALA:HB3	3	0.11
(1,1321)	1:A:20:LEU:HD21	1:A:24:ALA:HB1	3	0.11
(1,1321)	1:A:20:LEU:HD21	1:A:24:ALA:HB2	3	0.11
(1,1321)	1:A:20:LEU:HD21	1:A:24:ALA:HB3	3	0.11
(1,1321)	1:A:20:LEU:HD22	1:A:24:ALA:HB1	3	0.11
(1,1321)	1:A:20:LEU:HD22	1:A:24:ALA:HB2	3	0.11
(1,1321)	1:A:20:LEU:HD22	1:A:24:ALA:HB3	3	0.11
(1,1321)	1:A:20:LEU:HD23	1:A:24:ALA:HB1	3	0.11
(1,1321)	1:A:20:LEU:HD23	1:A:24:ALA:HB2	3	0.11
(1,1321)	1:A:20:LEU:HD23	1:A:24:ALA:HB3	3	0.11
(1,1283)	1:A:17:ILE:HG21	1:A:69:TYR:HD1	12	0.11
(1,1283)	1:A:17:ILE:HG21	1:A:69:TYR:HD2	12	0.11
(1,1283)	1:A:17:ILE:HG22	1:A:69:TYR:HD1	12	0.11
(1,1283)	1:A:17:ILE:HG22	1:A:69:TYR:HD2	12	0.11
(1,1283)	1:A:17:ILE:HG23	1:A:69:TYR:HD1	12	0.11
(1,1283)	1:A:17:ILE:HG23	1:A:69:TYR:HD2	12	0.11
(1,1283)	1:A:17:ILE:HG21	1:A:69:TYR:HD1	15	0.11
(1,1283)	1:A:17:ILE:HG21	1:A:69:TYR:HD2	15	0.11
(1,1283)	1:A:17:ILE:HG22	1:A:69:TYR:HD1	15	0.11
(1,1283)	1:A:17:ILE:HG22	1:A:69:TYR:HD2	15	0.11
(1,1283)	1:A:17:ILE:HG23	1:A:69:TYR:HD1	15	0.11
(1,1283)	1:A:17:ILE:HG23	1:A:69:TYR:HD2	15	0.11
(1,1151)	1:A:121:LEU:HD11	1:A:127:TYR:HD1	14	0.11
(1,1151)	1:A:121:LEU:HD11	1:A:127:TYR:HD2	14	0.11
(1,1151)	1:A:121:LEU:HD12	1:A:127:TYR:HD1	14	0.11
(1,1151)	1:A:121:LEU:HD12	1:A:127:TYR:HD2	14	0.11
(1,1151)	1:A:121:LEU:HD13	1:A:127:TYR:HD1	14	0.11
(1,1151)	1:A:121:LEU:HD13	1:A:127:TYR:HD2	14	0.11
(1,1151)	1:A:121:LEU:HD21	1:A:127:TYR:HD1	14	0.11
(1,1151)	1:A:121:LEU:HD21	1:A:127:TYR:HD2	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:A:121:LEU:HD22	1:A:127:TYR:HD1	14	0.11
(1,1151)	1:A:121:LEU:HD22	1:A:127:TYR:HD2	14	0.11
(1,1151)	1:A:121:LEU:HD23	1:A:127:TYR:HD1	14	0.11
(1,1151)	1:A:121:LEU:HD23	1:A:127:TYR:HD2	14	0.11
(1,1151)	1:A:121:LEU:HD11	1:A:127:TYR:HD1	16	0.11
(1,1151)	1:A:121:LEU:HD11	1:A:127:TYR:HD2	16	0.11
(1,1151)	1:A:121:LEU:HD12	1:A:127:TYR:HD1	16	0.11
(1,1151)	1:A:121:LEU:HD12	1:A:127:TYR:HD2	16	0.11
(1,1151)	1:A:121:LEU:HD13	1:A:127:TYR:HD1	16	0.11
(1,1151)	1:A:121:LEU:HD13	1:A:127:TYR:HD2	16	0.11
(1,1151)	1:A:121:LEU:HD21	1:A:127:TYR:HD1	16	0.11
(1,1151)	1:A:121:LEU:HD21	1:A:127:TYR:HD2	16	0.11
(1,1151)	1:A:121:LEU:HD22	1:A:127:TYR:HD1	16	0.11
(1,1151)	1:A:121:LEU:HD22	1:A:127:TYR:HD2	16	0.11
(1,1151)	1:A:121:LEU:HD23	1:A:127:TYR:HD1	16	0.11
(1,1151)	1:A:121:LEU:HD23	1:A:127:TYR:HD2	16	0.11
(1,1143)	1:A:63:LEU:HD11	1:A:128:PHE:HE1	11	0.11
(1,1143)	1:A:63:LEU:HD11	1:A:128:PHE:HE2	11	0.11
(1,1143)	1:A:63:LEU:HD12	1:A:128:PHE:HE1	11	0.11
(1,1143)	1:A:63:LEU:HD12	1:A:128:PHE:HE2	11	0.11
(1,1143)	1:A:63:LEU:HD13	1:A:128:PHE:HE1	11	0.11
(1,1143)	1:A:63:LEU:HD13	1:A:128:PHE:HE2	11	0.11
(1,1143)	1:A:63:LEU:HD21	1:A:128:PHE:HE1	11	0.11
(1,1143)	1:A:63:LEU:HD21	1:A:128:PHE:HE2	11	0.11
(1,1143)	1:A:63:LEU:HD22	1:A:128:PHE:HE1	11	0.11
(1,1143)	1:A:63:LEU:HD22	1:A:128:PHE:HE2	11	0.11
(1,1143)	1:A:63:LEU:HD23	1:A:128:PHE:HE1	11	0.11
(1,1143)	1:A:63:LEU:HD23	1:A:128:PHE:HE2	11	0.11

## 10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value