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Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 07:57 pm BST

PDB ID	:	6SOW
BMRB ID	:	34430
Title	:	NMR solution structure of staphylococcal protein A, C domain
Authors	:	Backlund, S.M.; Iwai, H.
Deposited on	:	2019-08-30

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 96%.

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.
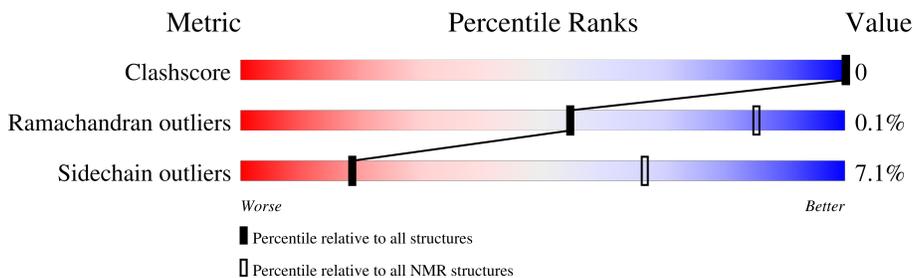
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	58	79% 5% 16%

2 Ensemble composition and analysis ⓘ

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:8-A:56 (49)	0.31	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 4 clusters and 6 single-model clusters were found.

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 930 atoms, of which 461 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Immunoglobulin G binding protein A.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	58	930	292	461	81	96	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q2UW48

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: Immunoglobulin G binding protein A

Chain A:
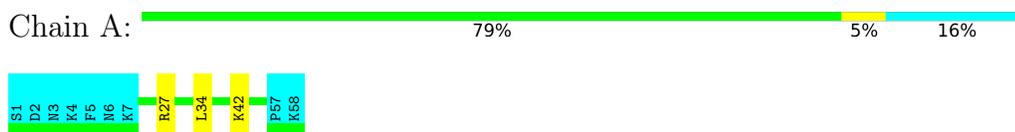
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
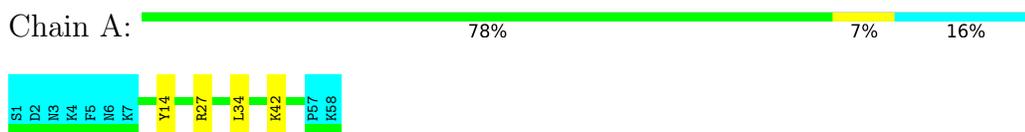
4.2.2 Score per residue for model 2

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
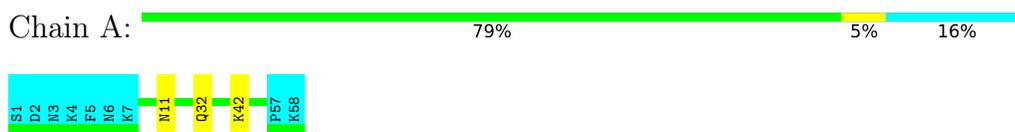
4.2.3 Score per residue for model 3

• Molecule 1: Immunoglobulin G binding protein A

Chain A: 78%   7%   16%

S1 D2 N3 K4 F5 N6 K7 Y14 R27 L34 K42 P57 K58
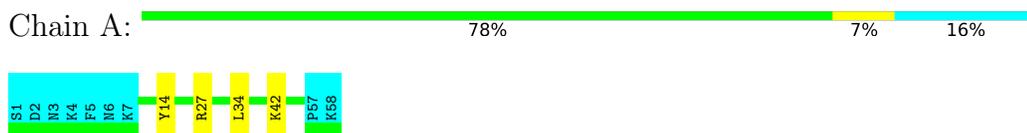
4.2.4 Score per residue for model 4

• Molecule 1: Immunoglobulin G binding protein A

Chain A: 78%   7%   16%

S1 D2 N3 K4 F5 N6 K7 R27 L34 K42 K50 P57 K58
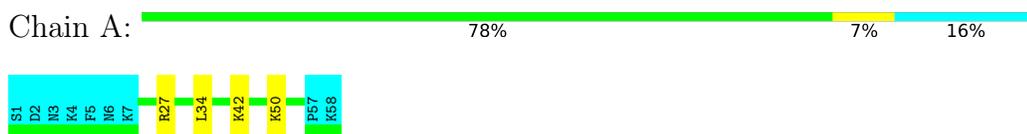
4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: Immunoglobulin G binding protein A

Chain A: 74%   10%   16%

S1 D2 N3 K4 F5 N6 K7 Y14 P20 R27 Q32 K42 K50 P57 K58
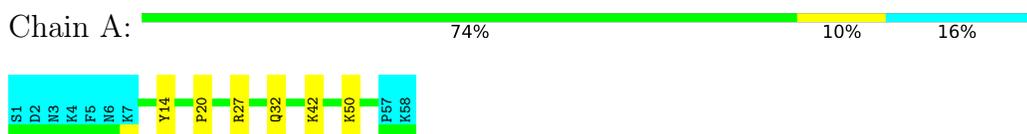
4.2.6 Score per residue for model 6

• Molecule 1: Immunoglobulin G binding protein A

Chain A: 76%   9%   16%

S1 D2 N3 K4 F5 N6 K7 R27 L34 K42 K50 L51 P57 K58
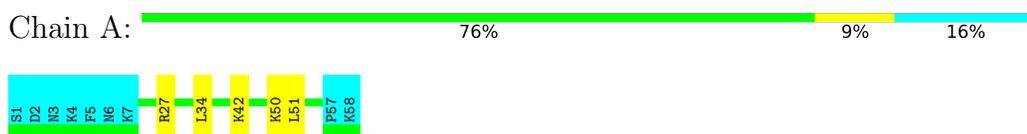
4.2.7 Score per residue for model 7

• Molecule 1: Immunoglobulin G binding protein A

Chain A: 78%   7%   16%

S1 D2 N3 K4 F5 N6 K7 H18 L34 K42 K50 P57 K58
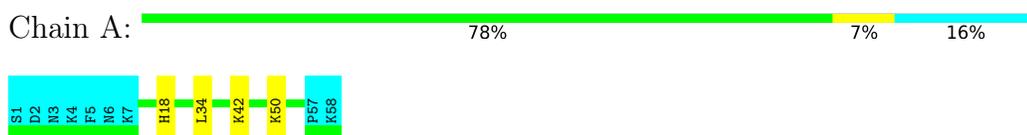
4.2.8 Score per residue for model 8

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
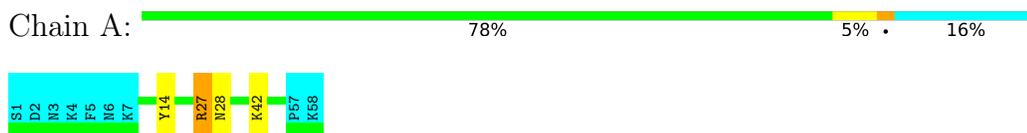
4.2.9 Score per residue for model 9

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
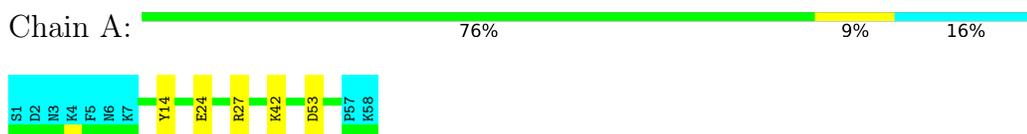
4.2.10 Score per residue for model 10

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
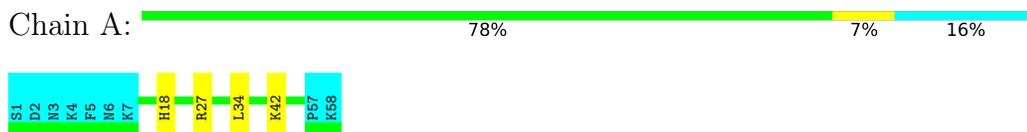
4.2.11 Score per residue for model 11

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
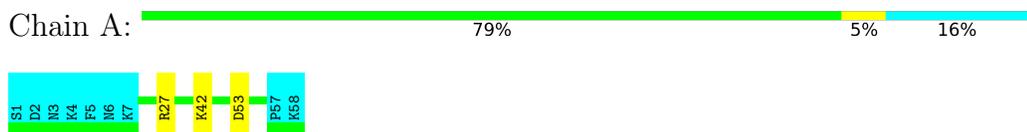
4.2.12 Score per residue for model 12

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
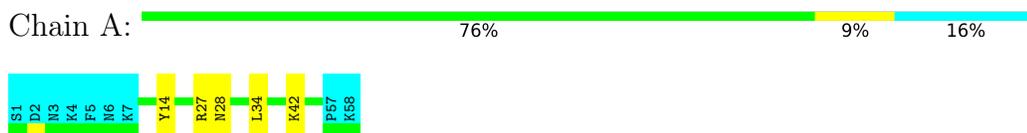
4.2.13　Score per residue for model 13

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
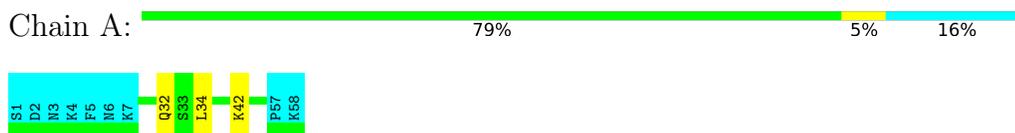
4.2.14　Score per residue for model 14

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
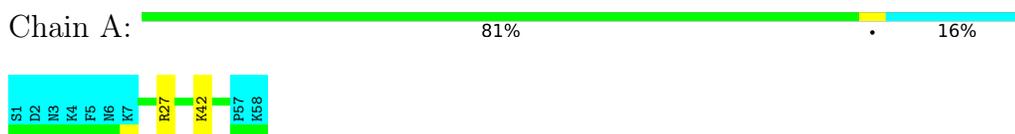
4.2.15　Score per residue for model 15

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
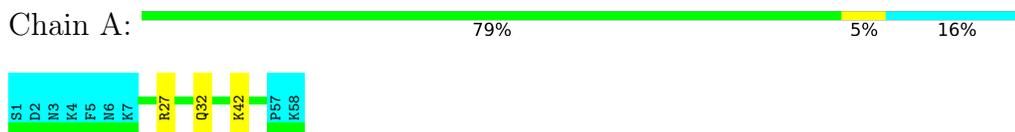
4.2.16　Score per residue for model 16

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
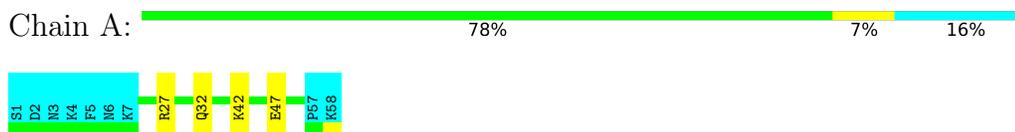
4.2.17　Score per residue for model 17

• Molecule 1: Immunoglobulin G binding protein A

Chain A:
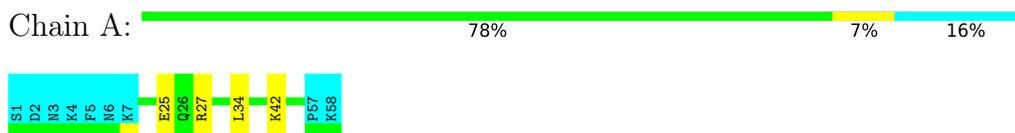
4.2.18 Score per residue for model 18

• Molecule 1: Immunoglobulin G binding protein A

Chain A:

74% 10% 16%

S1 D2 N3 K4 F5 N6 K7 R27 N28 G29 F30 I31 Q32 S33 L34 K42 P57 K58
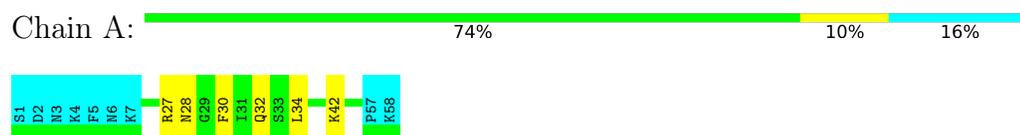
4.2.19 Score per residue for model 19

• Molecule 1: Immunoglobulin G binding protein A

Chain A:

78% 7% 16%

S1 D2 N3 K4 F5 N6 K7 R27 K42 K50 D53 P57 K58
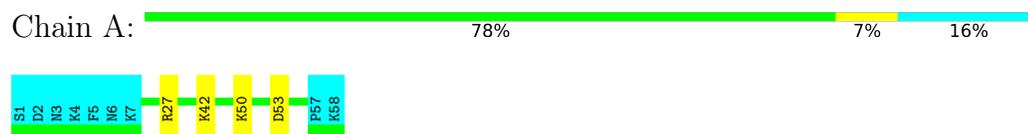
4.2.20 Score per residue for model 20

• Molecule 1: Immunoglobulin G binding protein A

Chain A:

78% 7% 16%

S1 D2 N3 K4 F5 N6 K7 R27 L34 S39 K42 P57 K58
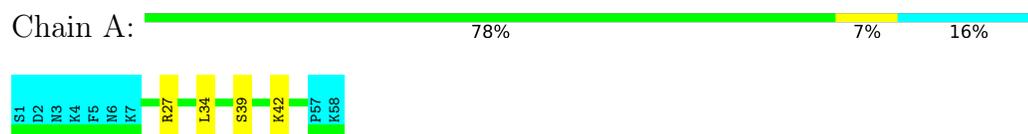
5 Refinement protocol and experimental data overview ⓘ

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	Classification	Version
CYANA	structure calculation	3.0
Amber	refinement	14

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	758
Number of shifts mapped to atoms	758
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	96%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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	0.62±0.01	0±0/399 (0.0± 0.0%)	1.02±0.04	1±1/540 (0.2± 0.1%)
All	All	0.62	0/7980 (0.0%)	1.02	18/10800 (0.2%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.4
All	All	0	3

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	27	ARG	NE-CZ-NH1	9.61	125.11	120.30	15	16
1	A	27	ARG	NE-CZ-NH2	-5.76	117.42	120.30	17	1
1	A	30	PHE	CB-CG-CD1	-5.14	117.20	120.80	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	27	ARG	Sidechain	2
1	A	14	TYR	Sidechain	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
All	All	7860	7660	7660	-

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 -.

There are no clashes.

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	49/58 (84%)	47±1 (96±2%)	2±1 (4±2%)	0±0 (0±0%)	54	85
All	All	980/1160 (84%)	941 (96%)	38 (4%)	1 (0%)	54	85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	20	PRO	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	43/52 (83%)	40±1 (93±2%)	3±1 (7±2%)	18	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	860/1040 (83%)	799 (93%)	61 (7%)	18 67

All 14 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	42	LYS	20
1	A	34	LEU	11
1	A	32	GLN	6
1	A	14	TYR	5
1	A	50	LYS	5
1	A	28	ASN	3
1	A	53	ASP	3
1	A	18	HIS	2
1	A	11	ASN	1
1	A	51	LEU	1
1	A	24	GLU	1
1	A	47	GLU	1
1	A	25	GLU	1
1	A	39	SER	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 96% for the well-defined parts and 95% 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	758
Number of shifts mapped to atoms	758
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 ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}\text{C}_\alpha$	58	-0.16 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	56	0.29 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	58	0.03 ± 0.08	None needed (< 0.5 ppm)
^{15}N	57	0.06 ± 0.39	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 96%, i.e. 645 atoms were assigned a chemical shift out of a possible 672. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	242/242 (100%)	97/97 (100%)	98/98 (100%)	47/47 (100%)
Sidechain	379/394 (96%)	247/252 (98%)	123/126 (98%)	9/16 (56%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	24/36 (67%)	15/18 (83%)	9/17 (53%)	0/1 (0%)
Overall	645/672 (96%)	359/367 (98%)	230/241 (95%)	56/64 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 95%, i.e. 755 atoms were assigned a chemical shift out of a possible 797. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	280/285 (98%)	110/114 (96%)	116/116 (100%)	54/55 (98%)
Sidechain	445/466 (95%)	289/296 (98%)	145/149 (97%)	11/21 (52%)
Aromatic	30/46 (65%)	19/23 (83%)	11/22 (50%)	0/1 (0%)
Overall	755/797 (95%)	418/433 (97%)	272/287 (95%)	65/77 (84%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:
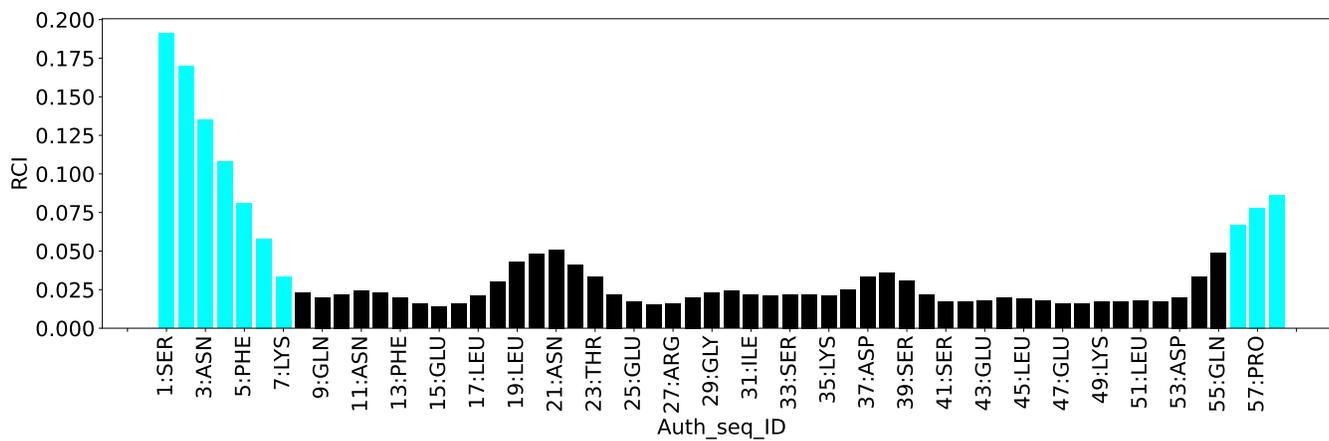
8 NMR restraints analysis ⓘ

8.1 Conformationally restricting restraints ⓘ

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

Description	Value
Total distance restraints	1105
Intra-residue ($|i\text{-}j|=0$)	251
Sequential ($|i\text{-}j|=1$)	254
Medium range ($|i\text{-}j|>1$ and $|i\text{-}j|<5$)	353
Long range ($|i\text{-}j|\geq5$)	247
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	19.1
Number of long range restraints per residue[1]	4.3

[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)	5.6	0.2
0.2-0.5 (Medium)	1.8	0.48
>0.5 (Large)	0.3	0.8

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8.2.2 Average number of dihedral-angle violations per model ⓘ

Dihedral-angle violations less than 1° 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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	251	22.7	2	0.8	0.2	0	0.0	0.0
Backbone-Backbone	3	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	191	17.3	2	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	57	5.2	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	254	23.0	4	1.6	0.4	0	0.0	0.0
Backbone-Backbone	54	4.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	153	13.8	3	2.0	0.3	0	0.0	0.0
Sidechain-Sidechain	47	4.3	1	2.1	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	353	31.9	17	4.8	1.5	0	0.0	0.0
Backbone-Backbone	102	9.2	4	3.9	0.4	0	0.0	0.0
Backbone-Sidechain	159	14.4	9	5.7	0.8	0	0.0	0.0
Sidechain-Sidechain	92	8.3	4	4.3	0.4	0	0.0	0.0
Long range (|i-j|≥5)	247	22.4	10	4.0	0.9	0	0.0	0.0
Backbone-Backbone	2	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	104	9.4	5	4.8	0.5	0	0.0	0.0
Sidechain-Sidechain	141	12.8	5	3.5	0.5	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
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
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	1105	100.0	33	3.0	3.0	0	0.0	0.0
Backbone-Backbone	161	14.6	4	2.5	0.4	0	0.0	0.0
Backbone-Sidechain	607	54.9	19	3.1	1.7	0	0.0	0.0
Sidechain-Sidechain	337	30.5	10	3.0	0.9	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 ⓘ
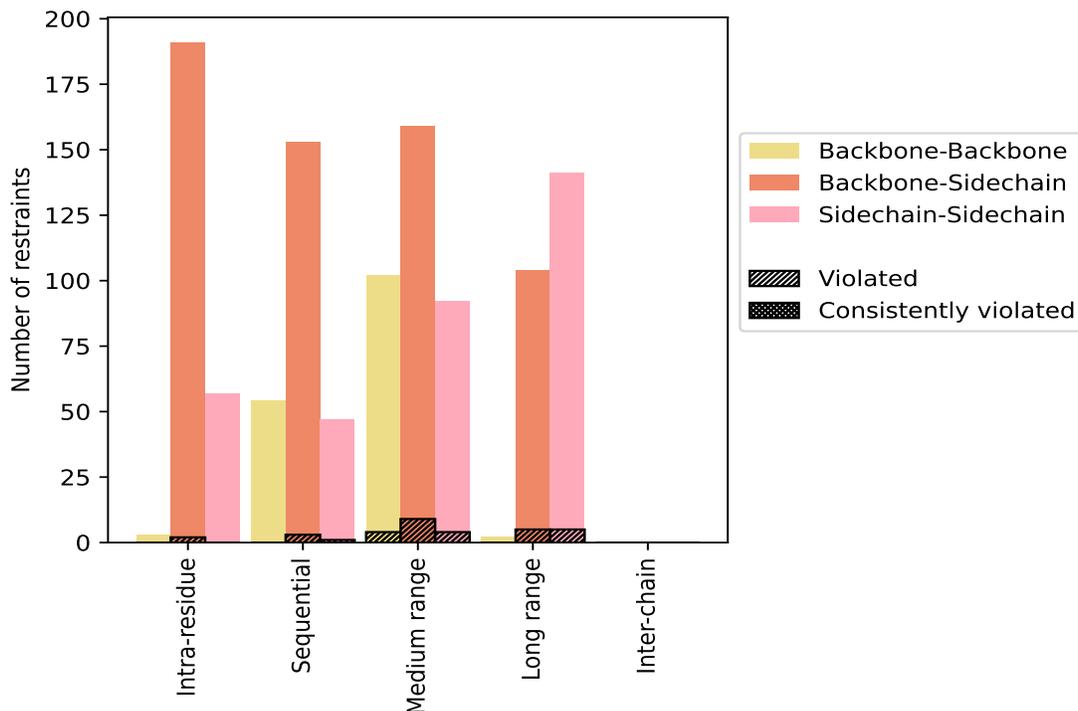
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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	0	1	1	5	0	7	0.34	0.65	0.15	0.29
2	0	2	3	1	0	6	0.12	0.15	0.01	0.12
3	0	1	1	5	0	7	0.21	0.48	0.12	0.15
4	0	2	3	3	0	8	0.24	0.71	0.19	0.17
5	0	1	3	2	0	6	0.13	0.15	0.01	0.12
6	0	3	3	2	0	8	0.16	0.32	0.07	0.12
7	0	1	2	5	0	8	0.22	0.68	0.18	0.16
8	0	3	7	2	0	12	0.14	0.22	0.03	0.12
9	0	3	2	2	0	7	0.17	0.39	0.09	0.12
10	0	2	3	4	0	9	0.25	0.45	0.11	0.23
11	0	1	2	3	0	6	0.16	0.34	0.08	0.12

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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	0	2	2	3	0	7	0.25	0.57	0.15	0.18
13	0	0	1	4	0	5	0.28	0.7	0.21	0.18
14	0	3	5	2	0	10	0.14	0.31	0.06	0.12
15	0	0	4	1	0	5	0.21	0.3	0.07	0.18
16	1	2	4	1	0	8	0.14	0.16	0.02	0.14
17	1	1	6	4	0	12	0.17	0.34	0.07	0.15
18	0	1	1	5	0	7	0.31	0.8	0.21	0.22
19	0	2	2	2	0	6	0.13	0.17	0.02	0.12
20	0	2	3	5	0	10	0.24	0.77	0.19	0.16

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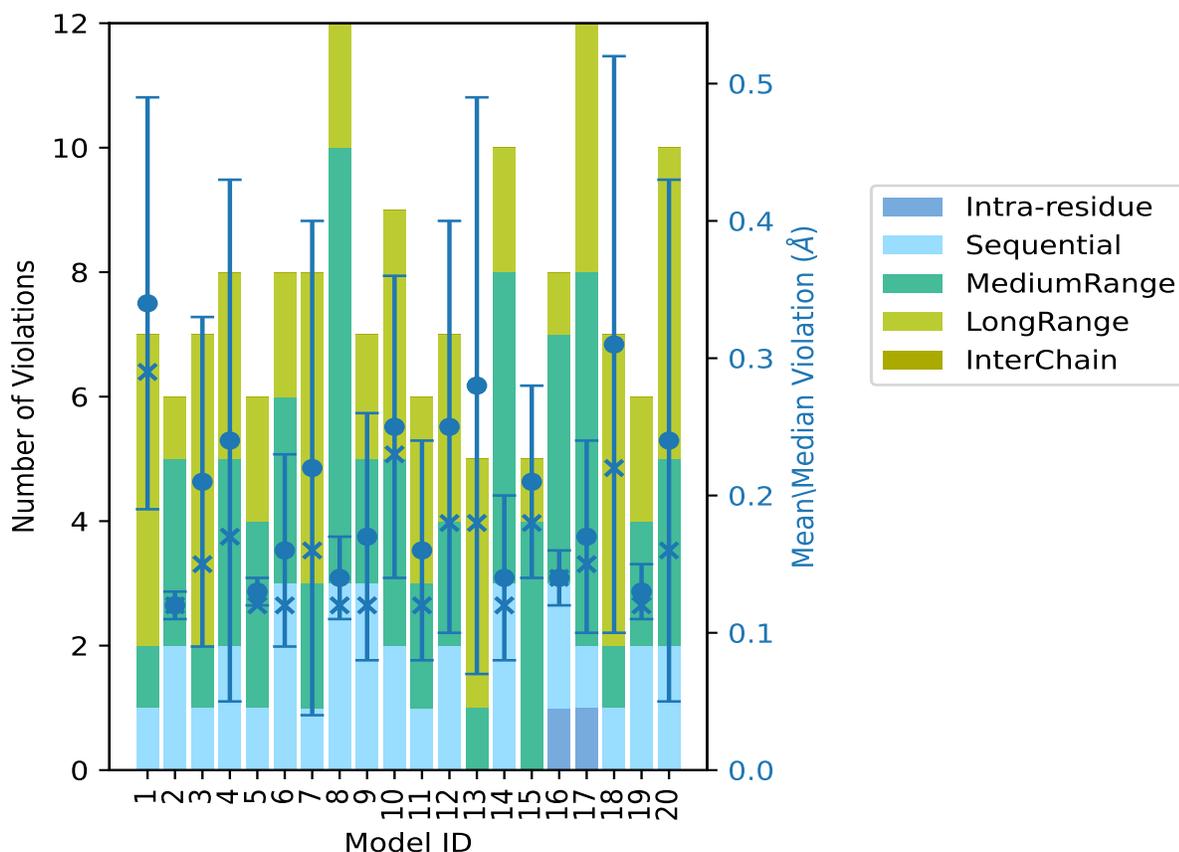
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis
on the right

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, 1072(IR:249, SQ:250, MR:336, LR:237, IC:0) 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]	%
2	0	7	3	0	12	1	5.0
0	0	4	1	0	5	2	10.0
0	1	0	0	0	1	3	15.0
0	0	2	0	0	2	4	20.0
0	0	0	0	0	0	5	25.0
0	1	1	0	0	2	6	30.0
0	0	1	3	0	4	7	35.0
0	0	1	0	0	1	8	40.0
0	0	0	0	0	0	9	45.0
0	1	0	1	0	2	10	50.0
0	0	0	1	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	1	1	1	0	3	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

[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 ⓘ
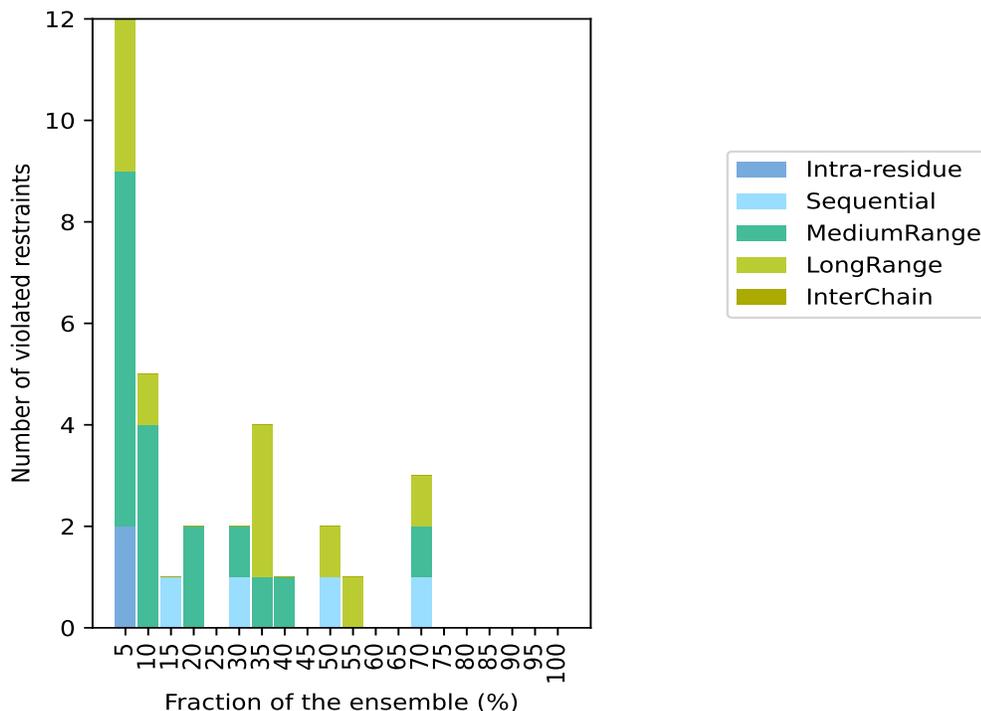
9.4 Most violated distance restraints in the ensemble ⓘ

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
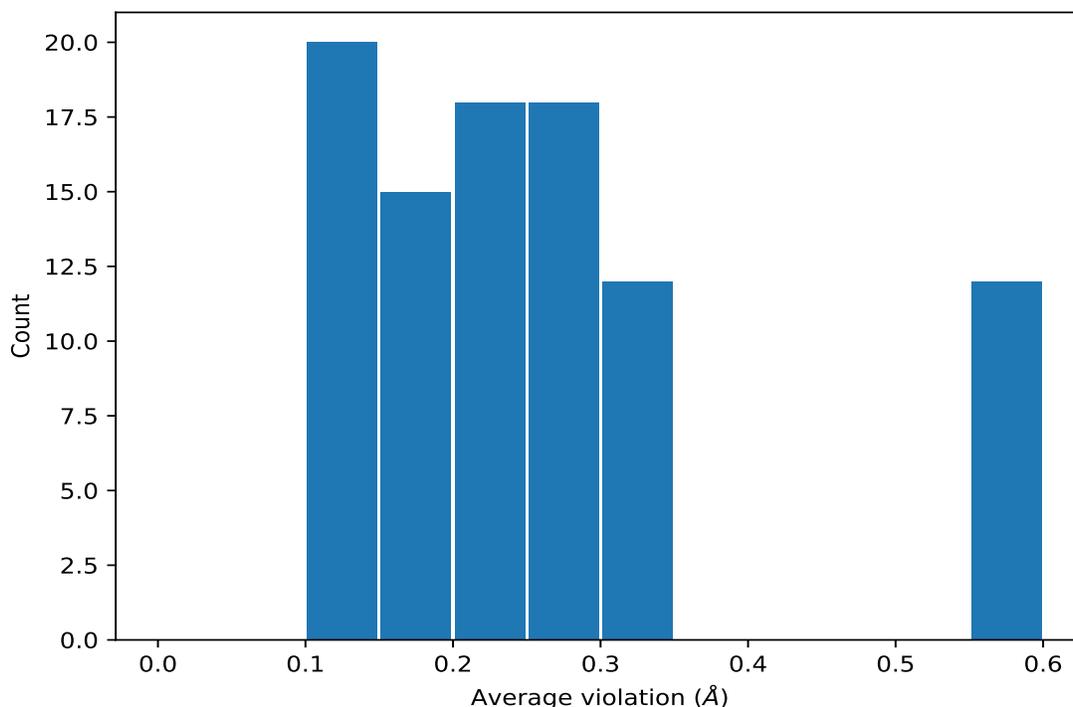
9.4.2　Table: Most violated distance restraints ⓘ

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)
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	14	0.18	0.03	0.17
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	14	0.16	0.03	0.16
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	14	0.13	0.02	0.14
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	11	0.55	0.19	0.57
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	11	0.55	0.19	0.57
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	11	0.55	0.19	0.57
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	11	0.55	0.19	0.57
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	11	0.55	0.19	0.57
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	11	0.55	0.19	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	11	0.55	0.19	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	11	0.55	0.19	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	11	0.55	0.19	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	11	0.55	0.19	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	11	0.55	0.19	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	11	0.55	0.19	0.57
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD11	10	0.27	0.1	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD12	10	0.27	0.1	0.26
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD13	10	0.27	0.1	0.26
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD21	10	0.27	0.1	0.26
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD22	10	0.27	0.1	0.26
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD23	10	0.27	0.1	0.26
(1,851)	1:A:25:GLU:HB3	1:A:26:GLN:HB2	10	0.15	0.04	0.14
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD2	8	0.3	0.16	0.29
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD3	8	0.3	0.16	0.29
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD2	8	0.3	0.16	0.29
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD3	8	0.3	0.16	0.29
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD2	8	0.3	0.16	0.29
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD3	8	0.3	0.16	0.29
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD2	8	0.3	0.16	0.29
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD3	8	0.3	0.16	0.29
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD2	8	0.3	0.16	0.29
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD3	8	0.3	0.16	0.29
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD2	8	0.3	0.16	0.29
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD3	8	0.3	0.16	0.29
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD11	7	0.23	0.07	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD12	7	0.23	0.07	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD13	7	0.23	0.07	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD21	7	0.23	0.07	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD22	7	0.23	0.07	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD23	7	0.23	0.07	0.22
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD11	7	0.21	0.08	0.19
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD12	7	0.21	0.08	0.19
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD13	7	0.21	0.08	0.19
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD21	7	0.21	0.08	0.19
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD22	7	0.21	0.08	0.19
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD23	7	0.21	0.08	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD11	7	0.21	0.08	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD12	7	0.21	0.08	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD13	7	0.21	0.08	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD21	7	0.21	0.08	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD22	7	0.21	0.08	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD23	7	0.21	0.08	0.19
(1,837)	1:A:13:PHE:HA	1:A:34:LEU:HG	7	0.13	0.01	0.12
(1,97)	1:A:50:LYS:HE2	1:A:53:ASP:H	7	0.12	0.01	0.12
(1,97)	1:A:50:LYS:HE3	1:A:53:ASP:H	7	0.12	0.01	0.12
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE2	6	0.27	0.08	0.28
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE3	6	0.27	0.08	0.28
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE2	6	0.27	0.08	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE3	6	0.27	0.08	0.28
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE2	6	0.27	0.08	0.28
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE3	6	0.27	0.08	0.28
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE2	6	0.27	0.08	0.28
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE3	6	0.27	0.08	0.28
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE2	6	0.27	0.08	0.28
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE3	6	0.27	0.08	0.28
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE2	6	0.27	0.08	0.28
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE3	6	0.27	0.08	0.28
(1,556)	1:A:34:LEU:HB3	1:A:35:LYS:HA	6	0.12	0.01	0.11
(1,739)	1:A:34:LEU:HD21	1:A:38:PRO:HA	4	0.12	0.01	0.12
(1,739)	1:A:34:LEU:HD22	1:A:38:PRO:HA	4	0.12	0.01	0.12
(1,739)	1:A:34:LEU:HD23	1:A:38:PRO:HA	4	0.12	0.01	0.12
(1,1087)	1:A:47:GLU:HA	1:A:50:LYS:HB2	4	0.12	0.01	0.12
(1,1087)	1:A:47:GLU:HA	1:A:50:LYS:HB3	4	0.12	0.01	0.12
(1,109)	1:A:31:ILE:HG13	1:A:32:GLN:H	3	0.11	0.0	0.11
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD11	2	0.18	0.02	0.18
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD12	2	0.18	0.02	0.18
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD13	2	0.18	0.02	0.18
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD21	2	0.18	0.02	0.18
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD22	2	0.18	0.02	0.18
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD23	2	0.18	0.02	0.18
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD11	2	0.16	0.01	0.16
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD12	2	0.16	0.01	0.16
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD13	2	0.16	0.01	0.16
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD21	2	0.16	0.01	0.16
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD22	2	0.16	0.01	0.16
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD23	2	0.16	0.01	0.16
(1,1042)	1:A:34:LEU:HD11	1:A:37:ASP:HB2	2	0.14	0.02	0.14
(1,1042)	1:A:34:LEU:HD12	1:A:37:ASP:HB2	2	0.14	0.02	0.14
(1,1042)	1:A:34:LEU:HD13	1:A:37:ASP:HB2	2	0.14	0.02	0.14
(1,1042)	1:A:34:LEU:HD21	1:A:37:ASP:HB2	2	0.14	0.02	0.14
(1,1042)	1:A:34:LEU:HD22	1:A:37:ASP:HB2	2	0.14	0.02	0.14
(1,1042)	1:A:34:LEU:HD23	1:A:37:ASP:HB2	2	0.14	0.02	0.14
(1,803)	1:A:47:GLU:HG2	1:A:49:LYS:H	2	0.12	0.01	0.12
(1,803)	1:A:47:GLU:HG3	1:A:49:LYS:H	2	0.12	0.01	0.12
(1,127)	1:A:13:PHE:H	1:A:15:GLU:HB2	2	0.12	0.0	0.12

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.
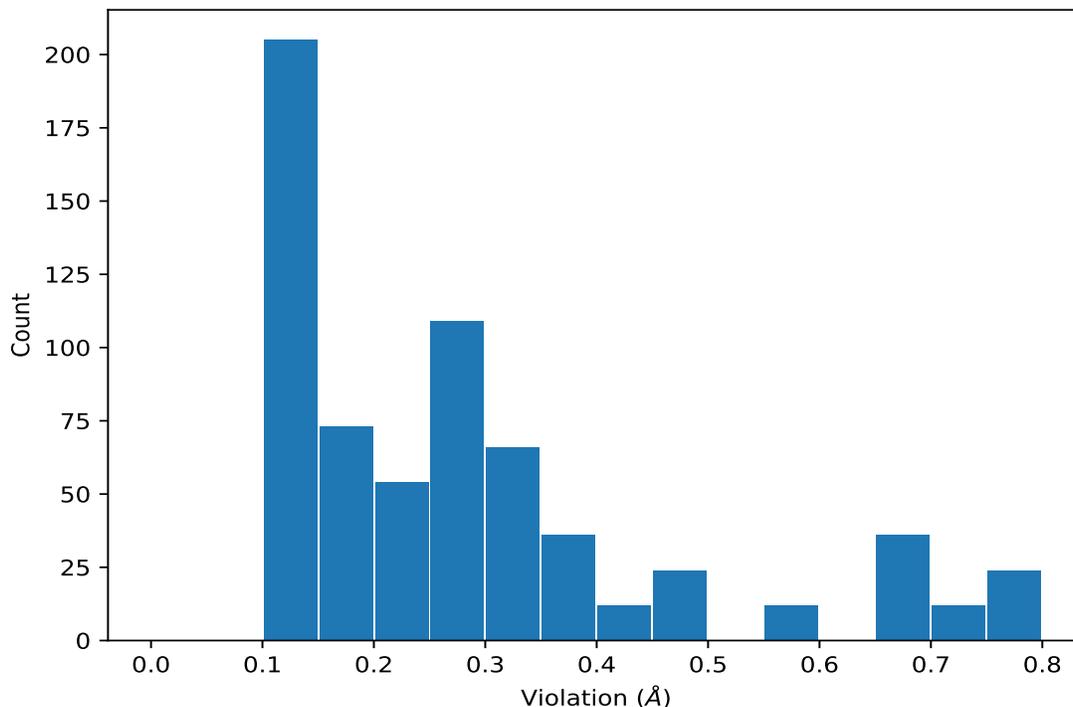
9.5.2 Table : All distance violations ⓘ

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)
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	18	0.8
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	18	0.8
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	18	0.8
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	18	0.8
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	18	0.8
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	18	0.8
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	18	0.8
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	18	0.8
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	18	0.8
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	18	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	18	0.8
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	18	0.8
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	20	0.77
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	20	0.77
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	20	0.77
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	20	0.77
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	20	0.77
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	20	0.77
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	20	0.77
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	20	0.77
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	20	0.77
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	20	0.77
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	20	0.77
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	20	0.77
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	4	0.71
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	4	0.71
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	4	0.71
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	4	0.71
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	4	0.71
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	4	0.71
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	4	0.71
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	4	0.71
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	4	0.71
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	4	0.71
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	4	0.71
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	4	0.71
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	13	0.7
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	13	0.7
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	13	0.7
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	13	0.7
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	13	0.7
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	13	0.7
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	13	0.7
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	13	0.7
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	13	0.7
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	13	0.7
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	13	0.7
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	13	0.7
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	7	0.68
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	7	0.68
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	7	0.68
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	7	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	7	0.68
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	7	0.68
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	7	0.68
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	7	0.68
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	7	0.68
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	7	0.68
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	7	0.68
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	7	0.68
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD2	1	0.65
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD3	1	0.65
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD2	1	0.65
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD3	1	0.65
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD2	1	0.65
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD3	1	0.65
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD2	1	0.65
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD3	1	0.65
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD2	1	0.65
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD3	1	0.65
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD2	1	0.65
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD3	1	0.65
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	12	0.57
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	12	0.57
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	12	0.57
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	12	0.57
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	12	0.57
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	12	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	12	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	12	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	12	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	12	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	12	0.57
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	12	0.57
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	3	0.48
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	3	0.48
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	3	0.48
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	3	0.48
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	3	0.48
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	3	0.48
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	3	0.48
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	3	0.48
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	3	0.48
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	3	0.48
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	3	0.48
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	10	0.45
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	10	0.45
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	10	0.45
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	10	0.45
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	10	0.45
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	10	0.45
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	10	0.45
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	10	0.45
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	10	0.45
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	10	0.45
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	10	0.45
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	10	0.45
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD11	1	0.44
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD12	1	0.44
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD13	1	0.44
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD21	1	0.44
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD22	1	0.44
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD23	1	0.44
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD11	10	0.42
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD12	10	0.42
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD13	10	0.42
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD21	10	0.42
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD22	10	0.42
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD23	10	0.42
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD2	9	0.39
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD3	9	0.39
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD2	9	0.39
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD3	9	0.39
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD2	9	0.39
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD3	9	0.39
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD2	9	0.39
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD3	9	0.39
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD2	9	0.39
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD3	9	0.39
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD2	9	0.39
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD3	9	0.39
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE2	12	0.38
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE3	12	0.38
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE2	12	0.38
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE3	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE2	12	0.38
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE3	12	0.38
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE2	12	0.38
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE3	12	0.38
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE2	12	0.38
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE3	12	0.38
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE2	12	0.38
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE3	12	0.38
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD2	4	0.36
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD3	4	0.36
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD2	4	0.36
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD3	4	0.36
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD2	4	0.36
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD3	4	0.36
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD2	4	0.36
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD3	4	0.36
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD2	4	0.36
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD3	4	0.36
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD2	4	0.36
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD3	4	0.36
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD11	20	0.35
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD12	20	0.35
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD13	20	0.35
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD21	20	0.35
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD22	20	0.35
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD23	20	0.35
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD11	17	0.34
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD12	17	0.34
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD13	17	0.34
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD21	17	0.34
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD22	17	0.34
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD23	17	0.34
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE2	11	0.34
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE3	11	0.34
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE2	11	0.34
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE3	11	0.34
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE2	11	0.34
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE3	11	0.34
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE2	11	0.34
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE3	11	0.34
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE2	11	0.34
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE3	11	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE2	11	0.34
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE3	11	0.34
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	6	0.32
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	6	0.32
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	6	0.32
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	6	0.32
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	6	0.32
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	6	0.32
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	6	0.32
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	6	0.32
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	6	0.32
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	6	0.32
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	6	0.32
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	6	0.32
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD11	18	0.31
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD12	18	0.31
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD13	18	0.31
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD21	18	0.31
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD22	18	0.31
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD23	18	0.31
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD11	18	0.31
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD12	18	0.31
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD13	18	0.31
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD21	18	0.31
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD22	18	0.31
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD23	18	0.31
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD11	1	0.31
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD12	1	0.31
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD13	1	0.31
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD21	1	0.31
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD22	1	0.31
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD23	1	0.31
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE2	14	0.31
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE3	14	0.31
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE2	14	0.31
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE3	14	0.31
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE2	14	0.31
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE3	14	0.31
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE2	14	0.31
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE3	14	0.31
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE2	14	0.31
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE3	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE2	14	0.31
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE3	14	0.31
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD11	20	0.3
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD12	20	0.3
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD13	20	0.3
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD21	20	0.3
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD22	20	0.3
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD23	20	0.3
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD11	20	0.3
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD12	20	0.3
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD13	20	0.3
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD21	20	0.3
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD22	20	0.3
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD23	20	0.3
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD11	3	0.3
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD12	3	0.3
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD13	3	0.3
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD21	3	0.3
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD22	3	0.3
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD23	3	0.3
(1,1080)	1:A:45:LEU:HD11	1:A:49:LYS:HG2	15	0.3
(1,1080)	1:A:45:LEU:HD12	1:A:49:LYS:HG2	15	0.3
(1,1080)	1:A:45:LEU:HD13	1:A:49:LYS:HG2	15	0.3
(1,1080)	1:A:45:LEU:HD21	1:A:49:LYS:HG2	15	0.3
(1,1080)	1:A:45:LEU:HD22	1:A:49:LYS:HG2	15	0.3
(1,1080)	1:A:45:LEU:HD23	1:A:49:LYS:HG2	15	0.3
(1,1080)	1:A:45:LEU:HD11	1:A:49:LYS:HG3	15	0.3
(1,1080)	1:A:45:LEU:HD12	1:A:49:LYS:HG3	15	0.3
(1,1080)	1:A:45:LEU:HD13	1:A:49:LYS:HG3	15	0.3
(1,1080)	1:A:45:LEU:HD21	1:A:49:LYS:HG3	15	0.3
(1,1080)	1:A:45:LEU:HD22	1:A:49:LYS:HG3	15	0.3
(1,1080)	1:A:45:LEU:HD23	1:A:49:LYS:HG3	15	0.3
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	1	0.29
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	1	0.29
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	1	0.29
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	1	0.29
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	1	0.29
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	1	0.29
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	1	0.29
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	1	0.29
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	1	0.29
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	1	0.29
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	1	0.29
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD11	1	0.29
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD12	1	0.29
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD13	1	0.29
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD21	1	0.29
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD22	1	0.29
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD23	1	0.29
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD11	1	0.29
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD12	1	0.29
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD13	1	0.29
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD21	1	0.29
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD22	1	0.29
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD23	1	0.29
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD2	10	0.29
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD3	10	0.29
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD2	10	0.29
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD3	10	0.29
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD2	10	0.29
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD3	10	0.29
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD2	10	0.29
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD3	10	0.29
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD2	10	0.29
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD3	10	0.29
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD2	10	0.29
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD3	10	0.29
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD11	18	0.28
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD12	18	0.28
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD13	18	0.28
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD21	18	0.28
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD22	18	0.28
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD23	18	0.28
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD2	15	0.28
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD3	15	0.28
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD2	15	0.28
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD3	15	0.28
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD2	15	0.28
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD3	15	0.28
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD2	15	0.28
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD3	15	0.28
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD2	15	0.28
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD3	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD2	15	0.28
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD3	15	0.28
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	10	0.25
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE2	17	0.25
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE3	17	0.25
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE2	17	0.25
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE3	17	0.25
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE2	17	0.25
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE3	17	0.25
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE2	17	0.25
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE3	17	0.25
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE2	17	0.25
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE3	17	0.25
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE2	17	0.25
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE3	17	0.25
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD2	13	0.25
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD3	13	0.25
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD2	13	0.25
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD3	13	0.25
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD2	13	0.25
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD3	13	0.25
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD2	13	0.25
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD3	13	0.25
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD2	13	0.25
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD3	13	0.25
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD2	13	0.25
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD3	13	0.25
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD11	17	0.24
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD12	17	0.24
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD13	17	0.24
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD21	17	0.24
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD22	17	0.24
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD23	17	0.24
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD11	17	0.23
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD12	17	0.23
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD13	17	0.23
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD21	17	0.23
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD22	17	0.23
(1,970)	1:A:13:PHE:HD1	1:A:34:LEU:HD23	17	0.23
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD11	17	0.23
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD12	17	0.23
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD13	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD21	17	0.23
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD22	17	0.23
(1,970)	1:A:13:PHE:HD2	1:A:34:LEU:HD23	17	0.23
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD11	10	0.23
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD12	10	0.23
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD13	10	0.23
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD21	10	0.23
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD22	10	0.23
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD23	10	0.23
(1,851)	1:A:25:GLU:HB3	1:A:26:GLN:HB2	6	0.23
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	12	0.23
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD11	7	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD12	7	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD13	7	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD21	7	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD22	7	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD23	7	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD11	18	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD12	18	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD13	18	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD21	18	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD22	18	0.22
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD23	18	0.22
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	8	0.22
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD11	7	0.21
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD12	7	0.21
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD13	7	0.21
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD21	7	0.21
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD22	7	0.21
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD23	7	0.21
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	1	0.21
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	9	0.2
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	18	0.2
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD11	20	0.2
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD12	20	0.2
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD13	20	0.2
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD21	20	0.2
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD22	20	0.2
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD23	20	0.2
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD11	10	0.19
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD12	10	0.19
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD13	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD21	10	0.19
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD22	10	0.19
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD23	10	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD11	10	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD12	10	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD13	10	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD21	10	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD22	10	0.19
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD23	10	0.19
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	7	0.19
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE2	18	0.19
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE3	18	0.19
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE2	18	0.19
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE3	18	0.19
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE2	18	0.19
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE3	18	0.19
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE2	18	0.19
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE3	18	0.19
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE2	18	0.19
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE3	18	0.19
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE2	18	0.19
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE3	18	0.19
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD11	13	0.18
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD12	13	0.18
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD13	13	0.18
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD21	13	0.18
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD22	13	0.18
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD23	13	0.18
(1,851)	1:A:25:GLU:HB3	1:A:26:GLN:HB2	10	0.18
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	6	0.18
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	12	0.18
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	15	0.18
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD11	12	0.17
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD12	12	0.17
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD13	12	0.17
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD21	12	0.17
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD22	12	0.17
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD23	12	0.17
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD11	1	0.17
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD12	1	0.17
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD13	1	0.17
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD21	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD22	1	0.17
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD23	1	0.17
(1,851)	1:A:25:GLU:HB3	1:A:26:GLN:HB2	4	0.17
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	3	0.17
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	4	0.17
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	9	0.17
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	11	0.17
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	14	0.17
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	17	0.17
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	19	0.17
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	13	0.17
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	4	0.17
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD11	8	0.17
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD12	8	0.17
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD13	8	0.17
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD21	8	0.17
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD22	8	0.17
(1,1068)	1:A:42:LYS:H	1:A:45:LEU:HD23	8	0.17
(1,851)	1:A:25:GLU:HB3	1:A:26:GLN:HB2	16	0.16
(1,161)	1:A:47:GLU:H	1:A:47:GLU:HG2	16	0.16
(1,161)	1:A:47:GLU:H	1:A:47:GLU:HG3	16	0.16
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	20	0.16
(1,1042)	1:A:34:LEU:HD11	1:A:37:ASP:HB2	15	0.16
(1,1042)	1:A:34:LEU:HD12	1:A:37:ASP:HB2	15	0.16
(1,1042)	1:A:34:LEU:HD13	1:A:37:ASP:HB2	15	0.16
(1,1042)	1:A:34:LEU:HD21	1:A:37:ASP:HB2	15	0.16
(1,1042)	1:A:34:LEU:HD22	1:A:37:ASP:HB2	15	0.16
(1,1042)	1:A:34:LEU:HD23	1:A:37:ASP:HB2	15	0.16
(1,97)	1:A:50:LYS:HE2	1:A:53:ASP:H	8	0.15
(1,97)	1:A:50:LYS:HE3	1:A:53:ASP:H	8	0.15
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD11	20	0.15
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD12	20	0.15
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD13	20	0.15
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD21	20	0.15
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD22	20	0.15
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD23	20	0.15
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD11	3	0.15
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD12	3	0.15
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD13	3	0.15
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD21	3	0.15
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD22	3	0.15
(1,951)	1:A:10:GLN:HA	1:A:34:LEU:HD23	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,837)	1:A:13:PHE:HA	1:A:34:LEU:HG	2	0.15
(1,380)	1:A:25:GLU:H	1:A:25:GLU:HG2	17	0.15
(1,380)	1:A:25:GLU:H	1:A:25:GLU:HG3	17	0.15
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	5	0.15
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	8	0.15
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE2	8	0.15
(1,1082)	1:A:45:LEU:HD11	1:A:49:LYS:HE3	8	0.15
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE2	8	0.15
(1,1082)	1:A:45:LEU:HD12	1:A:49:LYS:HE3	8	0.15
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE2	8	0.15
(1,1082)	1:A:45:LEU:HD13	1:A:49:LYS:HE3	8	0.15
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE2	8	0.15
(1,1082)	1:A:45:LEU:HD21	1:A:49:LYS:HE3	8	0.15
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE2	8	0.15
(1,1082)	1:A:45:LEU:HD22	1:A:49:LYS:HE3	8	0.15
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE2	8	0.15
(1,1082)	1:A:45:LEU:HD23	1:A:49:LYS:HE3	8	0.15
(1,97)	1:A:50:LYS:HE2	1:A:53:ASP:H	16	0.14
(1,97)	1:A:50:LYS:HE3	1:A:53:ASP:H	16	0.14
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD11	7	0.14
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD12	7	0.14
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD13	7	0.14
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD21	7	0.14
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD22	7	0.14
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD23	7	0.14
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD11	7	0.14
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD12	7	0.14
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD13	7	0.14
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD21	7	0.14
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD22	7	0.14
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD23	7	0.14
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD11	3	0.14
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD12	3	0.14
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD13	3	0.14
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD21	3	0.14
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD22	3	0.14
(1,965)	1:A:13:PHE:H	1:A:34:LEU:HD23	3	0.14
(1,851)	1:A:25:GLU:HB3	1:A:26:GLN:HB2	18	0.14
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	20	0.14
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	4	0.14
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	14	0.14
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	16	0.14
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	17	0.14
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	19	0.14
(1,851)	1:A:25:GLU:HB3	1:A:26:GLN:HB2	8	0.13
(1,837)	1:A:13:PHE:HA	1:A:34:LEU:HG	14	0.13
(1,837)	1:A:13:PHE:HA	1:A:34:LEU:HG	16	0.13
(1,803)	1:A:47:GLU:HG2	1:A:49:LYS:H	16	0.13
(1,803)	1:A:47:GLU:HG3	1:A:49:LYS:H	16	0.13
(1,739)	1:A:34:LEU:HD21	1:A:38:PRO:HA	5	0.13
(1,739)	1:A:34:LEU:HD22	1:A:38:PRO:HA	5	0.13
(1,739)	1:A:34:LEU:HD23	1:A:38:PRO:HA	5	0.13
(1,556)	1:A:34:LEU:HB3	1:A:35:LYS:HA	16	0.13
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	6	0.13
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	20	0.13
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	7	0.13
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	12	0.13
(1,1087)	1:A:47:GLU:HA	1:A:50:LYS:HB2	5	0.13
(1,1087)	1:A:47:GLU:HA	1:A:50:LYS:HB3	5	0.13
(1,97)	1:A:50:LYS:HE2	1:A:53:ASP:H	10	0.12
(1,97)	1:A:50:LYS:HE3	1:A:53:ASP:H	10	0.12
(1,97)	1:A:50:LYS:HE2	1:A:53:ASP:H	14	0.12
(1,97)	1:A:50:LYS:HE3	1:A:53:ASP:H	14	0.12
(1,97)	1:A:50:LYS:HE2	1:A:53:ASP:H	17	0.12
(1,97)	1:A:50:LYS:HE3	1:A:53:ASP:H	17	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD11	3	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD12	3	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD13	3	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD21	3	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD22	3	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD23	3	0.12
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD11	3	0.12
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD12	3	0.12
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD13	3	0.12
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD21	3	0.12
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD22	3	0.12
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD23	3	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD11	13	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD12	13	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD13	13	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD21	13	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD22	13	0.12
(1,969)	1:A:13:PHE:HB2	1:A:34:LEU:HD23	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD11	13	0.12
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD12	13	0.12
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD13	13	0.12
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD21	13	0.12
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD22	13	0.12
(1,969)	1:A:13:PHE:HB3	1:A:34:LEU:HD23	13	0.12
(1,851)	1:A:25:GLU:HB3	1:A:26:GLN:HB2	2	0.12
(1,851)	1:A:25:GLU:HB3	1:A:26:GLN:HB2	9	0.12
(1,837)	1:A:13:PHE:HA	1:A:34:LEU:HG	5	0.12
(1,837)	1:A:13:PHE:HA	1:A:34:LEU:HG	8	0.12
(1,837)	1:A:13:PHE:HA	1:A:34:LEU:HG	9	0.12
(1,818)	1:A:47:GLU:H	1:A:50:LYS:HE2	5	0.12
(1,818)	1:A:47:GLU:H	1:A:50:LYS:HE3	5	0.12
(1,739)	1:A:34:LEU:HD21	1:A:38:PRO:HA	8	0.12
(1,739)	1:A:34:LEU:HD22	1:A:38:PRO:HA	8	0.12
(1,739)	1:A:34:LEU:HD23	1:A:38:PRO:HA	8	0.12
(1,739)	1:A:34:LEU:HD21	1:A:38:PRO:HA	14	0.12
(1,739)	1:A:34:LEU:HD22	1:A:38:PRO:HA	14	0.12
(1,739)	1:A:34:LEU:HD23	1:A:38:PRO:HA	14	0.12
(1,564)	1:A:30:PHE:HD1	1:A:47:GLU:HG2	19	0.12
(1,564)	1:A:30:PHE:HD1	1:A:47:GLU:HG3	19	0.12
(1,564)	1:A:30:PHE:HD2	1:A:47:GLU:HG2	19	0.12
(1,564)	1:A:30:PHE:HD2	1:A:47:GLU:HG3	19	0.12
(1,556)	1:A:34:LEU:HB3	1:A:35:LYS:HA	14	0.12
(1,457)	1:A:32:GLN:HE21	1:A:33:SER:H	8	0.12
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	11	0.12
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	19	0.12
(1,289)	1:A:25:GLU:HA	1:A:28:ASN:H	8	0.12
(1,182)	1:A:6:ASN:H	1:A:10:GLN:HA	17	0.12
(1,127)	1:A:13:PHE:H	1:A:15:GLU:HB2	10	0.12
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	2	0.12
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	6	0.12
(1,1087)	1:A:47:GLU:HA	1:A:50:LYS:HB2	4	0.12
(1,1087)	1:A:47:GLU:HA	1:A:50:LYS:HB3	4	0.12
(1,1087)	1:A:47:GLU:HA	1:A:50:LYS:HB2	7	0.12
(1,1087)	1:A:47:GLU:HA	1:A:50:LYS:HB3	7	0.12
(1,97)	1:A:50:LYS:HE2	1:A:53:ASP:H	2	0.11
(1,97)	1:A:50:LYS:HE3	1:A:53:ASP:H	2	0.11
(1,97)	1:A:50:LYS:HE2	1:A:53:ASP:H	11	0.11
(1,97)	1:A:50:LYS:HE3	1:A:53:ASP:H	11	0.11
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD11	4	0.11
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD12	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD13	4	0.11
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD21	4	0.11
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD22	4	0.11
(1,967)	1:A:13:PHE:HA	1:A:34:LEU:HD23	4	0.11
(1,851)	1:A:25:GLU:HB3	1:A:26:GLN:HB2	12	0.11
(1,851)	1:A:25:GLU:HB3	1:A:26:GLN:HB2	20	0.11
(1,837)	1:A:13:PHE:HA	1:A:34:LEU:HG	11	0.11
(1,803)	1:A:47:GLU:HG2	1:A:49:LYS:H	2	0.11
(1,803)	1:A:47:GLU:HG3	1:A:49:LYS:H	2	0.11
(1,739)	1:A:34:LEU:HD21	1:A:38:PRO:HA	16	0.11
(1,739)	1:A:34:LEU:HD22	1:A:38:PRO:HA	16	0.11
(1,739)	1:A:34:LEU:HD23	1:A:38:PRO:HA	16	0.11
(1,659)	1:A:22:LEU:HD11	1:A:27:ARG:HB2	11	0.11
(1,659)	1:A:22:LEU:HD12	1:A:27:ARG:HB2	11	0.11
(1,659)	1:A:22:LEU:HD13	1:A:27:ARG:HB2	11	0.11
(1,556)	1:A:34:LEU:HB3	1:A:35:LYS:HA	5	0.11
(1,556)	1:A:34:LEU:HB3	1:A:35:LYS:HA	8	0.11
(1,556)	1:A:34:LEU:HB3	1:A:35:LYS:HA	9	0.11
(1,556)	1:A:34:LEU:HB3	1:A:35:LYS:HA	19	0.11
(1,463)	1:A:23:THR:H	1:A:25:GLU:H	17	0.11
(1,34)	1:A:16:ILE:H	1:A:22:LEU:HD21	7	0.11
(1,34)	1:A:16:ILE:H	1:A:22:LEU:HD22	7	0.11
(1,34)	1:A:16:ILE:H	1:A:22:LEU:HD23	7	0.11
(1,334)	1:A:51:LEU:HB2	1:A:54:ALA:H	6	0.11
(1,329)	1:A:26:GLN:HB2	1:A:55:GLN:HE21	17	0.11
(1,210)	1:A:52:ASN:HD21	1:A:55:GLN:H	17	0.11
(1,127)	1:A:13:PHE:H	1:A:15:GLU:HB2	8	0.11
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	9	0.11
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	14	0.11
(1,114)	1:A:28:ASN:H	1:A:32:GLN:H	15	0.11
(1,109)	1:A:31:ILE:HG13	1:A:32:GLN:H	2	0.11
(1,109)	1:A:31:ILE:HG13	1:A:32:GLN:H	6	0.11
(1,109)	1:A:31:ILE:HG13	1:A:32:GLN:H	14	0.11
(1,1087)	1:A:47:GLU:HA	1:A:50:LYS:HB2	6	0.11
(1,1087)	1:A:47:GLU:HA	1:A:50:LYS:HB3	6	0.11
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD2	19	0.11
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD3	19	0.11
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD2	19	0.11
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD3	19	0.11
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD2	19	0.11
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD3	19	0.11
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD3	19	0.11
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD2	19	0.11
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD3	19	0.11
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD2	19	0.11
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD3	19	0.11
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD2	20	0.11
(1,1081)	1:A:45:LEU:HD11	1:A:49:LYS:HD3	20	0.11
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD2	20	0.11
(1,1081)	1:A:45:LEU:HD12	1:A:49:LYS:HD3	20	0.11
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD2	20	0.11
(1,1081)	1:A:45:LEU:HD13	1:A:49:LYS:HD3	20	0.11
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD2	20	0.11
(1,1081)	1:A:45:LEU:HD21	1:A:49:LYS:HD3	20	0.11
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD2	20	0.11
(1,1081)	1:A:45:LEU:HD22	1:A:49:LYS:HD3	20	0.11
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD2	20	0.11
(1,1081)	1:A:45:LEU:HD23	1:A:49:LYS:HD3	20	0.11
(1,1042)	1:A:34:LEU:HD11	1:A:37:ASP:HB2	14	0.11
(1,1042)	1:A:34:LEU:HD12	1:A:37:ASP:HB2	14	0.11
(1,1042)	1:A:34:LEU:HD13	1:A:37:ASP:HB2	14	0.11
(1,1042)	1:A:34:LEU:HD21	1:A:37:ASP:HB2	14	0.11
(1,1042)	1:A:34:LEU:HD22	1:A:37:ASP:HB2	14	0.11
(1,1042)	1:A:34:LEU:HD23	1:A:37:ASP:HB2	14	0.11

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found