



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 5U6L / pdb_00005u6l
BMRB ID : 30208
Title : Solution structure of the zinc fingers 3 and 4 of MBNL1
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Deposited on : 2016-12-08

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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>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

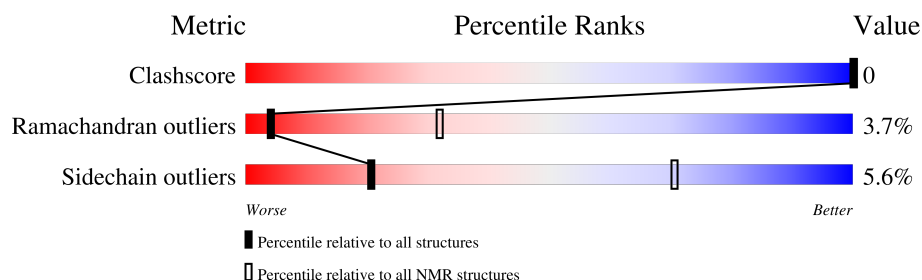
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 68%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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	83	

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:180-A:251 (72)	0.64	2

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 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1316 atoms, of which 644 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Muscleblind-like protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	83	Total	C	H	N	O	S	0
			1314	406	644	130	125	9	

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

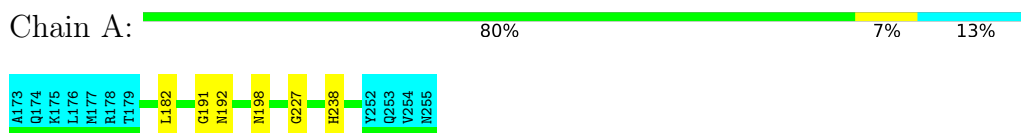
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Muscleblind-like protein 1

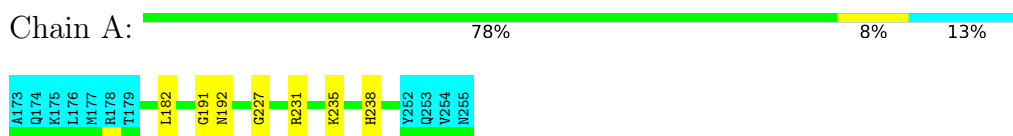


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

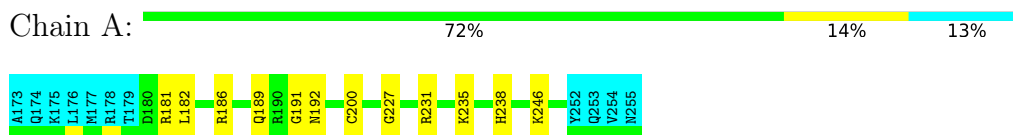
4.2.1 Score per residue for model 1

- Molecule 1: Muscleblind-like protein 1



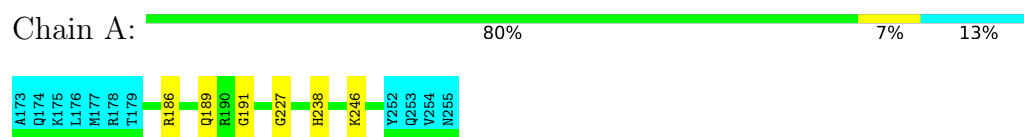
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Muscleblind-like protein 1



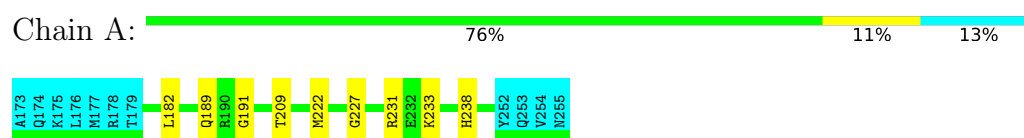
4.2.3 Score per residue for model 3

- Molecule 1: Muscleblind-like protein 1



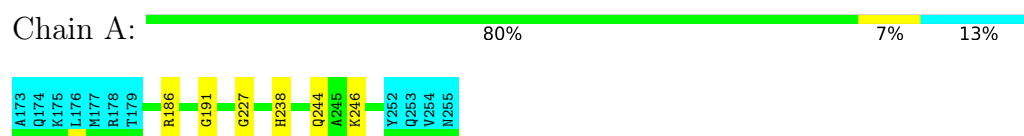
4.2.4 Score per residue for model 4

- Molecule 1: Muscleblind-like protein 1



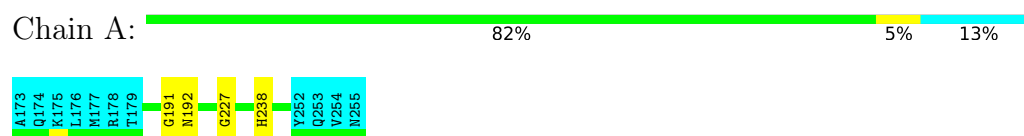
4.2.5 Score per residue for model 5

- Molecule 1: Muscleblind-like protein 1



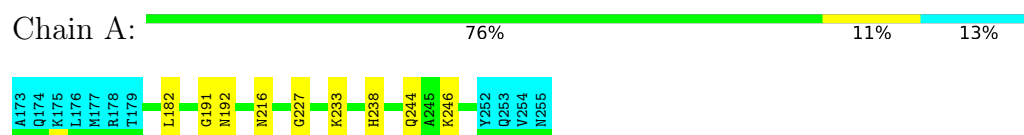
4.2.6 Score per residue for model 6

- Molecule 1: Muscleblind-like protein 1



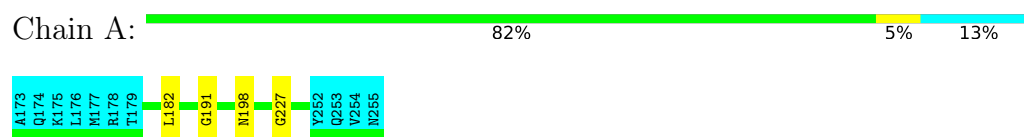
4.2.7 Score per residue for model 7

- Molecule 1: Muscleblind-like protein 1



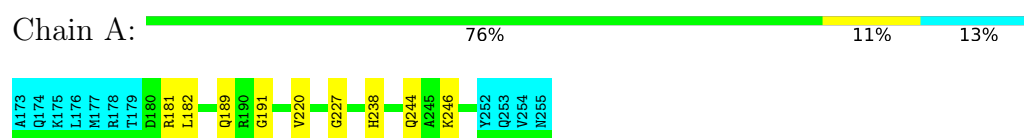
4.2.8 Score per residue for model 8

- Molecule 1: Muscleblind-like protein 1



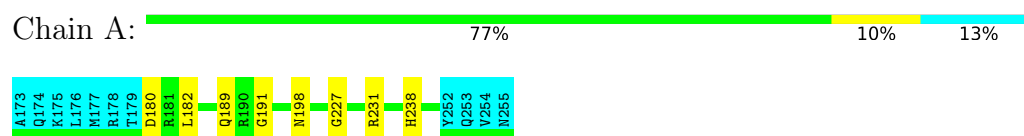
4.2.9 Score per residue for model 9

- Molecule 1: Muscleblind-like protein 1



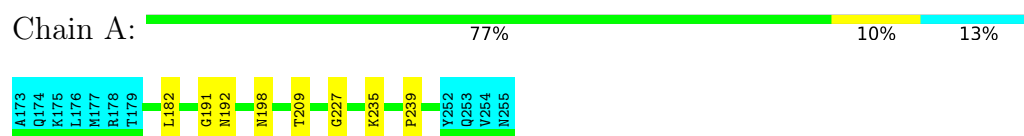
4.2.10 Score per residue for model 10

- Molecule 1: Muscleblind-like protein 1



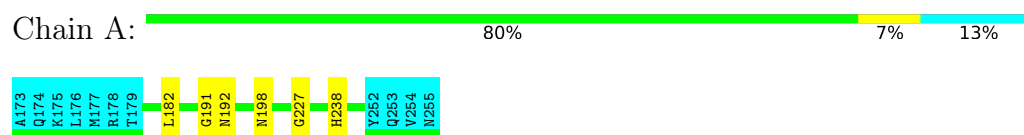
4.2.11 Score per residue for model 11

- Molecule 1: Muscleblind-like protein 1



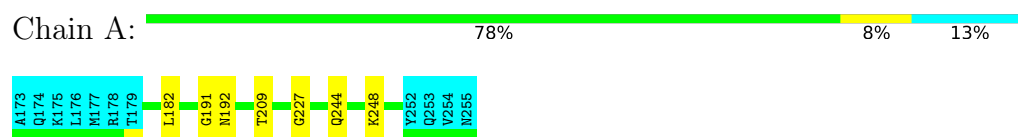
4.2.12 Score per residue for model 12

- Molecule 1: Muscleblind-like protein 1



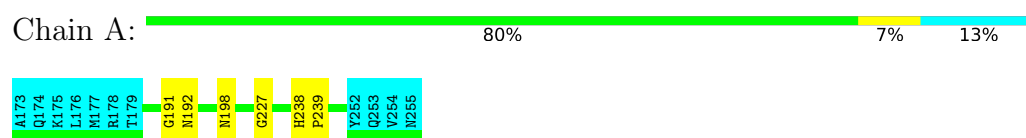
4.2.13 Score per residue for model 13

- Molecule 1: Muscleblind-like protein 1



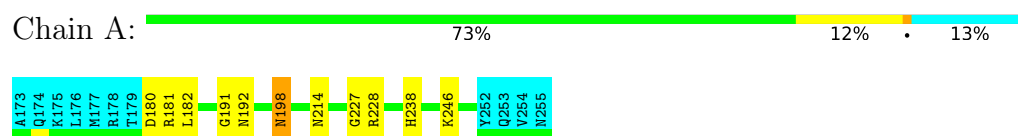
4.2.14 Score per residue for model 14

- Molecule 1: Muscleblind-like protein 1



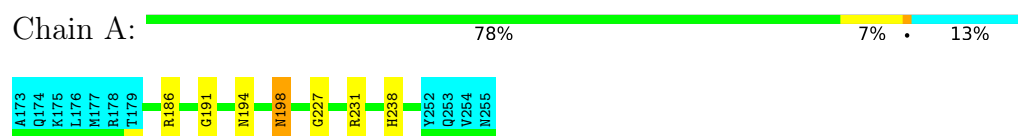
4.2.15 Score per residue for model 15

- Molecule 1: Muscleblind-like protein 1



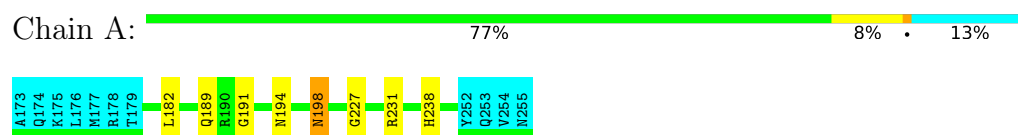
4.2.16 Score per residue for model 16

- Molecule 1: Muscleblind-like protein 1



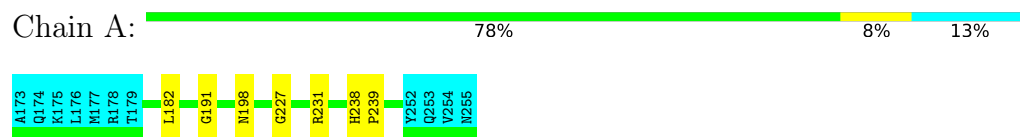
4.2.17 Score per residue for model 17

- Molecule 1: Muscleblind-like protein 1



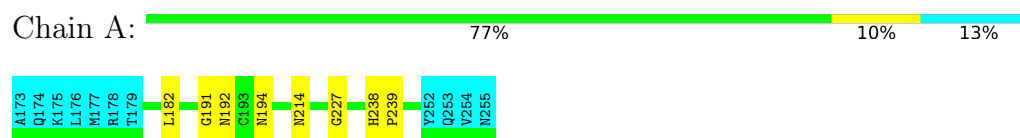
4.2.18 Score per residue for model 18

- Molecule 1: Muscleblind-like protein 1



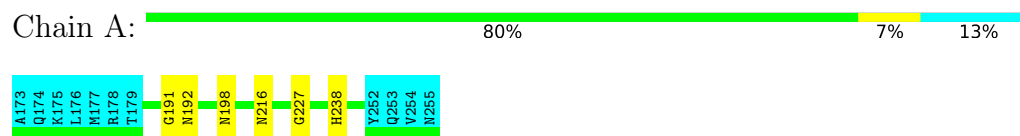
4.2.19 Score per residue for model 19

- Molecule 1: Muscleblind-like protein 1



4.2.20 Score per residue for model 20

- Molecule 1: Muscleblind-like protein 1



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
Amber	refinement	
CYANA	structure calculation	
TALOS	geometry optimization	

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	755
Number of shifts mapped to atoms	755
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	68%

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	0.88±0.01	0±0/588 (0.0± 0.0%)	1.51±0.03	2±1/791 (0.3± 0.1%)
All	All	0.88	0/11760 (0.0%)	1.51	43/15820 (0.3%)

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±0.3
All	All	0	2

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	238	HIS	CA-C-N	5.79	123.83	119.66	1	17
1	A	238	HIS	C-N-CA	5.79	123.83	119.66	1	17
1	A	181	ARG	NE-CZ-NH2	5.61	124.25	119.20	15	1
1	A	228	ARG	NE-CZ-NH2	5.40	124.06	119.20	15	1
1	A	231	ARG	NE-CZ-NH2	5.34	124.00	119.20	2	3
1	A	239	PRO	N-CA-C	5.20	116.14	110.58	14	4

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	181	ARG	Sidechain	2

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	11580	10920	10920	-

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 [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	72/83 (87%)	64±2 (89±3%)	5±2 (7±3%)	3±1 (4±1%)	4	32
All	All	1440/1660 (87%)	1284 (89%)	103 (7%)	53 (4%)	4	32

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	191	GLY	20
1	A	227	GLY	20
1	A	198	ASN	10
1	A	209	THR	3

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	63/73 (86%)	60±2 (94±3%)	4±2 (6±3%)	21 70
All	All	1260/1460 (86%)	1190 (94%)	70 (6%)	21 70

All 18 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	182	LEU	14
1	A	192	ASN	11
1	A	189	GLN	6
1	A	246	LYS	6
1	A	231	ARG	4
1	A	186	ARG	4
1	A	244	GLN	4
1	A	235	LYS	3
1	A	198	ASN	3
1	A	194	ASN	3
1	A	233	LYS	2
1	A	216	ASN	2
1	A	180	ASP	2
1	A	214	ASN	2
1	A	200	CYS	1
1	A	222	MET	1
1	A	220	VAL	1
1	A	248	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 68% for the well-defined parts and 66% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *chemical_shifts_zf34_str.txt*

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	755
Number of shifts mapped to atoms	755
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	80	-0.49 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	72	0.11 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	72	-1.59 ± 0.48	Should be applied

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 68%, i.e. 656 atoms were assigned a chemical shift out of a possible 971. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	267/357 (75%)	134/144 (93%)	70/144 (49%)	63/69 (91%)
Sidechain	371/546 (68%)	250/347 (72%)	121/165 (73%)	0/34 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	18/68 (26%)	18/34 (53%)	0/31 (0%)	0/3 (0%)
Overall	656/971 (68%)	402/525 (77%)	191/340 (56%)	63/106 (59%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 66%, i.e. 755 atoms were assigned a chemical shift out of a possible 1139. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	305/412 (74%)	153/166 (92%)	80/166 (48%)	72/80 (90%)
Sidechain	432/650 (66%)	292/414 (71%)	140/195 (72%)	0/41 (0%)
Aromatic	18/77 (23%)	18/38 (47%)	0/36 (0%)	0/3 (0%)
Overall	755/1139 (66%)	463/618 (75%)	220/397 (55%)	72/124 (58%)

7.1.4 Statistically unusual chemical shifts ⓘ

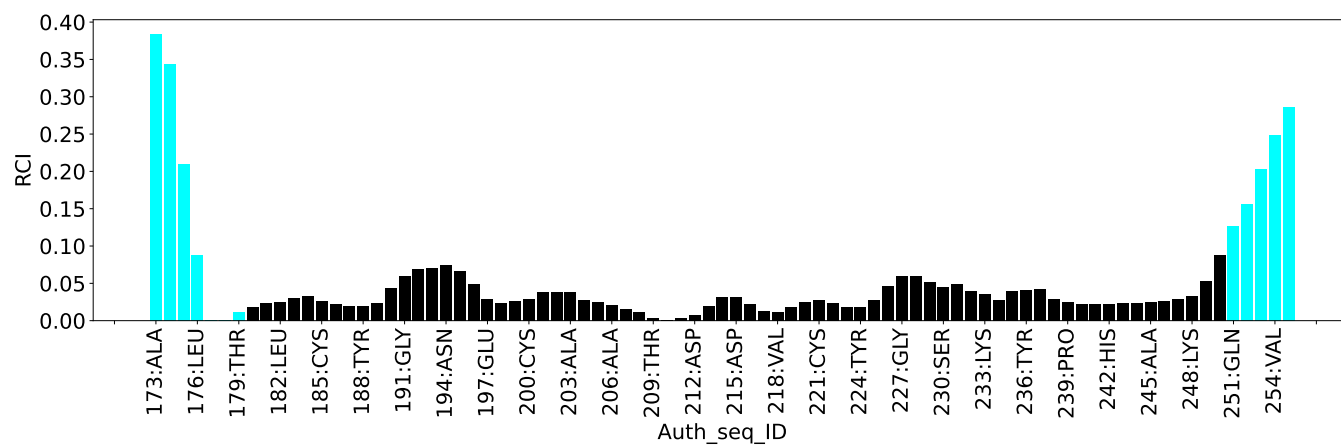
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	177	MET	H	177.00	5.39 – 11.10	295.5
1	A	178	ARG	H	178.00	5.25 – 11.22	284.4
1	A	211	ILE	N	9.27	100.55 – 142.30	-26.9
1	A	178	ARG	HB2	4.52	0.52 – 3.08	10.6
1	A	178	ARG	HA	8.46	2.06 – 6.51	9.4
1	A	177	MET	HA	8.47	2.11 – 6.67	8.9
1	A	177	MET	HB2	4.56	0.42 – 3.63	7.9
1	A	212	ASP	H	4.79	5.52 – 11.08	-6.3
1	A	181	ARG	HG3	3.24	0.15 – 2.94	6.1
1	A	238	HIS	HB2	1.24	1.36 – 4.85	-5.3

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	967
Intra-residue ($ i-j =0$)	204
Sequential ($ i-j =1$)	278
Medium range ($ i-j >1$ and $ i-j <5$)	199
Long range ($ i-j \geq 5$)	286
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	101
Number of unmapped restraints	0
Number of restraints per residue	12.6
Number of long range restraints per residue ¹	3.4

¹Long 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)	5.1	0.2
0.2-0.5 (Medium)	5.8	0.5
>0.5 (Large)	9.3	1.33

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

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

9 Distance violation analysis ⓘ

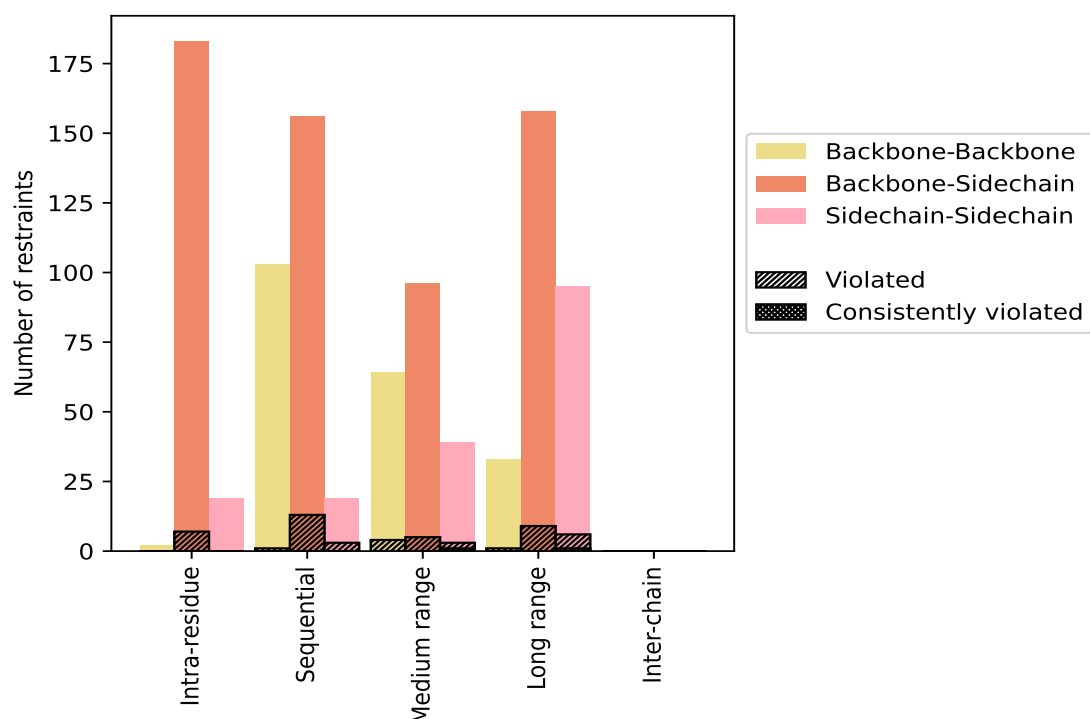
9.1 Summary of distance violations ⓘ

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	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	204	21.1	7	3.4	0.7	0	0.0	0.0
Backbone-Backbone	2	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	183	18.9	7	3.8	0.7	0	0.0	0.0
Sidechain-Sidechain	19	2.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	278	28.7	17	6.1	1.8	0	0.0	0.0
Backbone-Backbone	103	10.7	1	1.0	0.1	0	0.0	0.0
Backbone-Sidechain	156	16.1	13	8.3	1.3	0	0.0	0.0
Sidechain-Sidechain	19	2.0	3	15.8	0.3	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	199	20.6	12	6.0	1.2	1	0.5	0.1
Backbone-Backbone	64	6.6	4	6.2	0.4	0	0.0	0.0
Backbone-Sidechain	96	9.9	5	5.2	0.5	0	0.0	0.0
Sidechain-Sidechain	39	4.0	3	7.7	0.3	1	2.6	0.1
Long range (i-j ≥5)	286	29.6	16	5.6	1.7	1	0.3	0.1
Backbone-Backbone	33	3.4	1	3.0	0.1	0	0.0	0.0
Backbone-Sidechain	158	16.3	9	5.7	0.9	0	0.0	0.0
Sidechain-Sidechain	95	9.8	6	6.3	0.6	1	1.1	0.1
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	967	100.0	52	5.4	5.4	2	0.2	0.2
Backbone-Backbone	202	20.9	6	3.0	0.6	0	0.0	0.0
Backbone-Sidechain	593	61.3	34	5.7	3.5	0	0.0	0.0
Sidechain-Sidechain	172	17.8	12	7.0	1.2	2	1.2	0.2

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 [i](#)



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	6	8	8	0	23	0.44	1.03	0.28	0.31
2	2	6	7	5	0	20	0.51	1.29	0.32	0.46
3	2	6	8	7	0	23	0.54	1.29	0.3	0.51
4	2	6	7	5	0	20	0.51	1.28	0.34	0.49
5	2	6	8	5	0	21	0.42	1.08	0.29	0.37
6	1	5	7	6	0	19	0.46	1.08	0.28	0.5
7	1	3	7	7	0	18	0.49	1.09	0.28	0.46
8	3	5	5	6	0	19	0.47	1.32	0.35	0.33
9	2	5	6	8	0	21	0.47	1.09	0.32	0.36
10	2	9	8	5	0	24	0.5	1.33	0.34	0.47

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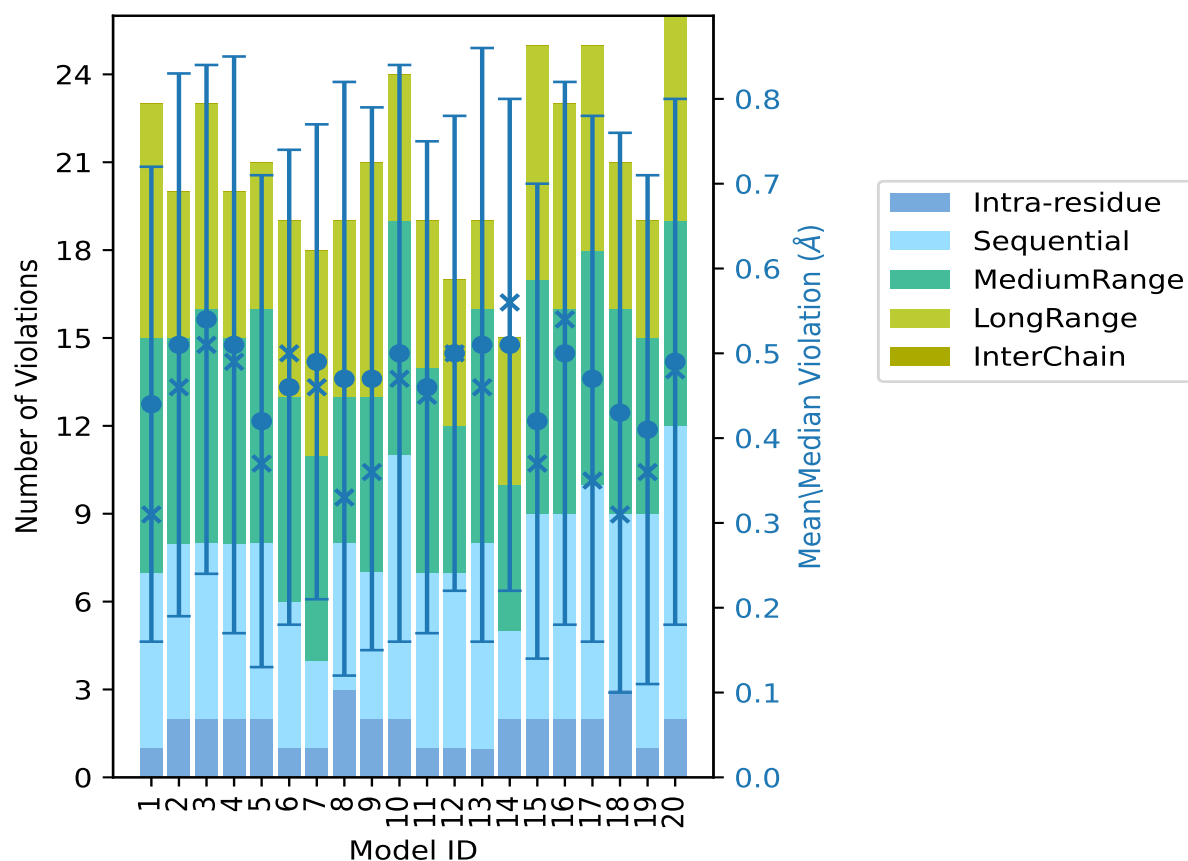
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	6	7	5	0	19	0.46	1.06	0.29	0.45
12	1	6	5	5	0	17	0.5	1.0	0.28	0.5
13	1	7	8	3	0	19	0.51	1.31	0.35	0.46
14	2	3	5	5	0	15	0.51	1.03	0.29	0.56
15	2	7	8	8	0	25	0.42	1.07	0.28	0.37
16	2	7	7	7	0	23	0.5	1.3	0.32	0.54
17	2	8	8	7	0	25	0.47	1.3	0.31	0.35
18	3	6	7	5	0	21	0.43	1.33	0.33	0.31
19	1	8	6	4	0	19	0.41	1.06	0.3	0.36
20	2	10	7	7	0	26	0.49	1.06	0.31	0.48

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

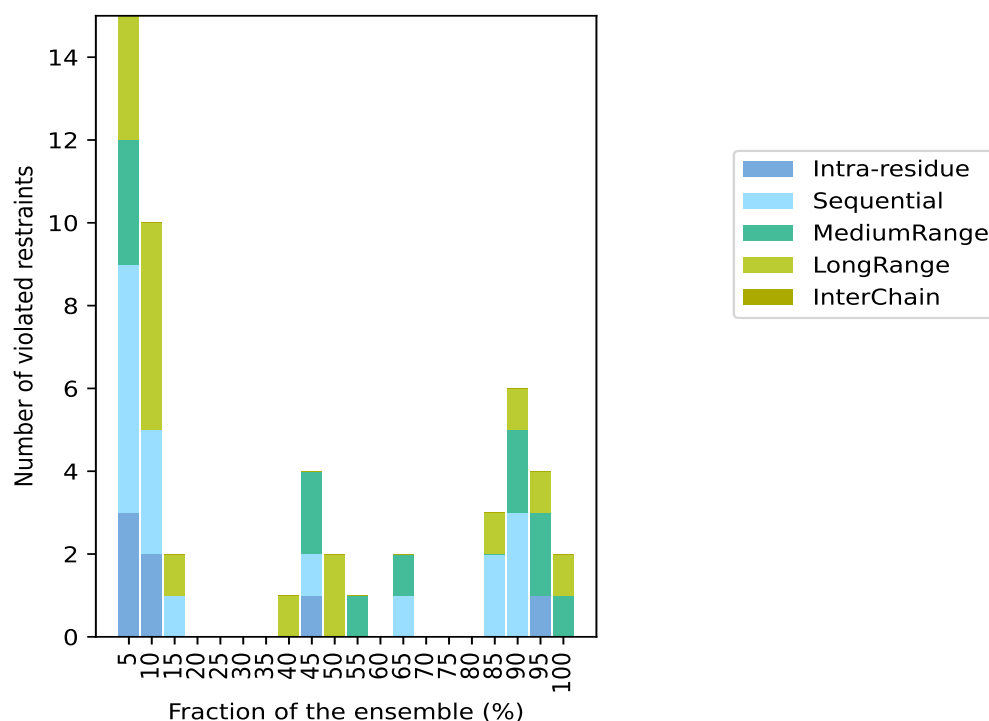
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 915(IR:197, SQ:261, MR:187, LR:270, IC:0) restraints are 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	%
3	6	3	3	0	15	1	5.0
2	3	0	5	0	10	2	10.0
0	1	0	1	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	1	0	1	8	40.0
1	1	2	0	0	4	9	45.0
0	0	0	2	0	2	10	50.0
0	0	1	0	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	1	1	0	0	2	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	2	0	1	0	3	17	85.0
0	3	2	1	0	6	18	90.0
1	0	2	1	0	4	19	95.0
0	0	1	1	0	2	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

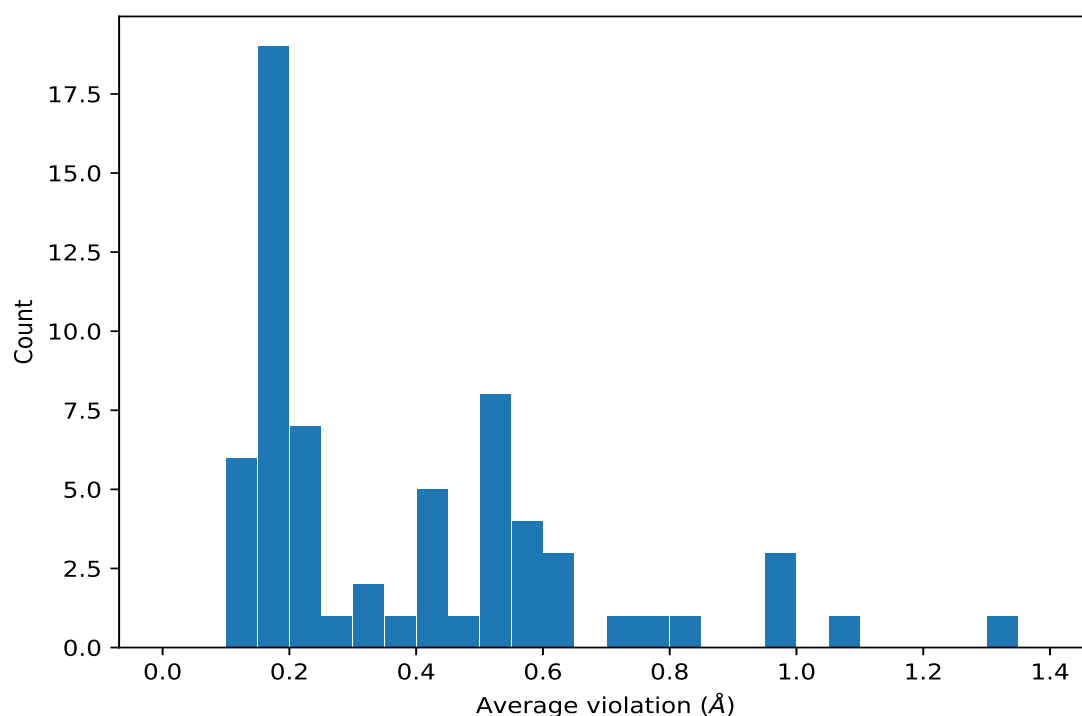
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	20	0.99	0.01	0.99
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	20	0.99	0.01	0.99
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	20	0.6	0.05	0.59
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	19	0.82	0.11	0.84
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	19	0.53	0.16	0.52
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	19	0.23	0.05	0.26
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	19	0.22	0.07	0.22
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	18	1.06	0.04	1.06
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	18	0.75	0.02	0.74
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	18	0.61	0.05	0.6
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	18	0.55	0.06	0.55
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	18	0.55	0.06	0.55
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	18	0.23	0.11	0.2
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	18	0.23	0.11	0.2
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	18	0.23	0.11	0.2
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	18	0.15	0.01	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	17	0.53	0.16	0.55
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	17	0.23	0.1	0.23
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	17	0.17	0.04	0.16
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	13	0.39	0.13	0.41
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	13	0.2	0.07	0.18
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	11	0.11	0.01	0.1
(1,668)	1:224:A:TYR:HE1	1:239:A:PRO:HD3	10	0.56	0.16	0.56
(1,668)	1:224:A:TYR:HE2	1:239:A:PRO:HD3	10	0.56	0.16	0.56
(1,156)	1:184:A:VAL:H	1:216:A:ASN:HB2	10	0.33	0.13	0.3
(1,310)	1:192:A:ASN:HB3	1:194:A:ASN:H	9	1.31	0.02	1.3
(1,296)	1:191:A:GLY:H	1:192:A:ASN:HB2	9	0.47	0.01	0.47
(1,307)	1:192:A:ASN:H	1:192:A:ASN:HB2	9	0.32	0.03	0.33
(1,230)	1:186:A:ARG:H	1:189:A:GLN:HB2	9	0.29	0.14	0.28
(1,76)	1:181:A:ARG:HD2	1:218:A:VAL:H	8	0.6	0.13	0.6
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD11	3	0.19	0.03	0.21
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD12	3	0.19	0.03	0.21
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD13	3	0.19	0.03	0.21
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD11	3	0.19	0.03	0.21
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD12	3	0.19	0.03	0.21
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD13	3	0.19	0.03	0.21
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD11	3	0.19	0.03	0.21
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD12	3	0.19	0.03	0.21
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD13	3	0.19	0.03	0.21
(1,533)	1:218:A:VAL:HG21	1:219:A:THR:HB	3	0.13	0.02	0.13
(1,533)	1:218:A:VAL:HG22	1:219:A:THR:HB	3	0.13	0.02	0.13
(1,533)	1:218:A:VAL:HG23	1:219:A:THR:HB	3	0.13	0.02	0.13
(1,358)	1:197:A:GLU:HA	1:198:A:ASN:HB2	2	0.96	0.03	0.96
(1,730)	1:226:A:LYS:H	1:226:A:LYS:HG3	2	0.74	0.03	0.74
(1,570)	1:220:A:VAL:HG21	1:238:A:HIS:H	2	0.5	0.3	0.5
(1,570)	1:220:A:VAL:HG22	1:238:A:HIS:H	2	0.5	0.3	0.5
(1,570)	1:220:A:VAL:HG23	1:238:A:HIS:H	2	0.5	0.3	0.5
(1,555)	1:220:A:VAL:HG21	1:239:A:PRO:HA	2	0.5	0.32	0.5
(1,555)	1:220:A:VAL:HG22	1:239:A:PRO:HA	2	0.5	0.32	0.5
(1,555)	1:220:A:VAL:HG23	1:239:A:PRO:HA	2	0.5	0.32	0.5
(1,66)	1:181:A:ARG:HD3	1:218:A:VAL:H	2	0.43	0.08	0.43
(1,563)	1:220:A:VAL:HG21	1:238:A:HIS:HA	2	0.42	0.26	0.42
(1,563)	1:220:A:VAL:HG22	1:238:A:HIS:HA	2	0.42	0.26	0.42
(1,563)	1:220:A:VAL:HG23	1:238:A:HIS:HA	2	0.42	0.26	0.42
(1,723)	1:226:A:LYS:HG3	1:227:A:GLY:H	2	0.42	0.04	0.42
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD11	2	0.18	0.06	0.18
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD12	2	0.18	0.06	0.18
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD13	2	0.18	0.06	0.18

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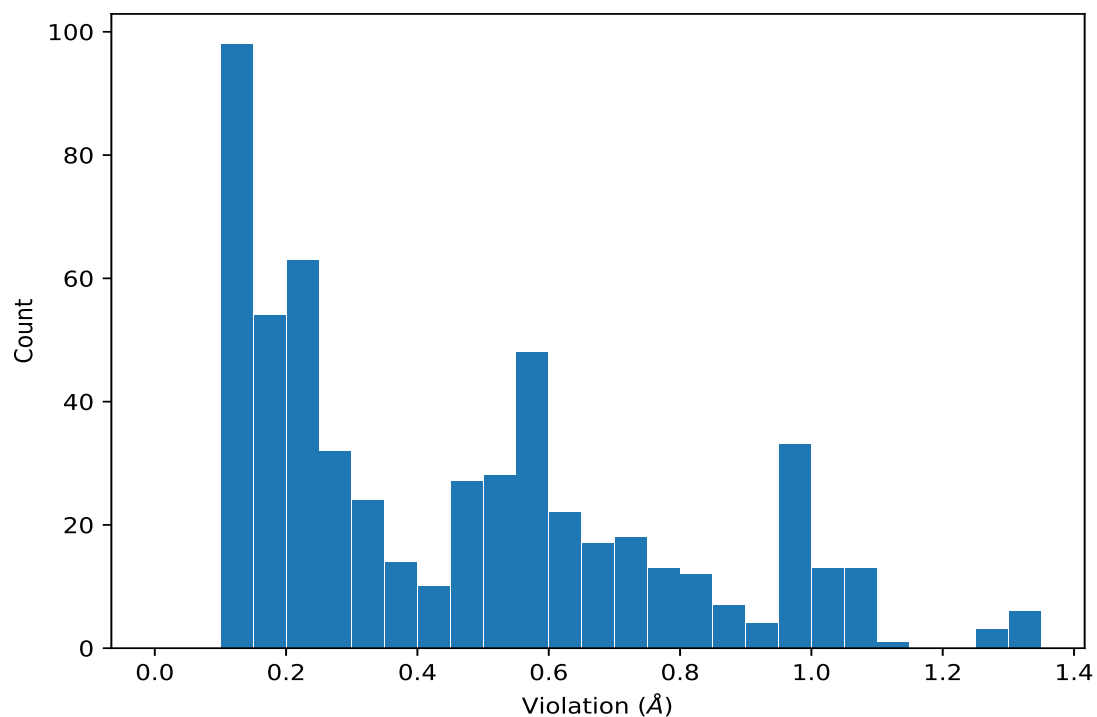
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD21	2	0.18	0.06	0.18
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD22	2	0.18	0.06	0.18
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD23	2	0.18	0.06	0.18
(1,945)	1:248:A:LYS:H	1:248:A:LYS:HG2	2	0.18	0.03	0.18
(1,945)	1:248:A:LYS:H	1:248:A:LYS:HG3	2	0.18	0.03	0.18
(1,250)	1:187:A:GLU:H	1:188:A:TYR:HD1	2	0.12	0.0	0.12
(1,250)	1:187:A:GLU:H	1:188:A:TYR:HD2	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,310)	1:192:A:ASN:HB3	1:194:A:ASN:H	10	1.33
(1,310)	1:192:A:ASN:HB3	1:194:A:ASN:H	18	1.33
(1,310)	1:192:A:ASN:HB3	1:194:A:ASN:H	8	1.32
(1,310)	1:192:A:ASN:HB3	1:194:A:ASN:H	13	1.31
(1,310)	1:192:A:ASN:HB3	1:194:A:ASN:H	16	1.3
(1,310)	1:192:A:ASN:HB3	1:194:A:ASN:H	17	1.3
(1,310)	1:192:A:ASN:HB3	1:194:A:ASN:H	2	1.29
(1,310)	1:192:A:ASN:HB3	1:194:A:ASN:H	3	1.29
(1,310)	1:192:A:ASN:HB3	1:194:A:ASN:H	4	1.28
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	17	1.1
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	3	1.09
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	7	1.09
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	9	1.09
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	5	1.08
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	6	1.08
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	13	1.08
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	16	1.08
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	15	1.07
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	2	1.06
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	10	1.06
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	11	1.06
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	19	1.06
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	20	1.06
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	1	1.03
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	14	1.03
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	2	1.01
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	2	1.01
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	4	1.01
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	4	1.01
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	10	1.0
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	10	1.0
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	12	1.0
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	12	1.0
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	19	1.0
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	19	1.0
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	20	1.0
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	6	0.99
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	6	0.99
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	8	0.99
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	8	0.99
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	9	0.99
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	9	0.99
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	13	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	13	0.99
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	14	0.99
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	14	0.99
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	15	0.99
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	15	0.99
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	16	0.99
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	16	0.99
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	17	0.99
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	17	0.99
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	18	0.99
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	18	0.99
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	20	0.99
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	20	0.99
(1,358)	1:197:A:GLU:HA	1:198:A:ASN:HB2	20	0.99
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	1	0.98
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	1	0.98
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	3	0.98
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	3	0.98
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	5	0.98
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	5	0.98
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	7	0.98
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	7	0.98
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	4	0.98
(1,819)	1:237:A:PHE:HE1	1:239:A:PRO:HD2	11	0.97
(1,819)	1:237:A:PHE:HE2	1:239:A:PRO:HD2	11	0.97
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	1	0.96
(1,634)	1:223:A:ASP:HA	1:226:A:LYS:HG2	12	0.95
(1,358)	1:197:A:GLU:HA	1:198:A:ASN:HB2	10	0.94
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	13	0.93
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	10	0.9
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	8	0.89
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	4	0.88
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	5	0.87
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	9	0.87
(1,668)	1:224:A:TYR:HE1	1:239:A:PRO:HD3	8	0.86
(1,668)	1:224:A:TYR:HE2	1:239:A:PRO:HD3	8	0.86
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	16	0.86
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	7	0.85
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	3	0.84
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	12	0.83
(1,555)	1:220:A:VAL:HG21	1:239:A:PRO:HA	9	0.82
(1,555)	1:220:A:VAL:HG22	1:239:A:PRO:HA	9	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:220:A:VAL:HG23	1:239:A:PRO:HA	9	0.82
(1,570)	1:220:A:VAL:HG21	1:238:A:HIS:H	9	0.81
(1,570)	1:220:A:VAL:HG22	1:238:A:HIS:H	9	0.81
(1,570)	1:220:A:VAL:HG23	1:238:A:HIS:H	9	0.81
(1,76)	1:181:A:ARG:HD2	1:218:A:VAL:H	20	0.81
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	11	0.8
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	17	0.8
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	10	0.79
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	2	0.78
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	4	0.78
(1,730)	1:226:A:LYS:H	1:226:A:LYS:HG3	18	0.77
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	12	0.77
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	14	0.77
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	8	0.77
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	13	0.76
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	15	0.76
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	18	0.76
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	18	0.76
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	7	0.75
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	9	0.75
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	3	0.74
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	5	0.74
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	12	0.74
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	14	0.74
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	1	0.73
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	6	0.73
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	11	0.73
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	16	0.73
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	20	0.73
(1,76)	1:181:A:ARG:HD2	1:218:A:VAL:H	15	0.73
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	19	0.72
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	15	0.72
(1,730)	1:226:A:LYS:H	1:226:A:LYS:HG3	8	0.71
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	4	0.71
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	4	0.71
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	4	0.71
(1,668)	1:224:A:TYR:HE1	1:239:A:PRO:HD3	17	0.71
(1,668)	1:224:A:TYR:HE2	1:239:A:PRO:HD3	17	0.71
(1,711)	1:225:A:ILE:H	1:226:A:LYS:HG2	17	0.7
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	3	0.69
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	12	0.69
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	12	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:220:A:VAL:HG21	1:238:A:HIS:HA	9	0.69
(1,563)	1:220:A:VAL:HG22	1:238:A:HIS:HA	9	0.69
(1,563)	1:220:A:VAL:HG23	1:238:A:HIS:HA	9	0.69
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	3	0.68
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	8	0.68
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	3	0.68
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	1	0.67
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	2	0.67
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	15	0.67
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	20	0.67
(1,668)	1:224:A:TYR:HE1	1:239:A:PRO:HD3	3	0.65
(1,668)	1:224:A:TYR:HE2	1:239:A:PRO:HD3	3	0.65
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	11	0.65
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	2	0.64
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	11	0.64
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	16	0.64
(1,76)	1:181:A:ARG:HD2	1:218:A:VAL:H	6	0.64
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	20	0.63
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	15	0.63
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	13	0.63
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	6	0.62
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	10	0.62
(1,668)	1:224:A:TYR:HE1	1:239:A:PRO:HD3	2	0.62
(1,668)	1:224:A:TYR:HE2	1:239:A:PRO:HD3	2	0.62
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	1	0.62
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	2	0.62
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	17	0.62
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	1	0.62
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	6	0.62
(1,156)	1:184:A:VAL:H	1:216:A:ASN:HB2	20	0.62
(1,76)	1:181:A:ARG:HD2	1:218:A:VAL:H	7	0.62
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	20	0.61
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	19	0.61
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	5	0.61
(1,230)	1:186:A:ARG:H	1:189:A:GLN:HB2	20	0.61
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	19	0.6
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	7	0.6
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	15	0.6
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	16	0.6
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	19	0.6
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	12	0.59
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	18	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	9	0.59
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	13	0.59
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	14	0.59
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	9	0.59
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	14	0.59
(1,668)	1:224:A:TYR:HE1	1:239:A:PRO:HD3	20	0.58
(1,668)	1:224:A:TYR:HE2	1:239:A:PRO:HD3	20	0.58
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	10	0.58
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	16	0.58
(1,446)	1:205:A:PRO:HG2	1:218:A:VAL:HB	6	0.58
(1,76)	1:181:A:ARG:HD2	1:218:A:VAL:H	10	0.58
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	10	0.57
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	10	0.57
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	11	0.57
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	11	0.57
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	1	0.57
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	3	0.57
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	5	0.57
(1,694)	1:225:A:ILE:HB	1:226:A:LYS:HG2	17	0.57
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	7	0.57
(1,76)	1:181:A:ARG:HD2	1:218:A:VAL:H	14	0.57
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	2	0.56
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	2	0.56
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	6	0.56
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	6	0.56
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	14	0.56
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	14	0.56
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	15	0.56
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	15	0.56
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	19	0.56
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	19	0.56
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	12	0.56
(1,156)	1:184:A:VAL:H	1:216:A:ASN:HB2	7	0.56
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	3	0.55
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	11	0.55
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	14	0.55
(1,668)	1:224:A:TYR:HE1	1:239:A:PRO:HD3	16	0.55
(1,668)	1:224:A:TYR:HE2	1:239:A:PRO:HD3	16	0.55
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	13	0.55
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	19	0.55
(1,76)	1:181:A:ARG:HD2	1:218:A:VAL:H	16	0.55
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	16	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	16	0.54
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	16	0.54
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	4	0.54
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	11	0.54
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	18	0.54
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	1	0.53
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	4	0.53
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	10	0.53
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	13	0.53
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	13	0.53
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	20	0.53
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	20	0.53
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	17	0.53
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	9	0.52
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	9	0.52
(1,652)	1:224:A:TYR:HB2	1:239:A:PRO:HD2	6	0.52
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	4	0.52
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	1	0.51
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	1	0.51
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	5	0.51
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	5	0.51
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	17	0.51
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	17	0.51
(1,66)	1:181:A:ARG:HD3	1:218:A:VAL:H	3	0.51
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	16	0.5
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	6	0.5
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	12	0.5
(1,668)	1:224:A:TYR:HE1	1:239:A:PRO:HD3	5	0.49
(1,668)	1:224:A:TYR:HE2	1:239:A:PRO:HD3	5	0.49
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	15	0.48
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	3	0.48
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	3	0.48
(1,296)	1:191:A:GLY:H	1:192:A:ASN:HB2	3	0.48
(1,296)	1:191:A:GLY:H	1:192:A:ASN:HB2	8	0.48
(1,296)	1:191:A:GLY:H	1:192:A:ASN:HB2	10	0.48
(1,296)	1:191:A:GLY:H	1:192:A:ASN:HB2	17	0.48
(1,723)	1:226:A:LYS:HG3	1:227:A:GLY:H	18	0.47
(1,697)	1:225:A:ILE:HG12	1:226:A:LYS:HG2	7	0.47
(1,697)	1:225:A:ILE:HG13	1:226:A:LYS:HG2	7	0.47
(1,296)	1:191:A:GLY:H	1:192:A:ASN:HB2	16	0.47
(1,296)	1:191:A:GLY:H	1:192:A:ASN:HB2	18	0.47
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	7	0.46
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	10	0.46
(1,296)	1:191:A:GLY:H	1:192:A:ASN:HB2	2	0.46
(1,296)	1:191:A:GLY:H	1:192:A:ASN:HB2	4	0.46
(1,296)	1:191:A:GLY:H	1:192:A:ASN:HB2	13	0.46
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	13	0.46
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	13	0.46
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	13	0.46
(1,608)	1:222:A:MET:HG2	1:225:A:ILE:HB	14	0.45
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	11	0.45
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	11	0.45
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	11	0.45
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	17	0.44
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	2	0.44
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	15	0.44
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	20	0.43
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	5	0.41
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	7	0.41
(1,668)	1:224:A:TYR:HE1	1:239:A:PRO:HD3	7	0.41
(1,668)	1:224:A:TYR:HE2	1:239:A:PRO:HD3	7	0.41
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	20	0.41
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	10	0.4
(1,668)	1:224:A:TYR:HE1	1:239:A:PRO:HD3	15	0.39
(1,668)	1:224:A:TYR:HE2	1:239:A:PRO:HD3	15	0.39
(1,723)	1:226:A:LYS:HG3	1:227:A:GLY:H	8	0.38
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	5	0.37
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	15	0.37
(1,230)	1:186:A:ARG:H	1:189:A:GLN:HB2	5	0.37
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	19	0.36
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	20	0.36
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	9	0.36
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	9	0.36
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	9	0.36
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	19	0.36
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	19	0.36
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	19	0.36
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	6	0.35
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	3	0.35
(1,307)	1:192:A:ASN:H	1:192:A:ASN:HB2	4	0.35
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	5	0.35
(1,66)	1:181:A:ARG:HD3	1:218:A:VAL:H	17	0.35
(1,307)	1:192:A:ASN:H	1:192:A:ASN:HB2	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:192:A:ASN:H	1:192:A:ASN:HB2	16	0.34
(1,307)	1:192:A:ASN:H	1:192:A:ASN:HB2	17	0.34
(1,307)	1:192:A:ASN:H	1:192:A:ASN:HB2	8	0.33
(1,307)	1:192:A:ASN:H	1:192:A:ASN:HB2	10	0.33
(1,307)	1:192:A:ASN:H	1:192:A:ASN:HB2	18	0.33
(1,230)	1:186:A:ARG:H	1:189:A:GLN:HB2	1	0.33
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	9	0.32
(1,76)	1:181:A:ARG:HD2	1:218:A:VAL:H	2	0.32
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	20	0.31
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	17	0.31
(1,668)	1:224:A:TYR:HE1	1:239:A:PRO:HD3	1	0.31
(1,668)	1:224:A:TYR:HE2	1:239:A:PRO:HD3	1	0.31
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	8	0.31
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	18	0.31
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	12	0.31
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	13	0.31
(1,230)	1:186:A:ARG:H	1:189:A:GLN:HB2	17	0.31
(1,156)	1:184:A:VAL:H	1:216:A:ASN:HB2	12	0.31
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	11	0.3
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	15	0.3
(1,156)	1:184:A:VAL:H	1:216:A:ASN:HB2	3	0.3
(1,156)	1:184:A:VAL:H	1:216:A:ASN:HB2	6	0.3
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	4	0.29
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	6	0.29
(1,293)	1:190:A:ARG:H	1:190:A:ARG:HB2	15	0.29
(1,156)	1:184:A:VAL:H	1:216:A:ASN:HB2	10	0.29
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	1	0.28
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	20	0.28
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	11	0.28
(1,230)	1:186:A:ARG:H	1:189:A:GLN:HB2	3	0.28
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	14	0.27
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	18	0.27
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	1	0.27
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	17	0.27
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	5	0.27
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	3	0.27
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	3	0.27
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	3	0.27
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	16	0.26
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	17	0.26
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	19	0.26
(1,307)	1:192:A:ASN:H	1:192:A:ASN:HB2	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:184:A:VAL:H	1:216:A:ASN:HB2	1	0.26
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	12	0.25
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	15	0.25
(1,307)	1:192:A:ASN:H	1:192:A:ASN:HB2	13	0.25
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	1	0.25
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	7	0.25
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	7	0.25
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	7	0.25
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	8	0.24
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	6	0.24
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	7	0.24
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	11	0.24
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	13	0.24
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	17	0.23
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	3	0.23
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	12	0.23
(1,230)	1:186:A:ARG:H	1:189:A:GLN:HB2	12	0.23
(1,156)	1:184:A:VAL:H	1:216:A:ASN:HB2	5	0.23
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	4	0.23
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	4	0.23
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	4	0.23
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD11	9	0.23
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD12	9	0.23
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD13	9	0.23
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD21	9	0.23
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD22	9	0.23
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD23	9	0.23
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	1	0.22
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	16	0.22
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	10	0.22
(1,230)	1:186:A:ARG:H	1:189:A:GLN:HB2	18	0.22
(1,156)	1:184:A:VAL:H	1:216:A:ASN:HB2	17	0.22
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD11	9	0.22
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD12	9	0.22
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD13	9	0.22
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD11	9	0.22
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD12	9	0.22
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD13	9	0.22
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD11	9	0.22
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD12	9	0.22
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD13	9	0.22
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	10	0.21
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	18	0.21
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	17	0.21
(1,156)	1:184:A:VAL:H	1:216:A:ASN:HB2	4	0.21
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD11	15	0.21
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD12	15	0.21
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD13	15	0.21
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD11	15	0.21
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD12	15	0.21
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD13	15	0.21
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD11	15	0.21
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD12	15	0.21
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD13	15	0.21
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	8	0.21
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	8	0.21
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	8	0.21
(1,945)	1:248:A:LYS:H	1:248:A:LYS:HG2	5	0.2
(1,945)	1:248:A:LYS:H	1:248:A:LYS:HG3	5	0.2
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	2	0.2
(1,570)	1:220:A:VAL:HG21	1:238:A:HIS:H	1	0.2
(1,570)	1:220:A:VAL:HG22	1:238:A:HIS:H	1	0.2
(1,570)	1:220:A:VAL:HG23	1:238:A:HIS:H	1	0.2
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	12	0.2
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	2	0.2
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	15	0.2
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	19	0.2
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	2	0.2
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	2	0.2
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	2	0.2
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	19	0.19
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	14	0.19
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	14	0.19
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	14	0.19
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	15	0.19
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	15	0.19
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	15	0.19
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	3	0.18
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	15	0.18
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	8	0.18
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	18	0.18
(1,218)	1:186:A:ARG:H	1:202:A:PHE:HB3	8	0.18
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	7	0.17
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	9	0.17
(1,555)	1:220:A:VAL:HG21	1:239:A:PRO:HA	1	0.17
(1,555)	1:220:A:VAL:HG22	1:239:A:PRO:HA	1	0.17
(1,555)	1:220:A:VAL:HG23	1:239:A:PRO:HA	1	0.17
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	5	0.17
(1,472)	1:212:A:ASP:HB2	1:215:A:ASP:H	9	0.17
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	4	0.17
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	3	0.17
(1,230)	1:186:A:ARG:H	1:189:A:GLN:HB2	11	0.17
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	16	0.17
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	16	0.17
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	16	0.17
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	5	0.16
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	7	0.16
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	10	0.16
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	11	0.16
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	17	0.16
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	19	0.16
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	20	0.16
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	5	0.16
(1,844)	1:239:A:PRO:HD2	1:244:A:GLN:HG2	7	0.16
(1,563)	1:220:A:VAL:HG21	1:238:A:HIS:HA	1	0.16
(1,563)	1:220:A:VAL:HG22	1:238:A:HIS:HA	1	0.16
(1,563)	1:220:A:VAL:HG23	1:238:A:HIS:HA	1	0.16
(1,533)	1:218:A:VAL:HG21	1:219:A:THR:HB	6	0.16
(1,533)	1:218:A:VAL:HG22	1:219:A:THR:HB	6	0.16
(1,533)	1:218:A:VAL:HG23	1:219:A:THR:HB	6	0.16
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	4	0.16
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	11	0.16
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	20	0.16
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	1	0.16
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	12	0.16
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	20	0.16
(1,163)	1:184:A:VAL:H	1:216:A:ASN:HB3	16	0.16
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	12	0.16
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	12	0.16
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	12	0.16
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	17	0.16
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	17	0.16
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	17	0.16
(1,945)	1:248:A:LYS:H	1:248:A:LYS:HG2	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	1:248:A:LYS:H	1:248:A:LYS:HG3	9	0.15
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	6	0.15
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	9	0.15
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	13	0.15
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	14	0.15
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	15	0.15
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	13	0.15
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	5	0.15
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	8	0.15
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	11	0.15
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	13	0.15
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD11	11	0.15
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD12	11	0.15
(1,151)	1:184:A:VAL:HG21	1:211:A:ILE:HD13	11	0.15
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD11	11	0.15
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD12	11	0.15
(1,151)	1:184:A:VAL:HG22	1:211:A:ILE:HD13	11	0.15
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD11	11	0.15
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD12	11	0.15
(1,151)	1:184:A:VAL:HG23	1:211:A:ILE:HD13	11	0.15
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	3	0.14
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	16	0.14
(1,911)	1:246:A:LYS:HA	1:246:A:LYS:HD3	10	0.14
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	6	0.14
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	9	0.14
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	18	0.14
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	20	0.14
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	20	0.14
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	20	0.14
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	1	0.13
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	18	0.13
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	14	0.13
(1,533)	1:218:A:VAL:HG21	1:219:A:THR:HB	20	0.13
(1,533)	1:218:A:VAL:HG22	1:219:A:THR:HB	20	0.13
(1,533)	1:218:A:VAL:HG23	1:219:A:THR:HB	20	0.13
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	2	0.13
(1,479)	1:212:A:ASP:HB2	1:214:A:ASN:H	10	0.13
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	16	0.13
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	2	0.13
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	6	0.13
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	6	0.13
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,812)	1:235:A:LYS:HG2	1:236:A:TYR:HA	10	0.12
(1,812)	1:235:A:LYS:HG3	1:236:A:TYR:HA	10	0.12
(1,753)	1:230:A:SER:H	1:231:A:ARG:HG2	20	0.12
(1,753)	1:230:A:SER:H	1:231:A:ARG:HG3	20	0.12
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	18	0.12
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	17	0.12
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	9	0.12
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	16	0.12
(1,281)	1:188:A:TYR:H	1:189:A:GLN:HB2	19	0.12
(1,264)	1:188:A:TYR:HA	1:190:A:ARG:H	15	0.12
(1,250)	1:187:A:GLU:H	1:188:A:TYR:HD1	15	0.12
(1,250)	1:187:A:GLU:H	1:188:A:TYR:HD2	15	0.12
(1,129)	1:183:A:GLU:H	1:183:A:GLU:HG2	14	0.12
(1,129)	1:183:A:GLU:H	1:183:A:GLU:HG3	14	0.12
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	18	0.12
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	18	0.12
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	18	0.12
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD11	18	0.12
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD12	18	0.12
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD13	18	0.12
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD21	18	0.12
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD22	18	0.12
(1,91)	1:182:A:LEU:HB2	1:243:A:LEU:HD23	18	0.12
(1,928)	1:247:A:ILE:HA	1:250:A:ALA:HA	4	0.11
(1,855)	1:240:A:PRO:HG3	1:243:A:LEU:HG	4	0.11
(1,829)	1:238:A:HIS:H	1:238:A:HIS:HD2	20	0.11
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	6	0.11
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	7	0.11
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	10	0.11
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	13	0.11
(1,533)	1:218:A:VAL:HG21	1:219:A:THR:HB	18	0.11
(1,533)	1:218:A:VAL:HG22	1:219:A:THR:HB	18	0.11
(1,533)	1:218:A:VAL:HG23	1:219:A:THR:HB	18	0.11
(1,492)	1:213:A:THR:H	1:214:A:ASN:HB2	19	0.11
(1,475)	1:212:A:ASP:HB3	1:213:A:THR:H	8	0.11
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	8	0.11
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	16	0.11
(1,250)	1:187:A:GLU:H	1:188:A:TYR:HD1	10	0.11
(1,250)	1:187:A:GLU:H	1:188:A:TYR:HD2	10	0.11
(1,230)	1:186:A:ARG:H	1:189:A:GLN:HB2	13	0.11
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG11	5	0.11
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG12	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:182:A:LEU:H	1:218:A:VAL:HG13	5	0.11
(1,1)	1:175:A:LYS:HA	1:176:A:LEU:H	17	0.11
(1,929)	1:247:A:ILE:HA	1:251:A:GLN:H	8	0.1
(1,749)	1:230:A:SER:HB2	1:231:A:ARG:HA	20	0.1
(1,748)	1:229:A:CYS:H	1:230:A:SER:HB3	19	0.1
(1,688)	1:225:A:ILE:HA	1:248:A:LYS:HA	15	0.1
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	1	0.1
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	5	0.1
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	9	0.1
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	11	0.1
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	15	0.1
(1,678)	1:224:A:TYR:HA	1:226:A:LYS:H	19	0.1
(1,284)	1:189:A:GLN:HB2	1:190:A:ARG:H	19	0.1

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

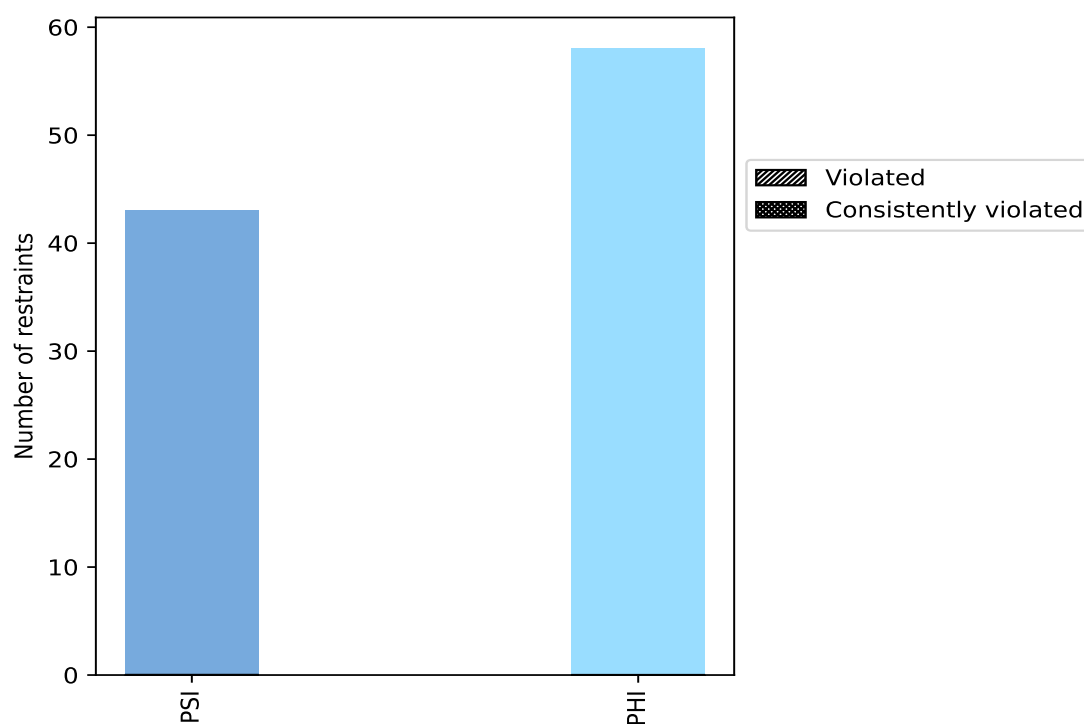
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	43	42.6	0	0.0	0.0	0	0.0	0.0
PHI	58	57.4	0	0.0	0.0	0	0.0	0.0
Total	101	100.0	0	0.0	0.0	0	0.0	0.0

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

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



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

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

No violations found

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

No violations found

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

No violations found

10.5 All violated dihedral-angle restraints [i](#)

No violations found