wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	8K31
BMRB ID	:	50583
Title	:	The complex of WRKY33 C terminal DBD and SIB1
Authors	:	Dong, X.; Gong, Z.; Hu, Y.F.
Deposited on	:	2023-07-14

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

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

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

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

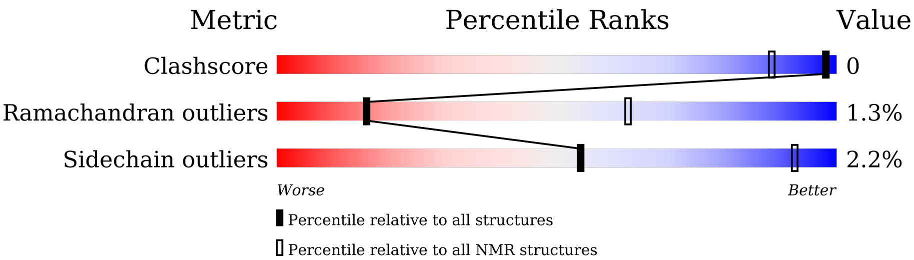
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 1%.

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	98	17% 5% 13% 64%
2	B	101	60% 15% • 22%

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 20 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:49-A:70, B:346-B:421 (98)	1.14	5

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1820 atoms, of which 904 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sigma factor binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	35	544	170	269	47	56	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	initiating methionine	UNP Q9LDH1
A	101	LEU	-	expression tag	UNP Q9LDH1
A	102	GLU	-	expression tag	UNP Q9LDH1
A	103	HIS	-	expression tag	UNP Q9LDH1
A	104	HIS	-	expression tag	UNP Q9LDH1
A	105	HIS	-	expression tag	UNP Q9LDH1
A	106	HIS	-	expression tag	UNP Q9LDH1
A	107	HIS	-	expression tag	UNP Q9LDH1

- Molecule 2 is a protein called Probable WRKY transcription factor 33.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	79	1275	397	635	123	115	5	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	330	MET	-	initiating methionine	UNP Q8S8P5
B	357	CYS	ASP	engineered mutation	UNP Q8S8P5
B	376	CYS	LYS	engineered mutation	UNP Q8S8P5
B	423	LEU	-	expression tag	UNP Q8S8P5
B	424	GLU	-	expression tag	UNP Q8S8P5
B	425	HIS	-	expression tag	UNP Q8S8P5
B	426	HIS	-	expression tag	UNP Q8S8P5
B	427	HIS	-	expression tag	UNP Q8S8P5
B	428	HIS	-	expression tag	UNP Q8S8P5
B	429	HIS	-	expression tag	UNP Q8S8P5
B	430	HIS	-	expression tag	UNP Q8S8P5

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

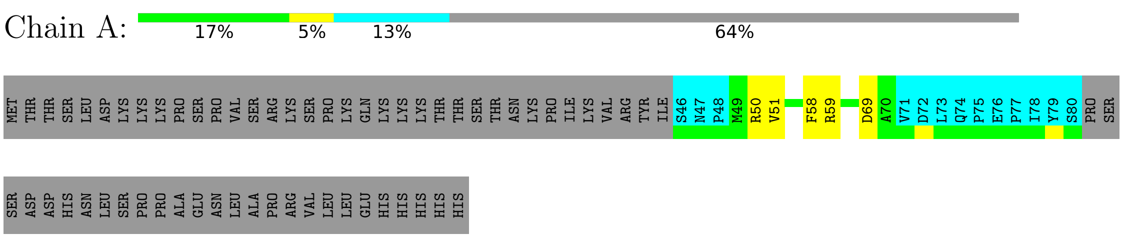
Mol	Chain	Residues	Atoms	
			Total	Zn
3	B	1	1	1

4 Residue-property plots (i)

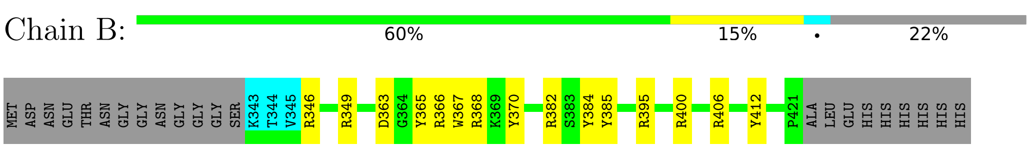
4.1 Average score per residue in the NMR ensemble

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: Sigma factor binding protein 1, chloroplastic



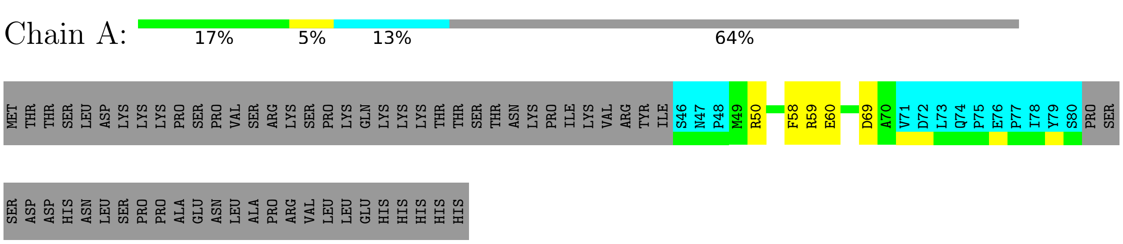
- Molecule 2: Probable WRKY transcription factor 33



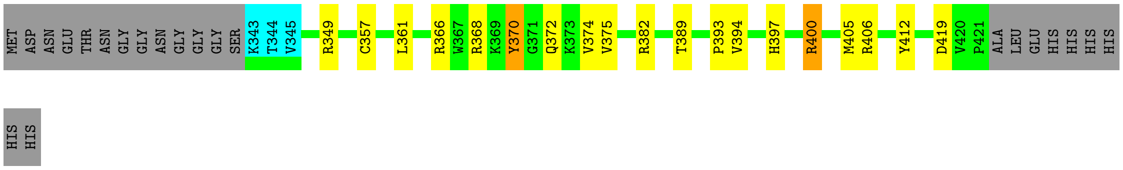
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 5. Colouring as in section 4.1 above.

- Molecule 1: Sigma factor binding protein 1, chloroplastic



- Molecule 2: Probable WRKY transcription factor 33


MET
ASP
ASN
GLU
THR
ASN
GLY
GLY
ASN
GLY
GLY
GLY
SER
K343
T344
V345
R349
C357
L361
R366
W367
R368
K369
Y370
G371
Q372
K373
V374
V375
R382
T389
P393
V394
H397
R400
M405
R406
Y412
D419
V420
P421
ALA
LEU
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5 Refinement protocol and experimental data overview (i)

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

Of the 240 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	structure calculation	
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	30
Number of shifts mapped to atoms	30
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

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	1.55±0.09	1±1/174 (0.4± 0.4%)	2.06±0.13	5±2/233 (2.3± 0.9%)
2	B	1.57±0.05	4±2/632 (0.6± 0.3%)	2.12±0.13	22±3/856 (2.6± 0.3%)
All	All	1.57	87/16120 (0.5%)	2.11	556/21780 (2.6%)

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	0.3±0.6
2	B	0.0±0.0	3.0±1.8
All	All	0	67

5 of 58 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	356	SER	CB-OG	9.70	1.54	1.42	18	1
2	B	412	TYR	CG-CD2	7.91	1.49	1.39	2	1
2	B	385	TYR	CE2-CZ	7.79	1.48	1.38	8	7
2	B	382	ARG	CZ-NH2	-7.63	1.23	1.33	8	1
2	B	368	ARG	CZ-NH1	-7.51	1.23	1.33	19	3

5 of 183 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
2	B	400	ARG	NE-CZ-NH1	20.66	130.63	120.30	10	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	368	ARG	NE-CZ-NH1	19.31	129.96	120.30	8	12
2	B	346	ARG	NE-CZ-NH1	18.67	129.63	120.30	10	6
2	B	382	ARG	NE-CZ-NH1	17.97	129.29	120.30	15	10
2	B	365	TYR	CB-CG-CD2	-17.76	110.34	121.00	11	6

There are no chirality outliers.

5 of 26 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	406	ARG	Sidechain	7
2	B	385	TYR	Sidechain	6
2	B	400	ARG	Sidechain	6
2	B	412	TYR	Sidechain,Peptide	5
2	B	370	TYR	Sidechain	4

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	173	174	174	0±0
2	B	617	606	606	0±1
All	All	15820	15600	15600	9

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 0.

5 of 7 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:PHE:CZ	2:B:415:LYS:HE3	0.57	2.33	2	1
2:B:367:TRP:CD2	2:B:396:LYS:HE2	0.50	2.41	8	3
2:B:347:GLU:N	2:B:348:PRO:CD	0.49	2.75	3	1
2:B:368:ARG:HG2	2:B:388:THR:HG22	0.46	1.86	4	1
2:B:347:GLU:HB3	2:B:348:PRO:HD3	0.43	1.90	2	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	22/98 (22%)	19±1 (85±5%)	3±1 (12±6%)	1±1 (4±3%)	6	34
2	B	75/101 (74%)	69±2 (92±2%)	5±2 (7±2%)	0±1 (1±1%)	26	73
All	All	1940/3980 (49%)	1755 (90%)	159 (8%)	26 (1%)	16	63

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

Mol	Chain	Res	Type	Models (Total)
1	A	51	VAL	10
1	A	68	GLN	4
2	B	346	ARG	3
2	B	377	GLY	2
2	B	360	ILE	2

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	19/93 (20%)	18±1 (97±4%)	0±1 (3±4%)	49	91
2	B	69/88 (78%)	68±1 (98±1%)	1±1 (2±1%)	57	93
All	All	1760/3620 (49%)	1722 (98%)	38 (2%)	54	92

5 of 21 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)
2	B	375	VAL	5
2	B	409	ILE	3

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Mol	Chain	Res	Type	Models (Total)
2	B	397	HIS	3
2	B	372	GLN	3
2	B	405	MET	3

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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 1% for the well-defined parts and 2% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *wk11_CS*

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	30
Number of shifts mapped to atoms	30
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 1%, i.e. 16 atoms were assigned a chemical shift out of a possible 1362. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	16/486 (3%)	8/197 (4%)	0/196 (0%)	8/93 (9%)
Sidechain	0/781 (0%)	0/502 (0%)	0/235 (0%)	0/44 (0%)
Aromatic	0/95 (0%)	0/47 (0%)	0/43 (0%)	0/5 (0%)
Overall	16/1362 (1%)	8/746 (1%)	0/474 (0%)	8/142 (6%)

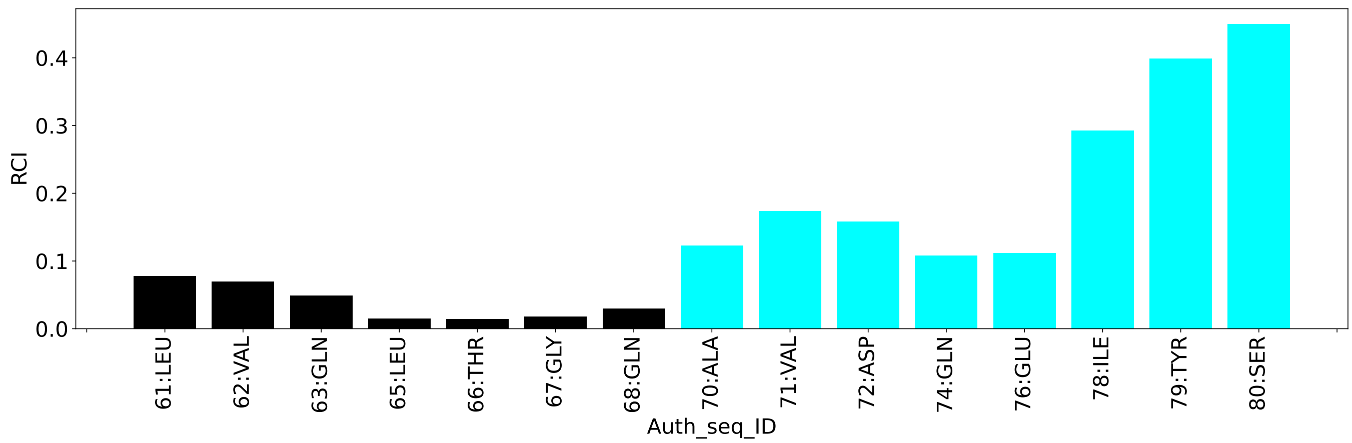
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	17
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	0
Medium range (|i-j|>1 and |i-j|<5)	0
Long range (|i-j|≥5)	0
Inter-chain	17
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue[1]	0.0

[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 (i)

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 (i)

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)	0.3	0.2
0.2-0.5 (Medium)	0.8	0.5
>0.5 (Large)	4.0	5.61

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

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

9 Distance violation analysis (i)

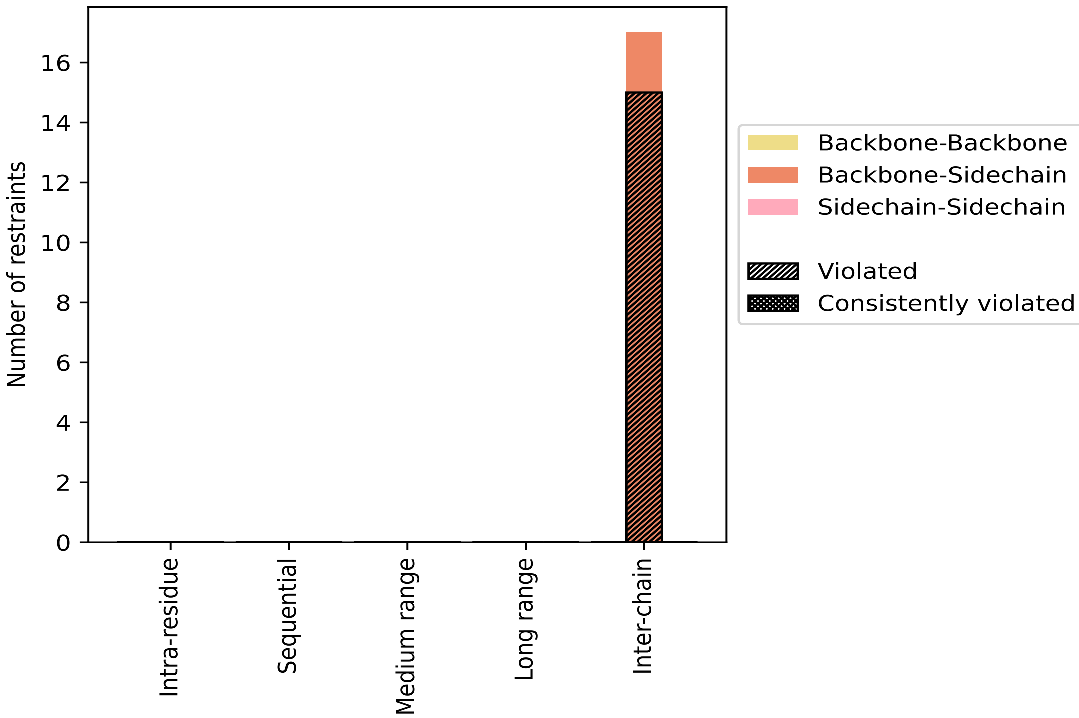
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	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
Sequential (|i-j|=1)	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
Medium range (|i-j|>1 & |i-j|<5)	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
Long range (|i-j|≥5)	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
Inter-chain	17	100.0	15	88.2	88.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	17	100.0	15	88.2	88.2	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	17	100.0	15	88.2	88.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	17	100.0	15	88.2	88.2	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	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 (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	0	0	0	0	7	7	1.54	4.31	1.27	1.05
2	0	0	0	0	5	5	1.39	2.84	0.84	1.27
3	0	0	0	0	6	6	0.9	2.89	0.9	0.56
4	0	0	0	0	3	3	0.77	1.36	0.42	0.48
5	0	0	0	0	3	3	0.81	1.57	0.59	0.75
6	0	0	0	0	3	3	0.34	0.54	0.14	0.24
7	0	0	0	0	3	3	0.48	0.67	0.2	0.56
8	0	0	0	0	4	4	1.58	3.18	1.08	1.5
9	0	0	0	0	5	5	0.94	1.97	0.59	0.8
10	0	0	0	0	4	4	0.83	1.54	0.43	0.68

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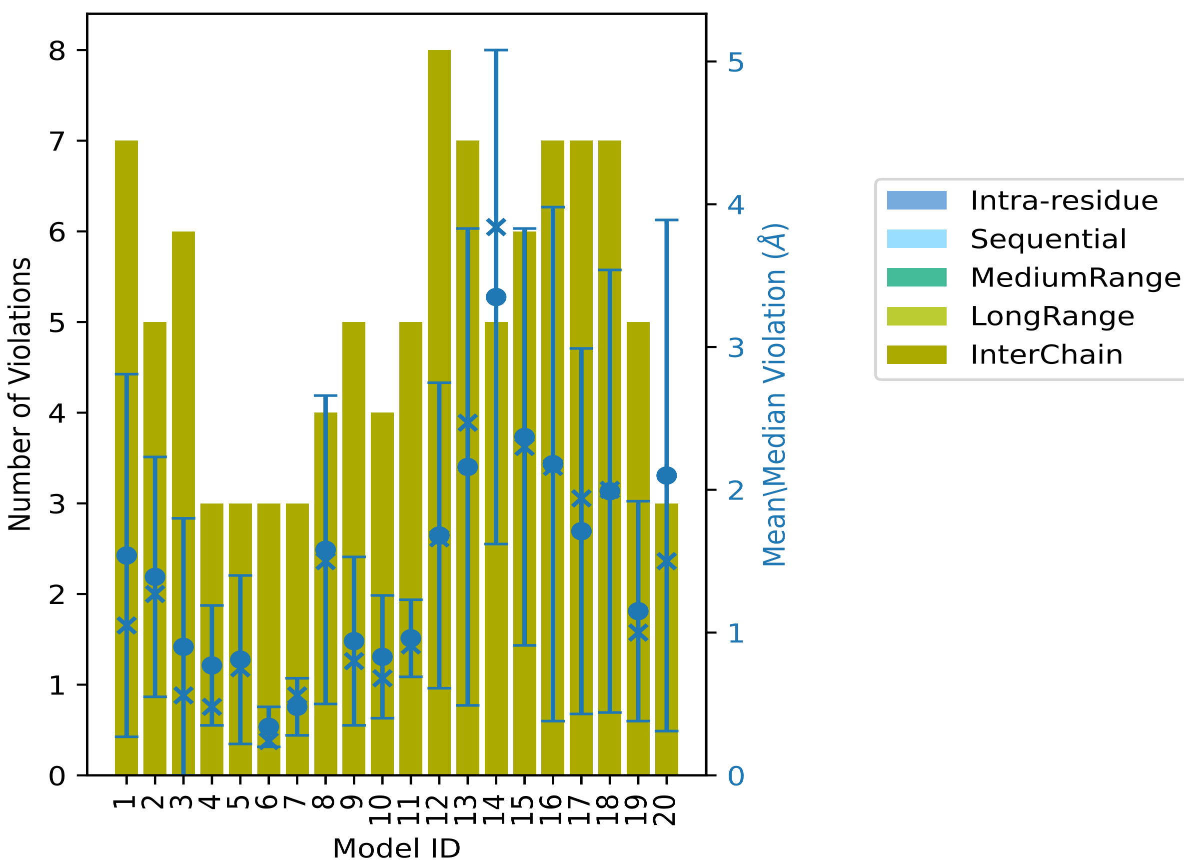
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	0	0	0	5	5	0.96	1.3	0.27	0.91
12	0	0	0	0	8	8	1.68	3.68	1.07	1.66
13	0	0	0	0	7	7	2.16	5.1	1.67	2.47
14	0	0	0	0	5	5	3.35	5.25	1.73	3.84
15	0	0	0	0	6	6	2.37	4.89	1.46	2.3
16	0	0	0	0	7	7	2.18	5.61	1.8	2.16
17	0	0	0	0	7	7	1.71	3.77	1.28	1.94
18	0	0	0	0	7	7	1.99	5.27	1.55	2.0
19	0	0	0	0	5	5	1.15	2.58	0.77	1.0
20	0	0	0	0	3	3	2.1	4.52	1.79	1.5

[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

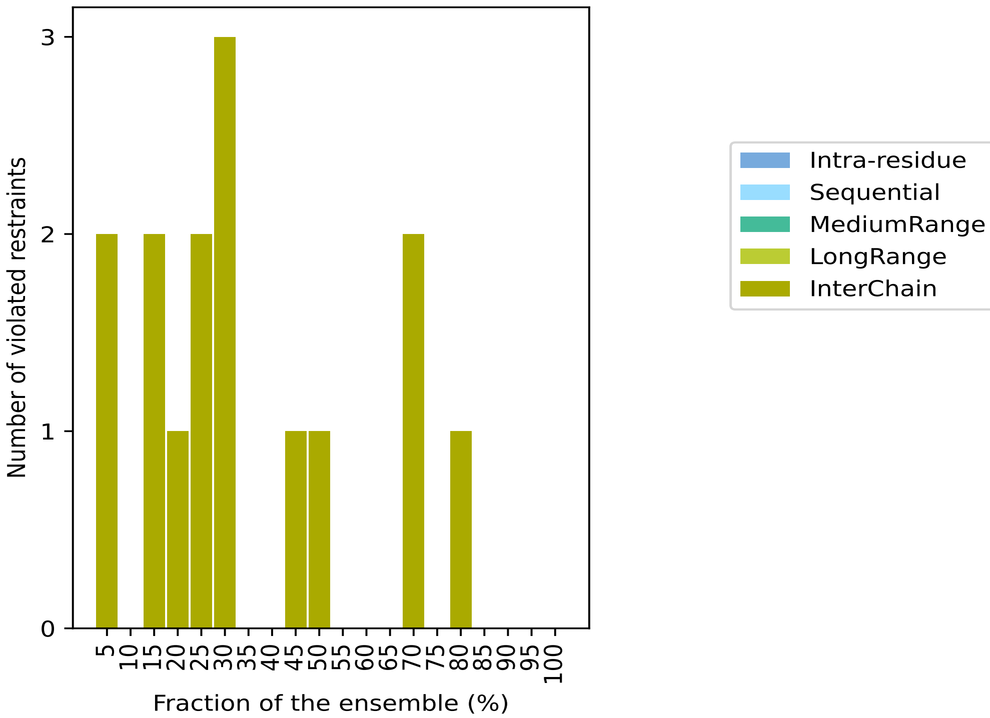
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2(IR:0, SQ:0, MR:0, LR:0, IC:2) 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]	%
0	0	0	0	2	2	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	2	2	3	15.0
0	0	0	0	1	1	4	20.0
0	0	0	0	2	2	5	25.0
0	0	0	0	3	3	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	1	1	9	45.0
0	0	0	0	1	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	2	2	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	1	1	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

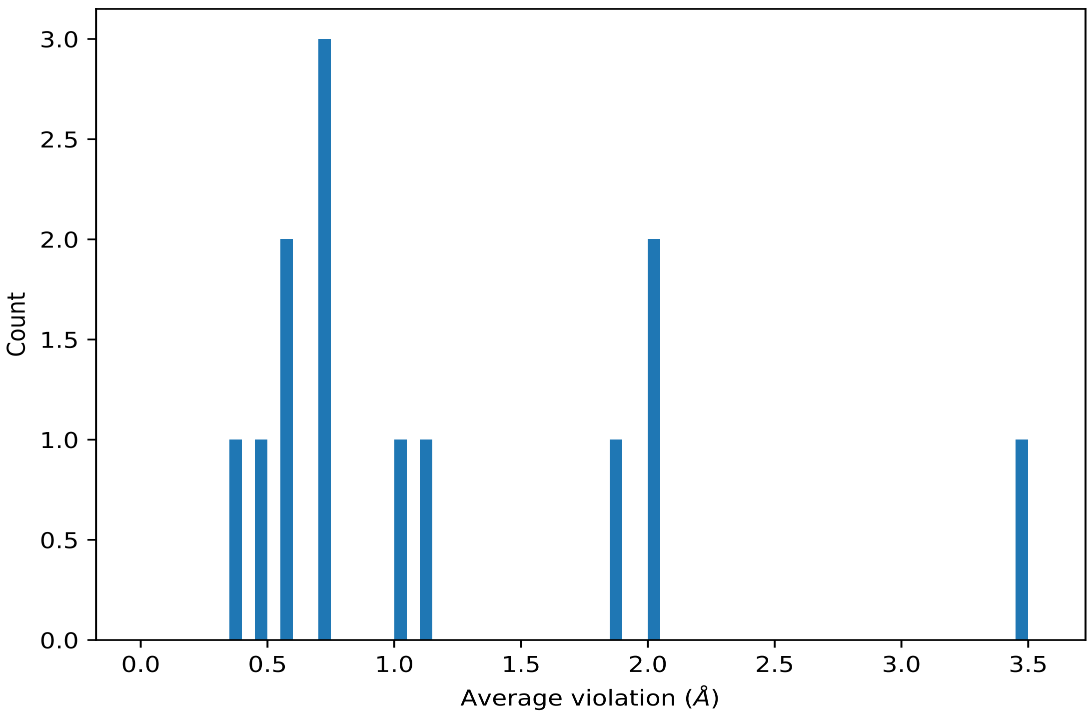
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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.

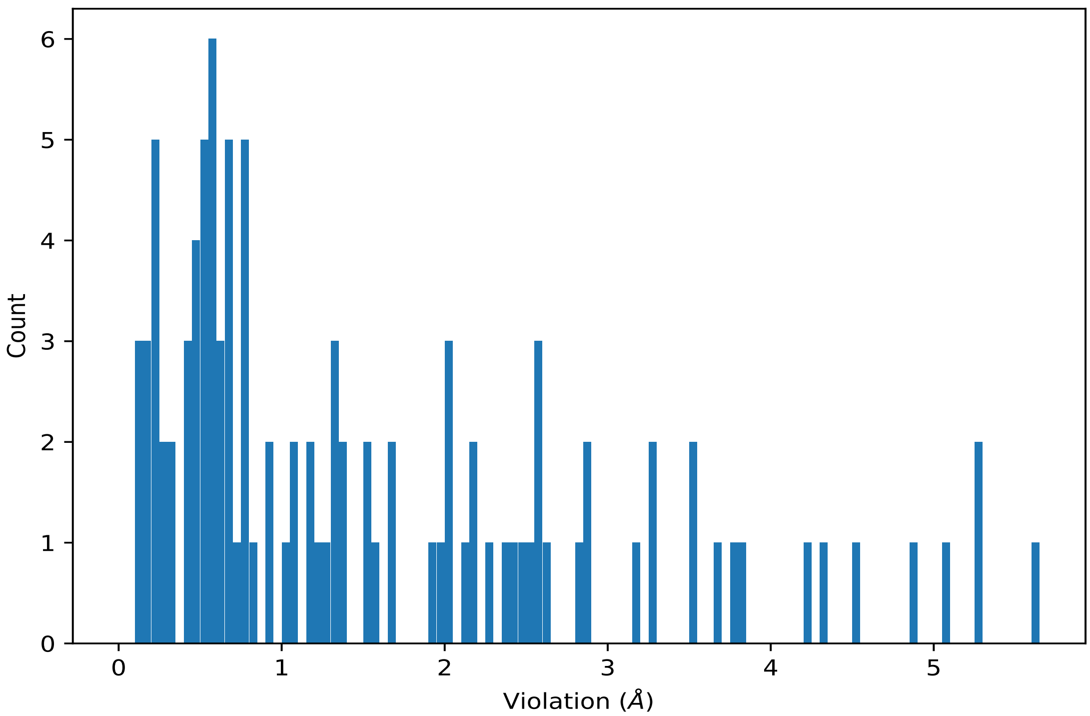
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	16	3.46	1.7	3.72
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	14	2.03	0.96	1.82
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	14	1.87	1.11	1.97
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	10	2.0	0.95	2.18
(1,17)	2:357:B:CYS:HG	1:80:A:SER:H	9	0.7	0.39	0.64
(1,14)	2:357:B:CYS:HG	1:76:A:GLU:H	6	0.7	0.41	0.52
(1,15)	2:357:B:CYS:HG	1:78:A:ILE:H	6	0.57	0.25	0.57
(1,13)	2:357:B:CYS:HG	1:71:A:VAL:H	6	0.49	0.32	0.4
(1,12)	2:357:B:CYS:HG	1:70:A:ALA:H	5	0.57	0.29	0.63
(1,8)	2:357:B:CYS:HG	1:63:A:GLN:H	5	0.35	0.19	0.33

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

The following table provides the 10 worst performing restraints, sorted by the violation 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)
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	16	5.61
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	18	5.27
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	14	5.25
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	13	5.1
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	15	4.89
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	20	4.52
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	1	4.31
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	14	4.21
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	14	3.84
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	17	3.77

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found