Full wwPDB NMR Structure Validation Report (i)

Dec 24, 2024 – 10:07 PM EST

PDB ID	:	2MJC
BMRB ID	:	19716
Title	:	Zn-binding domain of eukaryotic translation initiation factor 3, subunit G
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Deposited on	:	2014-01-03

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

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

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

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

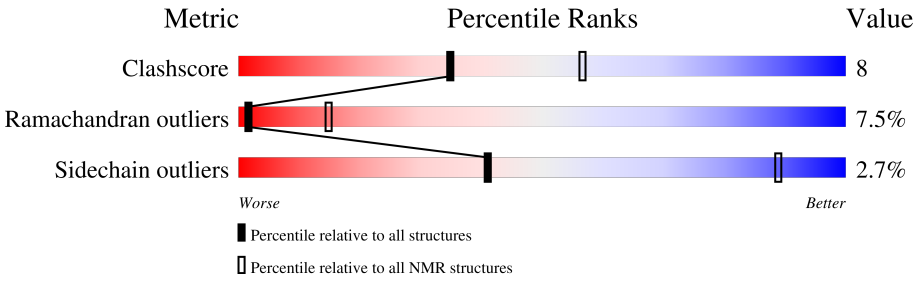
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 79%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	34	35% 12% 24% 29%

2 Ensemble composition and analysis

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:11-A:26 (16)	0.38	1

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 12, 14, 15
2	10, 13

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 384 atoms, of which 191 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	24	383	120	191	36	33	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	PRO	-	expression tag	UNP O75821
A	3	LEU	-	expression tag	UNP O75821
A	4	GLY	-	expression tag	UNP O75821
A	5	SER	-	expression tag	UNP O75821

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

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	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: Eukaryotic translation initiation factor 3 subunit G

Chain A:

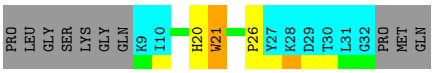
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

Chain A:



4.2.2 Score per residue for model 2

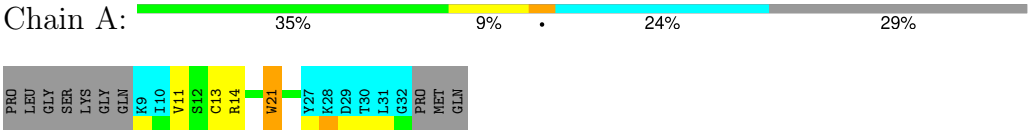
• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

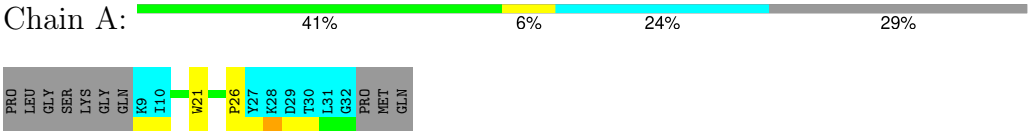
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

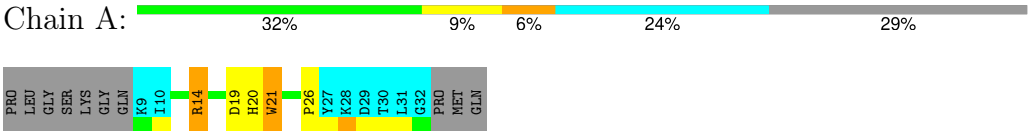
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

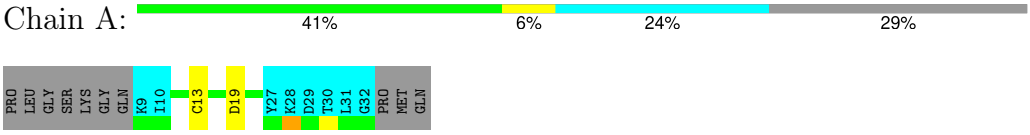
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

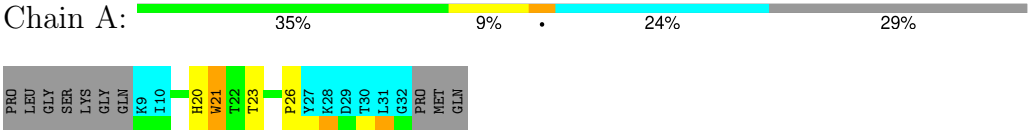
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

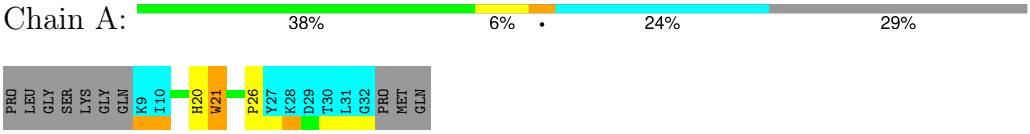
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

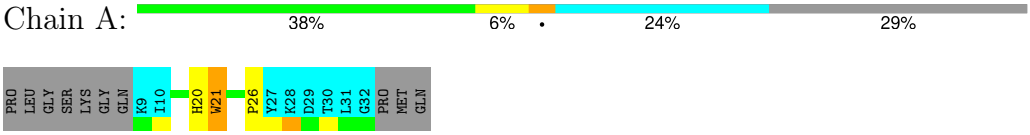
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

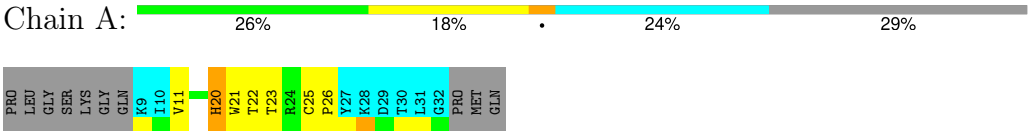
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

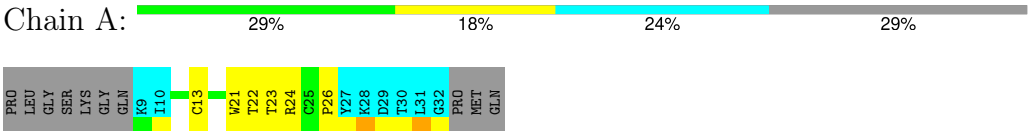
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

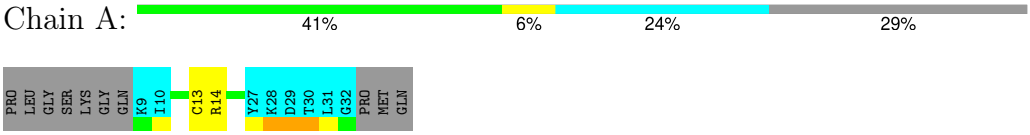
Chain A:



4.2.12 Score per residue for model 12

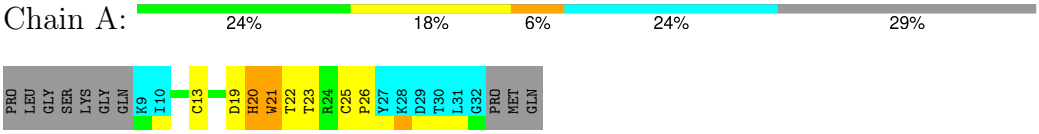
• Molecule 1: Eukaryotic translation initiation factor 3 subunit G

Chain A:



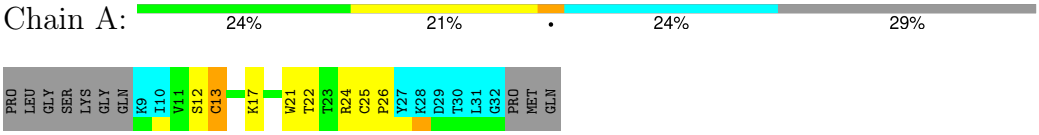
4.2.13 Score per residue for model 13

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G



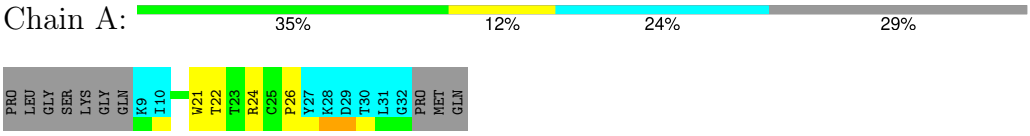
4.2.14 Score per residue for model 14

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G



4.2.15 Score per residue for model 15

• Molecule 1: Eukaryotic translation initiation factor 3 subunit G



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 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
XPLOR-NIH	structure solution	
XPLOR-NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	345
Number of shifts mapped to atoms	254
Number of unparsed shifts	0
Number of shifts with mapping errors	91
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality

6.1 Standard geometry

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	127	120	121	2±2
All	All	1920	1800	1815	29

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:ARG:NE	1:A:14:ARG:O	0.52	2.42	5	1
1:A:21:TRP:O	1:A:23:THR:N	0.51	2.43	13	2
1:A:14:ARG:NE	1:A:14:ARG:C	0.47	2.67	5	1
1:A:13:CYS:SG	1:A:14:ARG:N	0.47	2.87	3	2
1:A:11:VAL:HG23	1:A:21:TRP:CD1	0.47	2.45	3	1
1:A:11:VAL:CG2	1:A:20:HIS:O	0.47	2.63	10	1
1:A:14:ARG:C	1:A:14:ARG:HE	0.46	2.13	5	1
1:A:22:THR:O	1:A:25:CYS:N	0.46	2.48	10	2
1:A:14:ARG:NE	1:A:14:ARG:CA	0.46	2.78	5	1
1:A:20:HIS:O	1:A:21:TRP:O	0.45	2.34	7	5
1:A:22:THR:C	1:A:24:ARG:N	0.43	2.71	11	3
1:A:19:ASP:O	1:A:19:ASP:OD2	0.43	2.37	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:THR:O	1:A:25:CYS:CB	0.41	2.67	13	2
1:A:22:THR:C	1:A:24:ARG:H	0.41	2.19	15	2
1:A:22:THR:O	1:A:24:ARG:N	0.41	2.53	14	1
1:A:19:ASP:H	1:A:20:HIS:CE1	0.41	2.34	13	1
1:A:19:ASP:OD2	1:A:19:ASP:O	0.40	2.39	5	1
1:A:12:SER:O	1:A:13:CYS:O	0.40	2.40	14	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	16/34 (47%)	10±1 (60±7%)	5±1 (32±7%)	1±1 (8±5%)	1 15
All	All	240/510 (47%)	145 (60%)	77 (32%)	18 (8%)	1 15

All 3 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	21	TRP	12
1	A	13	CYS	5
1	A	26	PRO	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	15/30 (50%)	15±0 (97±3%)	0±0 (3±3%)	41 89
All	All	225/450 (50%)	219 (97%)	6 (3%)	41 89

All 4 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	23	THR	2
1	A	20	HIS	2
1	A	14	ARG	1
1	A	17	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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 79% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	345
Number of shifts mapped to atoms	254
Number of unparsed shifts	0
Number of shifts with mapping errors	91
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	56

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 91 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	PRO	CA	35.3515	0.0000	1
1	A	2	PRO	HA	4.4659	0.0000	1
1	A	2	PRO	CB	32.3343	0.0000	1
1	A	2	PRO	HB2	2.3148	0.0000	2
1	A	2	PRO	CG	27.1066	0.0000	1
1	A	2	PRO	HG2	2.0099	0.0000	2
1	A	2	PRO	CD	49.7183	0.0000	1
1	A	2	PRO	HD2	3.5683	0.0000	2
1	A	3	LEU	N	122.6532	0.0000	1
1	A	3	LEU	H	8.5603	0.0000	1
1	A	3	LEU	CA	27.2875	0.0000	1
1	A	3	LEU	HA	4.343	0.0000	1
1	A	3	LEU	CB	43.0704	0.0000	1
1	A	3	LEU	HB2	1.6537	0.0000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	LEU	CG	27.099	0.0000	1
1	A	3	LEU	HG	1.6503	0.0000	1
1	A	3	LEU	CD1	24.876	0.0000	2
1	A	3	LEU	HD11	0.8942	0.0000	2
1	A	3	LEU	HD12	0.8942	0.0000	2
1	A	3	LEU	HD13	0.8942	0.0000	2
1	A	3	LEU	CD2	51.4641	0.0000	2
1	A	3	LEU	HD21	0.911	0.0000	2
1	A	3	LEU	HD22	0.911	0.0000	2
1	A	3	LEU	HD23	0.911	0.0000	2
1	A	4	GLY	N	109.8654	0.0000	1
1	A	4	GLY	H	8.4436	0.0000	1
1	A	4	GLY	CA	45.9357	0.0000	1
1	A	4	GLY	HA2	3.9513	0.0000	2
1	A	5	SER	N	115.8753	0.0000	1
1	A	5	SER	H	8.2676	0.0000	1
1	A	5	SER	CA	30.4234	0.0000	1
1	A	5	SER	HA	4.4489	0.0000	1
1	A	5	SER	CB	35.9952	0.0000	1
1	A	5	SER	HB2	3.8594	0.0000	2
1	A	6	LYS	N	123.354	0.0000	1
1	A	6	LYS	H	8.4447	0.0000	1
1	A	6	LYS	CA	28.4489	0.0000	1
1	A	6	LYS	HA	4.3464	0.0000	1
1	A	6	LYS	CB	33.4432	0.0000	1
1	A	6	LYS	HB2	1.7139	0.0000	2
1	A	6	LYS	HB3	1.3657	0.0000	2
1	A	6	LYS	CG	24.7879	0.0000	1
1	A	6	LYS	HG2	1.4075	0.0000	2
1	A	6	LYS	HG3	1.4099	0.0000	2
1	A	6	LYS	HD2	1.717	0.0000	2
1	A	6	LYS	HE2	2.9744	0.0000	2
1	A	7	GLY	N	109.8433	0.0000	1
1	A	7	GLY	H	8.4302	0.0000	1
1	A	7	GLY	CA	46.0171	0.0000	1
1	A	7	GLY	HA2	4.8107	0.0000	2
1	A	8	GLN	N	120.0368	0.0000	1
1	A	8	GLN	H	8.1927	0.0000	1
1	A	8	GLN	CA	56.3108	0.0000	1
1	A	8	GLN	HA	4.3063	0.0000	1
1	A	8	GLN	CB	30.4397	0.0000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	GLN	HB2	2.3152	0.0000	2
1	A	8	GLN	HB3	1.9513	0.0000	2
1	A	8	GLN	HG2	2.3152	0.0000	2
1	A	8	GLN	HG3	1.9513	0.0000	2
1	A	33	PRO	CA	35.2803	0.0000	1
1	A	33	PRO	HA	4.3975	0.0000	1
1	A	33	PRO	CB	32.1147	0.0000	1
1	A	33	PRO	HB2	2.219	0.0000	2
1	A	33	PRO	CG	27.1892	0.0000	1
1	A	33	PRO	HG2	1.9763	0.0000	2
1	A	33	PRO	CD	49.7856	0.0000	1
1	A	33	PRO	HD2	3.5583	0.0000	2
1	A	34	MET	N	120.7562	0.0000	1
1	A	34	MET	H	8.45	0.0000	1
1	A	34	MET	CA	27.566	0.0000	1
1	A	34	MET	HA	4.4415	0.0000	1
1	A	34	MET	CB	32.8394	0.0000	1
1	A	34	MET	HB2	2.1	0.0000	2
1	A	34	MET	HB3	1.9965	0.0000	2
1	A	34	MET	CG	32.1922	0.0000	1
1	A	34	MET	HG2	2.6019	0.0000	2
1	A	34	MET	HG3	2.5447	0.0000	2
1	A	34	MET	CE	44.9347	0.0000	1
1	A	34	MET	HE1	2.0744	0.0000	1
1	A	34	MET	HE2	2.0744	0.0000	1
1	A	34	MET	HE3	2.0744	0.0000	1
1	A	35	GLN	N	126.2075	0.0000	1
1	A	35	GLN	H	7.929	0.0000	1
1	A	35	GLN	CA	29.3391	0.0000	1
1	A	35	GLN	HA	4.1533	0.0000	1
1	A	35	GLN	CB	30.4888	0.0000	1
1	A	35	GLN	HB2	2.0977	0.0000	2
1	A	35	GLN	HB3	1.9189	0.0000	2
1	A	35	GLN	CG	34.2691	0.0000	1
1	A	35	GLN	HG2	2.2711	0.0000	2
1	A	35	GLN	HG3	1.7531	0.0000	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	34	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	29	1.04 ± 0.56	None needed (imprecise)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	31	-0.57 ± 1.06	None needed (imprecise)

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 79%, i.e. 168 atoms were assigned a chemical shift out of a possible 212. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	63/79 (80%)	32/32 (100%)	16/32 (50%)	15/15 (100%)
Sidechain	89/115 (77%)	59/74 (80%)	30/34 (88%)	0/7 (0%)
Aromatic	16/18 (89%)	8/10 (80%)	7/7 (100%)	1/1 (100%)
Overall	168/212 (79%)	99/116 (85%)	53/73 (73%)	16/23 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 254 atoms were assigned a chemical shift out of a possible 327. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	95/120 (79%)	48/49 (98%)	24/48 (50%)	23/23 (100%)
Sidechain	139/180 (77%)	94/116 (81%)	45/55 (82%)	0/9 (0%)
Aromatic	20/27 (74%)	10/14 (71%)	9/12 (75%)	1/1 (100%)
Overall	254/327 (78%)	152/179 (85%)	78/115 (68%)	24/33 (73%)

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	27	TYR	CE2	34.12	111.68 – 124.17	-67.1
1	A	21	TRP	CZ2	30.73	107.20 – 121.33	-59.1
1	A	27	TYR	CD2	49.20	125.28 – 140.14	-56.2
1	A	21	TRP	CH2	40.90	116.19 – 131.43	-54.4
1	A	21	TRP	CZ3	38.03	113.48 – 129.28	-52.8
1	A	20	HIS	CE1	25.61	126.08 – 149.12	-48.6
1	A	21	TRP	CE3	36.83	111.58 – 129.41	-46.9

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	21	TRP	CD1	42.03	117.34 – 135.80	-45.8
1	A	22	THR	CG2	50.86	16.06 – 27.03	26.7
1	A	23	THR	CG2	50.74	16.06 – 27.03	26.6
1	A	30	THR	CG2	49.78	16.06 – 27.03	25.7
1	A	28	LYS	CG	52.03	19.35 – 30.45	24.4
1	A	20	HIS	CD2	44.37	103.95 – 136.66	-23.2
1	A	10	ILE	CG2	45.27	10.93 – 24.12	21.0
1	A	15	ILE	CD1	46.01	5.18 – 21.60	19.9
1	A	11	VAL	CG1	48.23	14.71 – 28.29	19.7
1	A	33	PRO	CA	35.28	55.85 – 70.84	-18.7
1	A	2	PRO	CA	35.35	55.85 – 70.84	-18.7
1	A	5	SER	CB	36.00	56.28 – 71.32	-18.5
1	A	26	PRO	CA	35.88	55.85 – 70.84	-18.3
1	A	15	ILE	CG2	41.53	10.93 – 24.12	18.2
1	A	12	SER	CB	36.52	56.28 – 71.32	-18.1
1	A	11	VAL	CG2	48.44	13.71 – 28.88	17.9
1	A	23	THR	CB	40.88	61.12 – 78.27	-16.8
1	A	10	ILE	CD1	40.62	5.18 – 21.60	16.6
1	A	3	LEU	CD2	51.46	15.73 – 32.47	16.4
1	A	30	THR	CB	41.92	61.12 – 78.27	-16.2
1	A	31	LEU	CD2	51.20	15.73 – 32.47	16.2
1	A	22	THR	CB	42.00	61.12 – 78.27	-16.1
1	A	34	MET	CE	44.93	8.39 – 25.85	15.9
1	A	19	ASP	CA	24.84	44.71 – 64.67	-15.0
1	A	12	SER	CA	29.11	48.46 – 68.96	-14.4
1	A	29	ASP	CA	26.99	44.71 – 64.67	-13.9
1	A	5	SER	CA	30.42	48.46 – 68.96	-13.8
1	A	31	LEU	CA	27.09	45.17 – 66.21	-13.6
1	A	24	ARG	CA	26.03	45.44 – 68.13	-13.6
1	A	3	LEU	CA	27.29	45.17 – 66.21	-13.5
1	A	20	HIS	CA	25.99	45.04 – 67.94	-13.3
1	A	9	LYS	CA	28.38	46.18 – 67.77	-13.2
1	A	6	LYS	CA	28.45	46.18 – 67.77	-13.2
1	A	34	MET	CA	27.57	45.26 – 67.07	-13.1
1	A	35	GLN	CA	29.34	46.17 – 66.97	-13.1
1	A	17	LYS	CA	30.68	46.18 – 67.77	-12.2
1	A	28	LYS	CA	30.70	46.18 – 67.77	-12.2
1	A	27	TYR	CA	28.90	45.75 – 70.63	-11.8
1	A	21	TRP	CA	28.74	45.21 – 70.26	-11.6
1	A	14	ARG	CA	30.67	45.44 – 68.13	-11.5
1	A	30	THR	CA	34.44	49.41 – 75.05	-10.8
1	A	10	ILE	CA	33.21	48.30 – 75.08	-10.6

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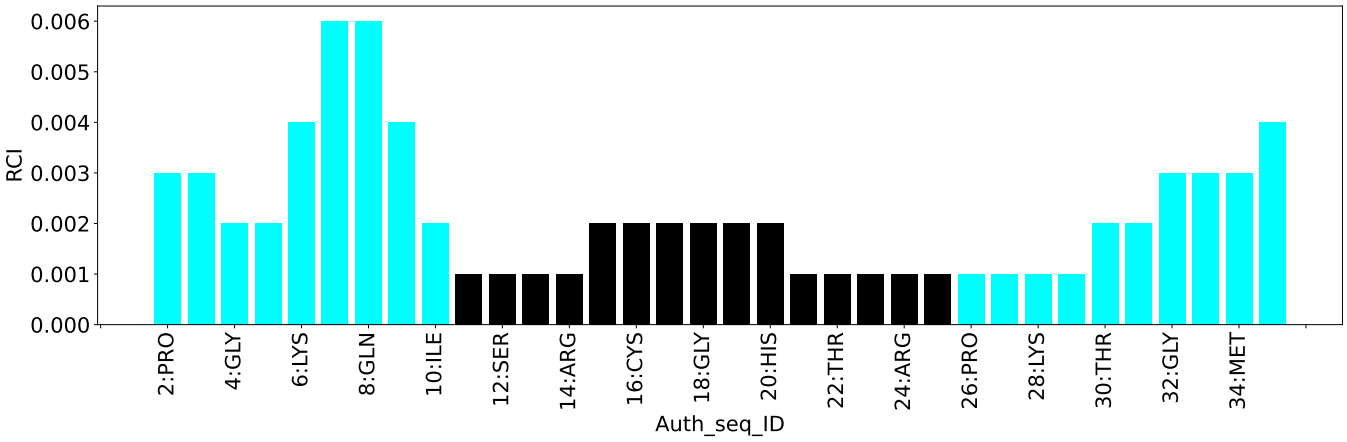
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	23	THR	CA	35.62	49.41 – 75.05	-10.4
1	A	11	VAL	CA	33.84	48.38 – 76.73	-10.1
1	A	22	THR	CA	37.99	49.41 – 75.05	-9.4
1	A	15	ILE	CA	36.41	48.30 – 75.08	-9.4
1	A	16	CYS	CA	30.67	40.80 – 75.33	-7.9
1	A	25	CYS	CA	30.89	40.80 – 75.33	-7.9
1	A	13	CYS	CA	31.86	40.80 – 75.33	-7.6

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	548
Intra-residue (|i-j|=0)	250
Sequential (|i-j|=1)	131
Medium range (|i-j|>1 and |i-j|<5)	74
Long range (|i-j|≥5)	93
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	22
Number of unmapped restraints	0
Number of restraints per residue	16.3
Number of long range restraints per residue[1]	2.7

[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)	4.8	0.19
0.2-0.5 (Medium)	4.5	0.5
>0.5 (Large)	1.0	3.0

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.5	1.99
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

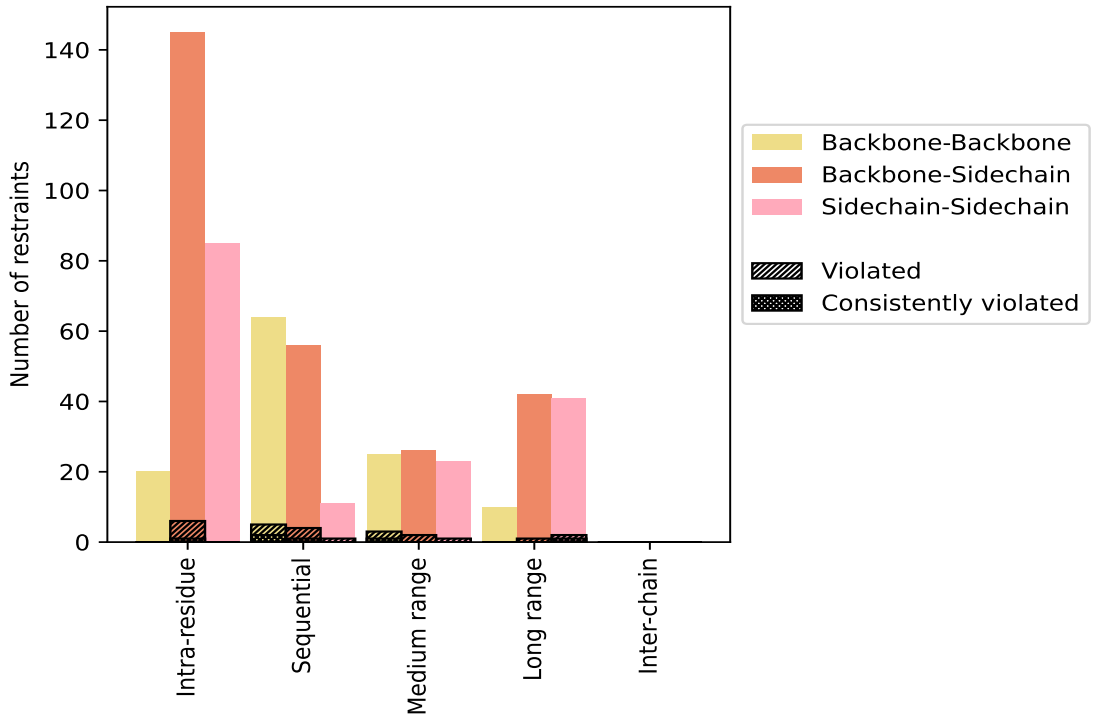
9.1 Summary of distance violations (i)

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)	250	45.6	6	2.4	1.1	1	0.4	0.2
Backbone-Backbone	20	3.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	145	26.5	6	4.1	1.1	1	0.7	0.2
Sidechain-Sidechain	85	15.5	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	131	23.9	10	7.6	1.8	3	2.3	0.5
Backbone-Backbone	64	11.7	5	7.8	0.9	2	3.1	0.4
Backbone-Sidechain	56	10.2	4	7.1	0.7	1	1.8	0.2
Sidechain-Sidechain	11	2.0	1	9.1	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	74	13.5	6	8.1	1.1	1	1.4	0.2
Backbone-Backbone	25	4.6	3	12.0	0.5	1	4.0	0.2
Backbone-Sidechain	26	4.7	2	7.7	0.4	0	0.0	0.0
Sidechain-Sidechain	23	4.2	1	4.3	0.2	0	0.0	0.0
Long range (|i-j|≥5)	93	17.0	3	3.2	0.5	1	1.1	0.2
Backbone-Backbone	10	1.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	42	7.7	1	2.4	0.2	0	0.0	0.0
Sidechain-Sidechain	41	7.5	2	4.9	0.4	1	2.4	0.2
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	548	100.0	25	4.6	4.6	6	1.1	1.1
Backbone-Backbone	119	21.7	8	6.7	1.5	3	2.5	0.5
Backbone-Sidechain	269	49.1	13	4.8	2.4	2	0.7	0.4
Sidechain-Sidechain	160	29.2	4	2.5	0.7	1	0.6	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



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	3	6	1	1	0	11	0.42	2.74	0.74	0.13
2	1	6	2	1	0	10	0.48	3.0	0.85	0.18
3	2	5	1	1	0	9	0.27	0.59	0.15	0.24
4	1	4	2	2	0	9	0.51	2.9	0.85	0.24
5	2	6	1	1	0	10	0.41	2.34	0.65	0.17
6	2	5	2	1	0	10	0.4	1.89	0.51	0.23
7	3	8	2	2	0	15	0.3	2.04	0.47	0.13
8	3	5	1	1	0	10	0.43	2.24	0.61	0.26
9	2	5	1	1	0	9	0.48	2.55	0.74	0.27
10	3	5	2	1	0	11	0.44	2.6	0.69	0.25

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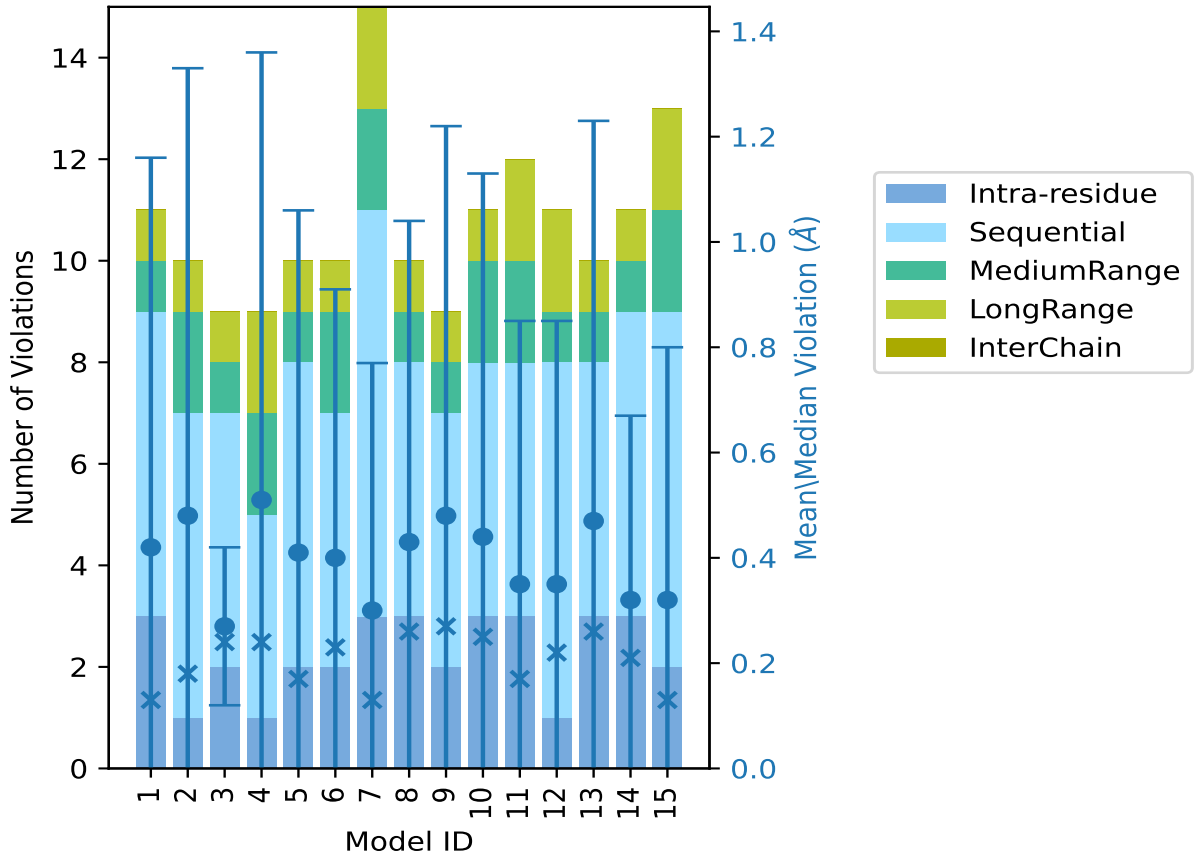
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	3	5	2	2	0	12	0.35	1.98	0.5	0.17
12	1	7	1	2	0	11	0.35	1.9	0.5	0.22
13	3	5	1	1	0	10	0.47	2.73	0.76	0.26
14	3	6	1	1	0	11	0.32	1.37	0.35	0.21
15	2	7	2	2	0	13	0.32	1.95	0.48	0.13

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

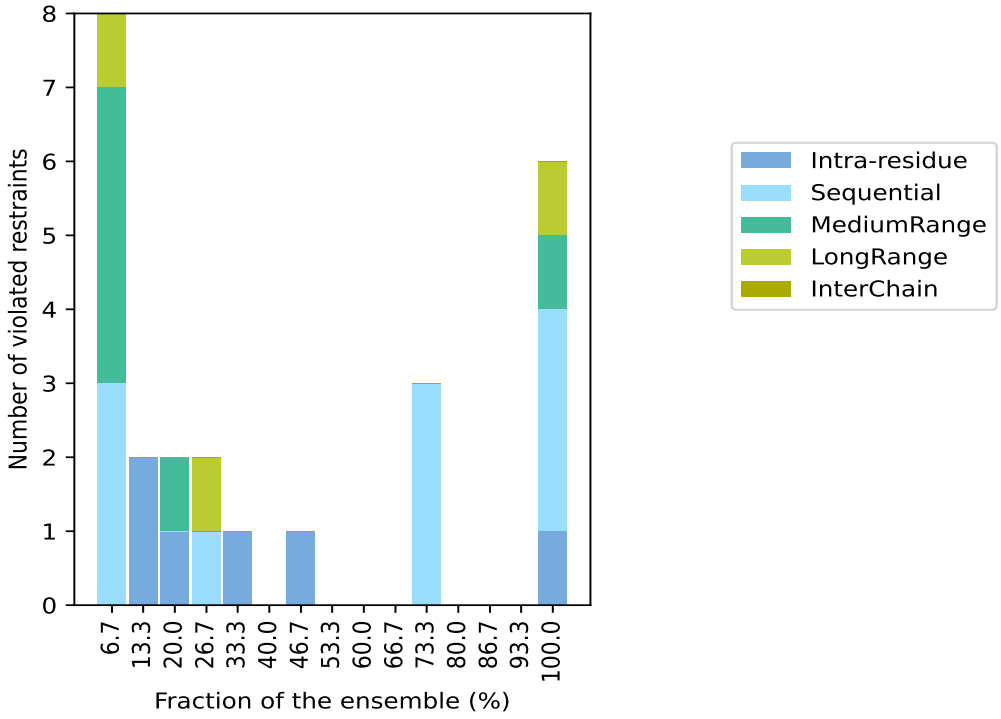
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 523(IR:244, SQ:121, MR:68, LR:90, 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]	%
0	3	4	1	0	8	1	6.7
2	0	0	0	0	2	2	13.3
1	0	1	0	0	2	3	20.0
0	1	0	1	0	2	4	26.7
1	0	0	0	0	1	5	33.3
0	0	0	0	0	0	6	40.0
1	0	0	0	0	1	7	46.7
0	0	0	0	0	0	8	53.3
0	0	0	0	0	0	9	60.0
0	0	0	0	0	0	10	66.7
0	3	0	0	0	3	11	73.3
0	0	0	0	0	0	12	80.0
0	0	0	0	0	0	13	86.7
0	0	0	0	0	0	14	93.3
1	3	1	1	0	6	15	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

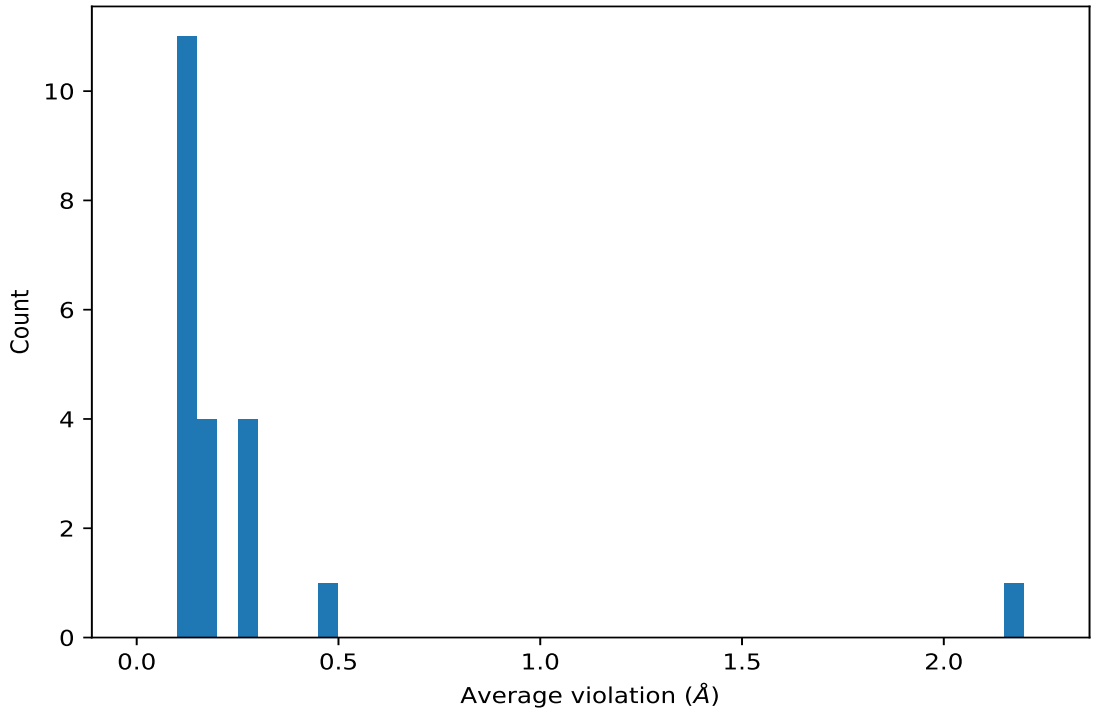
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 theviolation 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)
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	15	2.19	0.61	2.24
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	15	0.46	0.01	0.46
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	15	0.27	0.01	0.28
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	15	0.25	0.01	0.25
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	15	0.25	0.01	0.25
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	15	0.25	0.03	0.25
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	15	0.18	0.07	0.14
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	11	0.13	0.03	0.12
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	11	0.12	0.02	0.11
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	11	0.12	0.01	0.12
(1,284)	1:10:A:ILE:H	1:10:A:ILE:HB	7	0.15	0.05	0.13
(1,302)	1:16:A:CYS:H	1:16:A:CYS:HB3	5	0.11	0.0	0.11
(1,485)	1:14:A:ARG:H	1:25:A:CYS:HB3	4	0.12	0.02	0.12
(1,421)	1:29:A:ASP:H	1:28:A:LYS:HA	4	0.11	0.01	0.11
(1,330)	1:28:A:LYS:H	1:28:A:LYS:HG2	3	0.19	0.03	0.21
(1,330)	1:28:A:LYS:H	1:28:A:LYS:HG3	3	0.19	0.03	0.21

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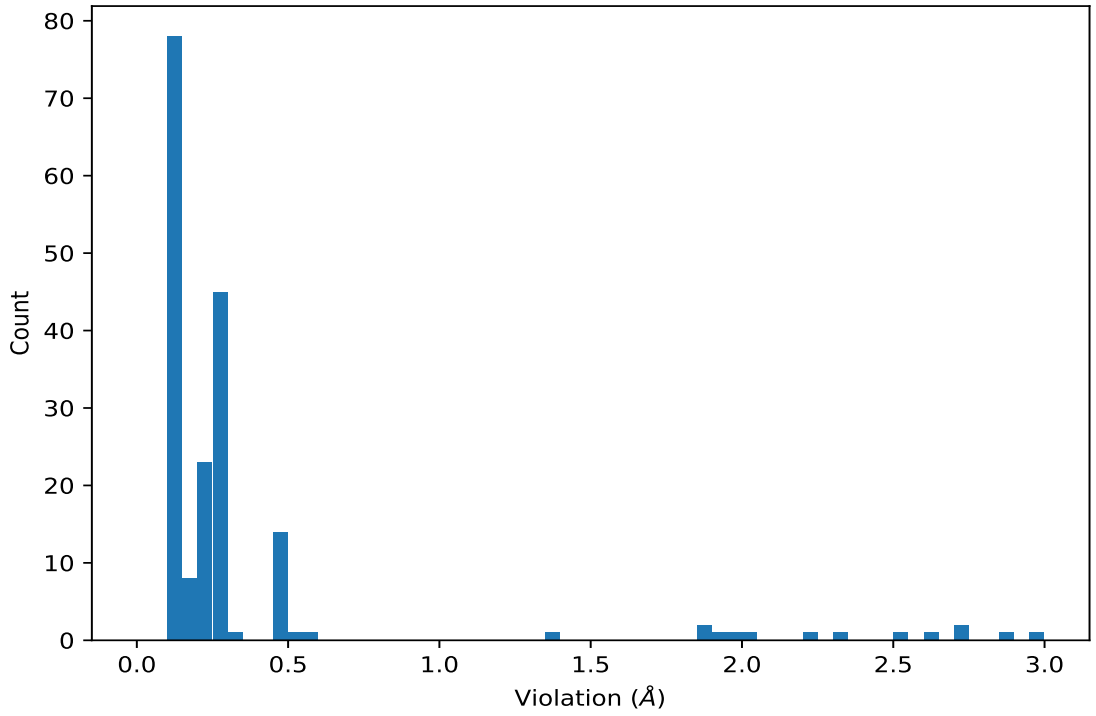
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,441)	1:17:A:LYS:H	1:13:A:CYS:H	3	0.1	0.0	0.1
(1,310)	1:19:A:ASP:H	1:19:A:ASP:HB3	2	0.16	0.01	0.16
(1,107)	1:23:A:THR:HG21	1:23:A:THR:HA	2	0.14	0.01	0.14
(1,107)	1:23:A:THR:HG22	1:23:A:THR:HA	2	0.14	0.01	0.14
(1,107)	1:23:A:THR:HG23	1:23:A:THR:HA	2	0.14	0.01	0.14

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	2	3.0
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	4	2.9
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	1	2.74
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	13	2.73
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	10	2.6
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	9	2.55
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	5	2.34
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	8	2.24
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	7	2.04
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	11	1.98
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	15	1.95
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	12	1.9
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	6	1.89
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	14	1.37
(1,528)	1:16:A:CYS:HB2	1:27:A:TYR:HE1	3	0.59
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	14	0.5
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	3	0.47
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	4	0.47
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	12	0.47
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	15	0.47
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	2	0.46
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	6	0.46
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	7	0.46
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	8	0.46
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	9	0.46
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	10	0.46
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	11	0.46
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	13	0.46
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	1	0.45
(1,334)	1:29:A:ASP:H	1:29:A:ASP:HB2	5	0.45
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	10	0.34
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	6	0.29
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	1	0.28
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	2	0.28
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	4	0.28
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	5	0.28
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	8	0.28
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	9	0.28
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	11	0.28
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	15	0.28
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	13	0.28
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	12	0.27
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	9	0.27
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	10	0.27
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	11	0.27
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	6	0.27
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	8	0.27
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	8	0.27
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	9	0.27
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	9	0.27
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	14	0.27
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	14	0.27
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	3	0.26
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	7	0.26
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	13	0.26
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	14	0.26
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	4	0.26
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	7	0.26
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	13	0.26
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	5	0.26
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	5	0.26
(1,284)	1:10:A:ILE:H	1:10:A:ILE:HB	8	0.26
(1,434)	1:13:A:CYS:H	1:11:A:VAL:HA	10	0.25
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	3	0.25
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	15	0.25
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	6	0.25
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	6	0.25
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	7	0.25
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	7	0.25
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	10	0.25
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	10	0.25
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	11	0.25
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	11	0.25
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	13	0.25
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	13	0.25
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	2	0.24
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	12	0.24
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	14	0.24
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	1	0.24
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	1	0.24
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	2	0.24
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	2	0.24
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	3	0.24
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	4	0.24
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	4	0.24
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	12	0.24
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	12	0.24
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	1	0.23
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	7	0.23
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB2	15	0.23
(1,352)	1:13:A:CYS:H	1:12:A:SER:HB3	15	0.23
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	12	0.22
(1,330)	1:28:A:LYS:H	1:28:A:LYS:HG2	3	0.22
(1,330)	1:28:A:LYS:H	1:28:A:LYS:HG3	3	0.22
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	6	0.21
(1,330)	1:28:A:LYS:H	1:28:A:LYS:HG2	14	0.21
(1,330)	1:28:A:LYS:H	1:28:A:LYS:HG3	14	0.21
(1,531)	1:16:A:CYS:HB3	1:27:A:TYR:HE2	11	0.19
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	8	0.19
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	14	0.19
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	5	0.17
(1,426)	1:30:A:THR:H	1:29:A:ASP:HA	5	0.17
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	14	0.17
(1,310)	1:19:A:ASP:H	1:19:A:ASP:HB3	10	0.17
(1,206)	1:20:A:HIS:HB3	1:24:A:ARG:HB3	6	0.17
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	11	0.15
(1,485)	1:14:A:ARG:H	1:25:A:CYS:HB3	15	0.15
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	6	0.15
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	4	0.15
(1,330)	1:28:A:LYS:H	1:28:A:LYS:HG2	6	0.15
(1,330)	1:28:A:LYS:H	1:28:A:LYS:HG3	6	0.15
(1,310)	1:19:A:ASP:H	1:19:A:ASP:HB3	13	0.15
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	14	0.14
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	3	0.14
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	3	0.14
(1,284)	1:10:A:ILE:H	1:10:A:ILE:HB	11	0.14
(1,107)	1:23:A:THR:HG21	1:23:A:THR:HA	7	0.14
(1,107)	1:23:A:THR:HG22	1:23:A:THR:HA	7	0.14
(1,107)	1:23:A:THR:HG23	1:23:A:THR:HA	7	0.14
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	1	0.13
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	15	0.13
(1,485)	1:14:A:ARG:H	1:25:A:CYS:HB3	7	0.13
(1,421)	1:29:A:ASP:H	1:28:A:LYS:HA	15	0.13
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	9	0.13
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	7	0.13
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	15	0.13
(1,284)	1:10:A:ILE:H	1:10:A:ILE:HB	1	0.13
(1,284)	1:10:A:ILE:H	1:10:A:ILE:HB	5	0.13
(1,284)	1:10:A:ILE:H	1:10:A:ILE:HB	9	0.13
(1,107)	1:23:A:THR:HG21	1:23:A:THR:HA	11	0.13
(1,107)	1:23:A:THR:HG22	1:23:A:THR:HA	11	0.13
(1,107)	1:23:A:THR:HG23	1:23:A:THR:HA	11	0.13
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	2	0.12
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	5	0.12
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	9	0.12
(1,471)	1:30:A:THR:H	1:28:A:LYS:HD2	2	0.12
(1,471)	1:30:A:THR:H	1:28:A:LYS:HD3	2	0.12
(1,456)	1:20:A:HIS:H	1:17:A:LYS:HA	10	0.12
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	1	0.12
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	2	0.12
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	1	0.12
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	5	0.12
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	8	0.12
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	4	0.12
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	10	0.12
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	12	0.12
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	13	0.12
(1,284)	1:10:A:ILE:H	1:10:A:ILE:HB	14	0.12
(1,284)	1:10:A:ILE:H	1:10:A:ILE:HB	15	0.12
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	6	0.11
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	7	0.11
(1,497)	1:16:A:CYS:H	1:17:A:LYS:HB3	10	0.11
(1,485)	1:14:A:ARG:H	1:25:A:CYS:HB3	4	0.11
(1,485)	1:14:A:ARG:H	1:25:A:CYS:HB3	12	0.11
(1,458)	1:24:A:ARG:H	1:21:A:TRP:HB3	7	0.11
(1,441)	1:17:A:LYS:H	1:13:A:CYS:H	15	0.11
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	3	0.11
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	7	0.11
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	12	0.11
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	15	0.11
(1,421)	1:29:A:ASP:H	1:28:A:LYS:HA	9	0.11
(1,421)	1:29:A:ASP:H	1:28:A:LYS:HA	12	0.11
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	2	0.11
(1,395)	1:21:A:TRP:H	1:20:A:HIS:H	15	0.11
(1,375)	1:17:A:LYS:H	1:16:A:CYS:H	7	0.11
(1,373)	1:16:A:CYS:H	1:17:A:LYS:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	1	0.11
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	2	0.11
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	11	0.11
(1,302)	1:16:A:CYS:H	1:16:A:CYS:HB3	1	0.11
(1,302)	1:16:A:CYS:H	1:16:A:CYS:HB3	7	0.11
(1,302)	1:16:A:CYS:H	1:16:A:CYS:HB3	10	0.11
(1,302)	1:16:A:CYS:H	1:16:A:CYS:HB3	13	0.11
(1,201)	1:27:A:TYR:HB3	1:28:A:LYS:HD2	12	0.11
(1,201)	1:27:A:TYR:HB3	1:28:A:LYS:HD3	12	0.11
(1,441)	1:17:A:LYS:H	1:13:A:CYS:H	4	0.1
(1,441)	1:17:A:LYS:H	1:13:A:CYS:H	11	0.1
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	8	0.1
(1,428)	1:30:A:THR:H	1:29:A:ASP:HB3	13	0.1
(1,421)	1:29:A:ASP:H	1:28:A:LYS:HA	14	0.1
(1,344)	1:12:A:SER:H	1:11:A:VAL:HB	5	0.1
(1,302)	1:16:A:CYS:H	1:16:A:CYS:HB3	8	0.1

10 Dihedral-angle violation analysis

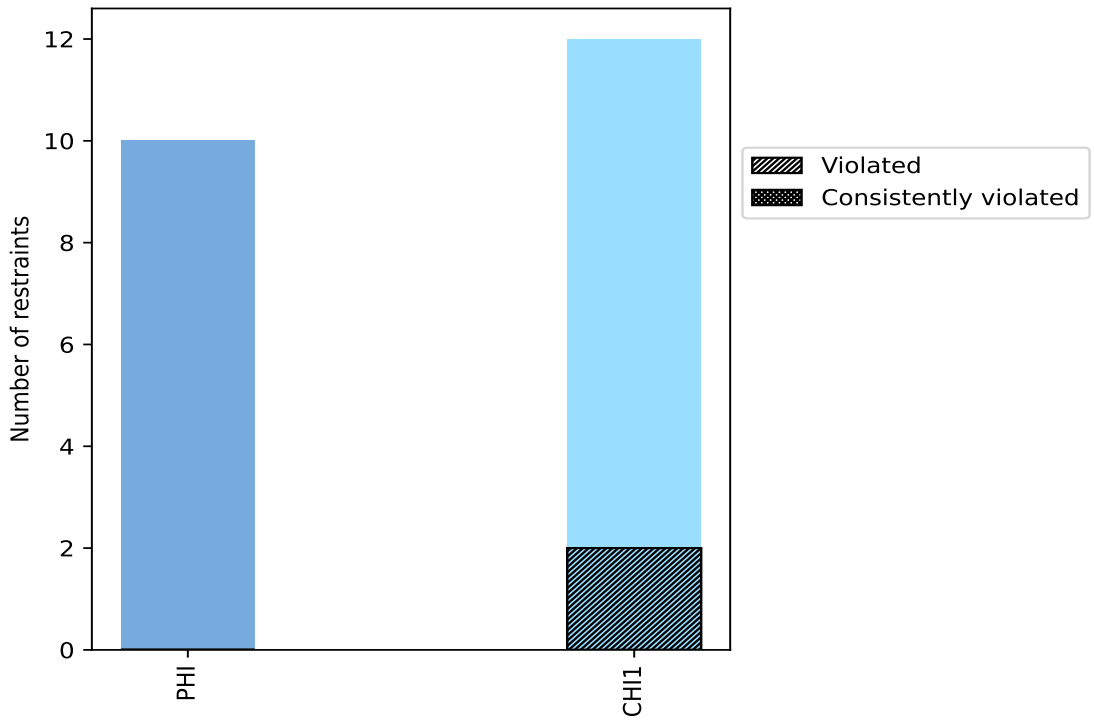
10.1 Summary of dihedral-angle violations

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]
PHI	10	45.5	0	0.0	0.0	0	0.0	0.0
CHI1	12	54.5	2	16.7	9.1	0	0.0	0.0
Total	22	100.0	2	9.1	9.1	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



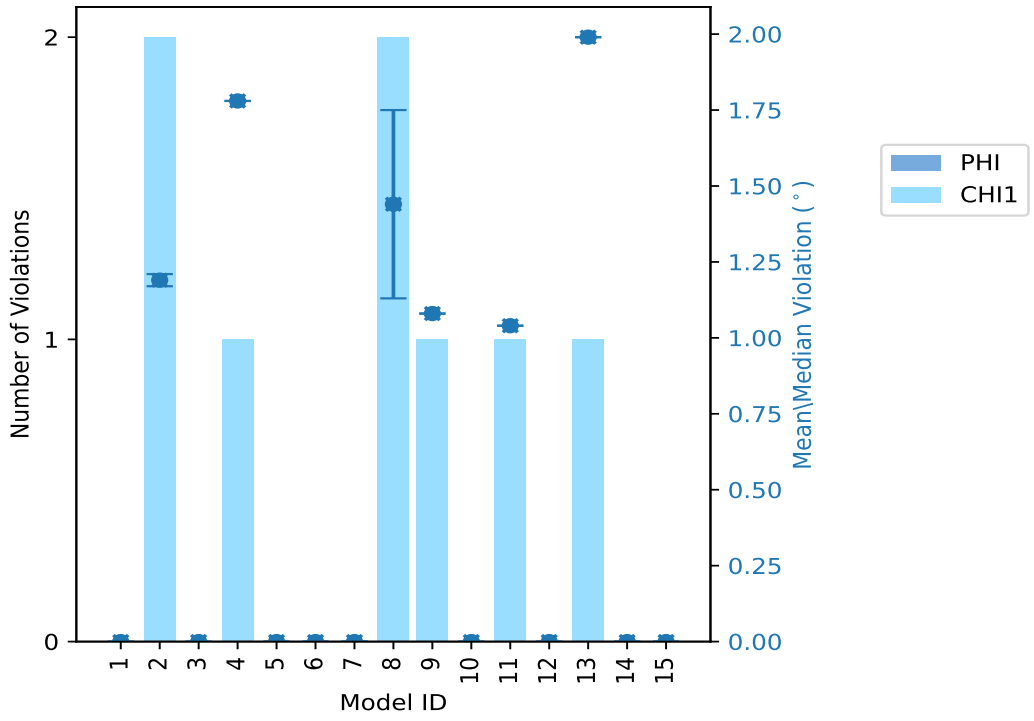
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	CHI1	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	2	2	1.19	1.21	0.02	1.19
3	0	0	0	0.0	0.0	0.0	0.0
4	0	1	1	1.78	1.78	0.0	1.78
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0.0	0.0	0.0	0.0
8	0	2	2	1.44	1.74	0.31	1.44
9	0	1	1	1.08	1.08	0.0	1.08
10	0	0	0	0.0	0.0	0.0	0.0
11	0	1	1	1.04	1.04	0.0	1.04
12	0	0	0	0.0	0.0	0.0	0.0
13	0	1	1	1.99	1.99	0.0	1.99
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral 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

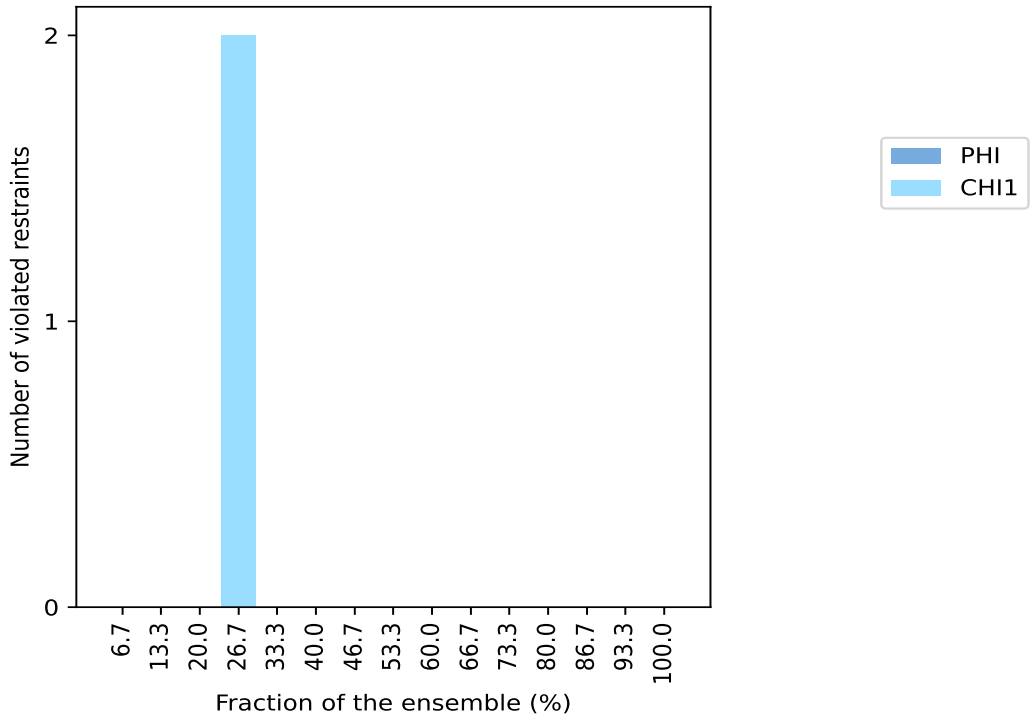
10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	CHI1	Total	Count[1]	%
0	0	0	1	6.7
0	0	0	2	13.3
0	0	0	3	20.0
0	2	2	4	26.7
0	0	0	5	33.3
0	0	0	6	40.0
0	0	0	7	46.7
0	0	0	8	53.3
0	0	0	9	60.0
0	0	0	10	66.7
0	0	0	11	73.3
0	0	0	12	80.0
0	0	0	13	86.7
0	0	0	14	93.3
0	0	0	15	100.0

[1] Number of models with violations

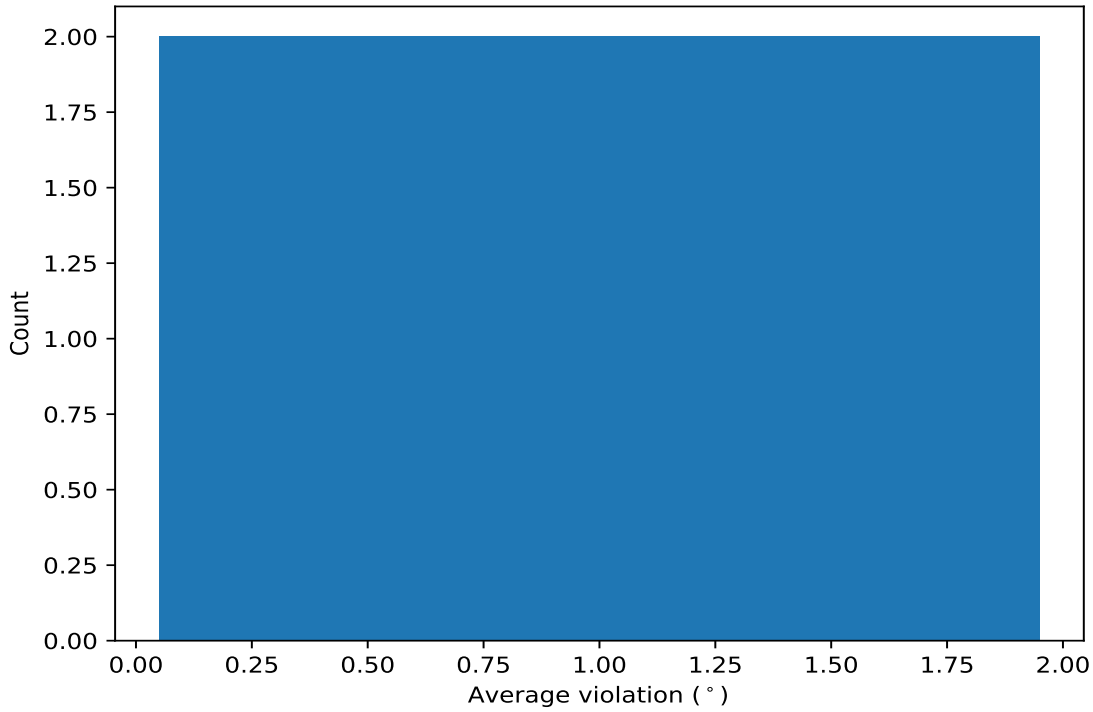
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle 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.

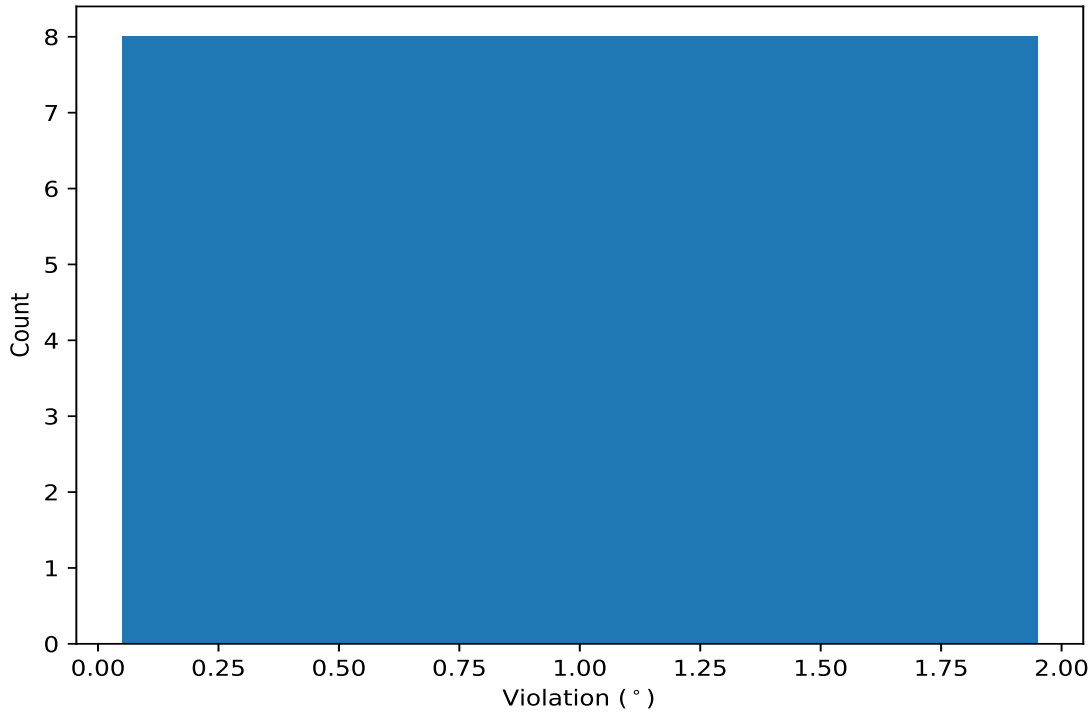
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,11)	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:CB	1:19:A:ASP:CG	4	1.67	0.3	1.76
(1,10)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:CB	1:14:A:ARG:CG	4	1.12	0.06	1.1

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints

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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,11)	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:CB	1:19:A:ASP:CG	13	1.99
(1,11)	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:CB	1:19:A:ASP:CG	4	1.78
(1,11)	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:CB	1:19:A:ASP:CG	8	1.74
(1,10)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:CB	1:14:A:ARG:CG	2	1.21
(1,11)	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:CB	1:19:A:ASP:CG	2	1.18
(1,10)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:CB	1:14:A:ARG:CG	8	1.13
(1,10)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:CB	1:14:A:ARG:CG	9	1.08
(1,10)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:CB	1:14:A:ARG:CG	11	1.04