



wwPDB NMR Structure Validation Summary Report ⓘ

Dec 25, 2024 – 12:00 AM EST

PDB ID : 2MY2
BMRB ID : 25442
Title : Snu17p-Bud13p structure intermediate during RES complex assembly
Authors : Wysoczanski, P.; Becker, S.; Zweckstetter, M.
Deposited on : 2015-01-19

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 ⓘ 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 : 4.02b-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

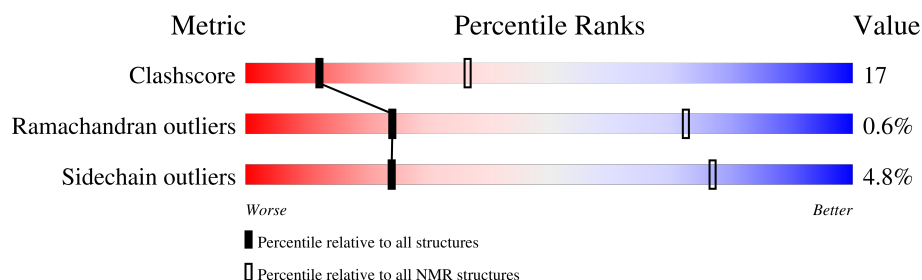
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR



The overall completeness of chemical shifts assignment is 82%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	118	
2	B	41	

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:44, A:53-A:89, B:311-B:325 (86)	0.80	10
2	B:328-B:338 (11)	0.50	18

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2549 atoms, of which 1251 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called U2 snRNP component IST3.

Mol	Chain	Residues	Atoms						Trace
1	A	118	Total	C	H	N	O	S	0
			1881	598	929	162	191	1	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P40565
A	2	ALA	-	expression tag	UNP P40565
A	3	MET	-	expression tag	UNP P40565
A	4	GLY	-	expression tag	UNP P40565

- Molecule 2 is a protein called Pre-mRNA-splicing factor CWC26.

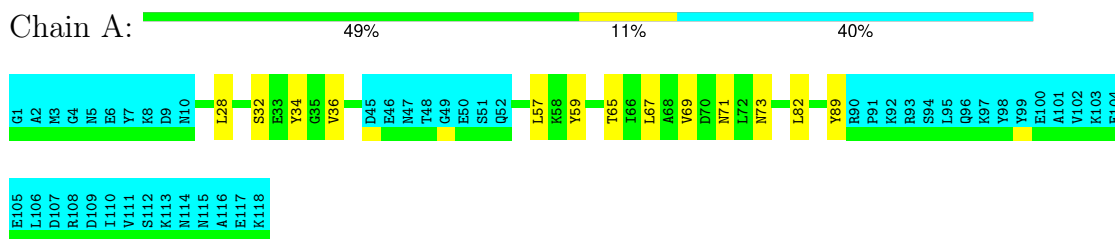
Mol	Chain	Residues	Atoms						Trace
2	B	41	Total	C	H	N	O	S	0
			668	218	322	63	64	1	

4 Residue-property plots

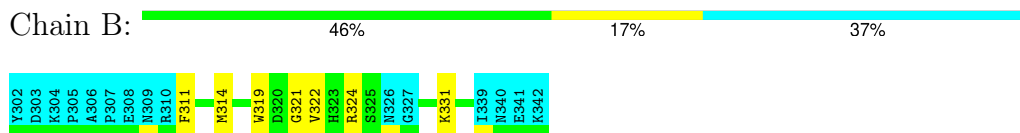
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: U2 snRNP component IST3



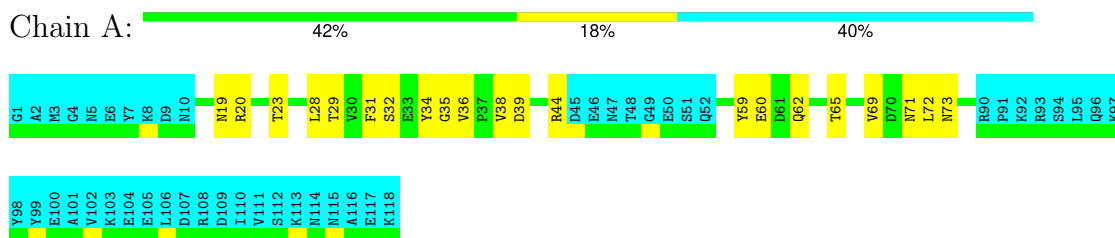
- Molecule 2: Pre-mRNA-splicing factor CWC26



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

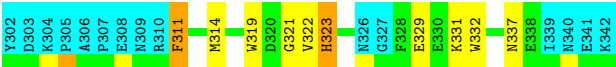
The representative model is number 10. Colouring as in section 4.1 above.

- Molecule 1: U2 snRNP component IST3



- Molecule 2: Pre-mRNA-splicing factor CWC26





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: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	3.0
CYANA	refinement	3.0

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	1688
Number of shifts mapped to atoms	1688
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [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	570	566	565	19±5
2	B	223	205	204	10±3
All	All	15860	15420	15380	529

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 17.

5 of 218 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ILE:HD11	1:A:57:LEU:HD12	0.86	1.46	8	3
1:A:67:LEU:HD21	2:B:311:PHE:CD1	0.82	2.10	19	10
1:A:57:LEU:H	1:A:57:LEU:HD12	0.70	1.45	11	1
2:B:323:HIS:H	2:B:323:HIS:CD2	0.69	2.05	10	1
1:A:65:THR:O	1:A:69:VAL:HG23	0.68	1.88	13	11

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	71/118 (60%)	67±1 (95±2%)	4±1 (5±2%)	0±0 (0±0%)	50	84
2	B	26/41 (63%)	24±1 (92±2%)	2±1 (6±3%)	0±0 (2±2%)	10	54
All	All	1940/3180 (61%)	1827 (94%)	102 (5%)	11 (1%)	24	72

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)
2	B	320	ASP	8
1	A	69	VAL	1
1	A	78	GLY	1
2	B	329	GLU	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	60/101 (59%)	58±1 (96±2%)	2±1 (4±2%)	30	82
2	B	22/35 (63%)	20±1 (93±5%)	2±1 (7±5%)	15	65
All	All	1640/2720 (60%)	1562 (95%)	78 (5%)	24	77

5 of 26 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	82	LEU	10
2	B	324	ARG	8
1	A	57	LEU	7
2	B	311	PHE	6
2	B	331	LYS	6

6.3.3 RNA ⓘ

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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 82% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *SHIFT_LIST*

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	1688
Number of shifts mapped to atoms	1688
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	157

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
$^{13}\text{C}_\alpha$	152	-0.35 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	128	-0.11 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	34	-0.38 ± 0.24	None needed (< 0.5 ppm)
^{15}N	137	-0.29 ± 0.34	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1120 atoms were assigned a chemical shift out of a possible 1365. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	405/490 (83%)	196/201 (98%)	117/194 (60%)	92/95 (97%)
Sidechain	596/711 (84%)	412/461 (89%)	178/220 (81%)	6/30 (20%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	119/164 (73%)	61/79 (77%)	56/79 (71%)	2/6 (33%)
Overall	1120/1365 (82%)	669/741 (90%)	351/493 (71%)	100/131 (76%)

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	B	331	LYS	CE	342.33	37.57 – 46.21	347.7
1	B	304	LYS	CE	342.31	37.57 – 46.21	347.7
1	B	335	LYS	CE	342.08	37.57 – 46.21	347.4
1	B	318	ARG	CD	342.64	38.57 – 47.75	326.2
1	B	310	ARG	CD	342.62	38.57 – 47.75	326.2
1	B	305	PRO	CD	350.65	45.11 – 55.58	286.8
1	B	307	PRO	CD	350.14	45.11 – 55.58	286.3
1	B	336	GLN	CG	333.03	28.36 – 39.21	275.8
1	B	331	LYS	CD	329.28	23.50 – 34.42	275.0
1	B	335	LYS	CD	328.70	23.50 – 34.42	274.5
1	B	305	PRO	CG	327.40	21.69 – 32.72	272.2
1	B	315	PRO	CG	327.32	21.69 – 32.72	272.1
1	B	307	PRO	CG	327.19	21.69 – 32.72	272.0
1	B	331	LYS	CG	325.49	19.35 – 30.45	270.8
1	B	304	LYS	CG	324.62	19.35 – 30.45	270.0
1	B	335	LYS	CG	324.56	19.35 – 30.45	270.0
1	B	315	PRO	CB	333.59	26.06 – 37.61	261.3
1	B	305	PRO	CB	332.15	26.06 – 37.61	260.0
1	B	307	PRO	CB	331.83	26.06 – 37.61	259.7
1	B	330	GLU	CG	337.23	30.20 – 42.01	255.0
1	B	338	GLU	CG	336.39	30.20 – 42.01	254.3
1	B	308	GLU	CG	336.32	30.20 – 42.01	254.2
1	B	324	ARG	CG	328.29	21.24 – 33.19	251.9
1	B	318	ARG	CG	327.43	21.24 – 33.19	251.2
1	B	327	GLY	CA	344.99	38.93 – 51.79	233.0
1	B	321	GLY	CA	344.17	38.93 – 51.79	232.4
1	B	314	MET	CG	332.69	25.46 – 38.60	228.8
1	B	339	ILE	CG2	317.62	10.93 – 24.12	227.5
1	B	313	ILE	CG2	317.53	10.93 – 24.12	227.4
1	B	322	VAL	CG1	321.19	14.71 – 28.29	220.7
1	B	325	SER	CB	365.09	56.28 – 71.32	200.3
1	B	305	PRO	CA	363.09	55.85 – 70.84	200.0

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	315	PRO	CA	362.82	55.85 – 70.84	199.8
1	B	307	PRO	CA	362.67	55.85 – 70.84	199.7
1	B	317	SER	CB	363.62	56.28 – 71.32	199.3
1	B	322	VAL	CG2	320.42	13.71 – 28.88	197.2
1	B	303	ASP	CB	341.27	32.98 – 48.76	190.4
1	B	320	ASP	CB	340.19	32.98 – 48.76	189.7
1	B	309	ASN	CB	342.80	30.50 – 46.89	185.5
1	B	340	ASN	CB	339.59	30.50 – 46.89	183.6
1	B	313	ILE	CD1	314.60	5.18 – 21.60	183.4
1	B	337	ASN	CB	339.18	30.50 – 46.89	183.3
1	B	326	ASN	CB	338.38	30.50 – 46.89	182.8
1	B	339	ILE	CD1	313.12	5.18 – 21.60	182.5
1	B	308	GLU	CB	330.83	21.56 – 38.37	179.0
1	B	338	GLU	CB	330.22	21.56 – 38.37	178.6
1	B	341	GLU	CB	330.17	21.56 – 38.37	178.6
1	B	330	GLU	CB	329.90	21.56 – 38.37	178.4
1	B	329	GLU	CB	329.69	21.56 – 38.37	178.3
1	B	313	ILE	CG1	329.29	19.24 – 36.26	177.2
1	B	336	GLN	NE2	412.16	103.38 – 120.35	177.0
1	B	339	ILE	CG1	327.47	19.24 – 36.26	176.1
1	B	304	LYS	CB	332.99	24.03 – 41.47	172.2
1	B	314	MET	CE	317.64	8.39 – 25.85	172.1
1	B	331	LYS	CB	332.04	24.03 – 41.47	171.6
1	B	335	LYS	CB	331.93	24.03 – 41.47	171.5
1	B	306	ALA	CB	318.87	10.19 – 27.75	170.8
1	B	334	ALA	CB	318.31	10.19 – 27.75	170.5
1	B	312	ALA	CB	316.77	10.19 – 27.75	169.6
1	B	336	GLN	CB	328.29	20.34 – 37.98	169.6
1	B	322	VAL	CB	331.75	23.86 – 41.50	169.5
1	B	318	ARG	CB	329.12	21.74 – 39.52	167.9
1	B	337	ASN	CA	354.02	44.28 – 62.79	162.3
1	B	326	ASN	CA	353.83	44.28 – 62.79	162.2
1	B	340	ASN	CA	353.48	44.28 – 62.79	162.0
1	B	309	ASN	CA	352.28	44.28 – 62.79	161.4
1	B	334	ALA	CA	354.70	43.52 – 62.81	156.3
1	B	312	ALA	CA	353.05	43.52 – 62.81	155.5
1	B	306	ALA	CA	350.08	43.52 – 62.81	153.9
1	B	313	ILE	CB	339.79	28.63 – 48.45	152.0
1	B	332	TRP	CB	328.80	20.06 – 39.75	151.8
1	B	319	TRP	CB	328.16	20.06 – 39.75	151.5
1	B	339	ILE	CB	338.69	28.63 – 48.45	151.4
1	B	303	ASP	CA	354.53	44.71 – 64.67	150.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	320	ASP	CA	353.54	44.71 – 64.67	149.7
1	B	311	PHE	CB	341.70	29.72 – 50.07	148.3
1	B	317	SER	CA	361.28	48.46 – 68.96	147.6
1	B	329	GLU	CA	360.83	47.03 – 67.62	147.4
1	B	328	PHE	CB	339.83	29.72 – 50.07	147.4
1	B	333	PHE	CB	339.31	29.72 – 50.07	147.1
1	B	330	GLU	CA	359.96	47.03 – 67.62	147.0
1	B	338	GLU	CA	357.36	47.03 – 67.62	145.7
1	B	341	GLU	CA	356.78	47.03 – 67.62	145.4
1	B	308	GLU	CA	356.37	47.03 – 67.62	145.2
1	B	325	SER	CA	356.12	48.46 – 68.96	145.1
1	B	336	GLN	CA	356.83	46.17 – 66.97	144.3
1	B	319	TRP	NE1	435.96	118.53 – 139.98	143.0
1	B	323	HIS	CB	329.05	19.76 – 40.75	142.3
1	B	302	TYR	CB	338.69	28.67 – 49.81	141.7
1	B	331	LYS	CA	359.22	46.18 – 67.77	140.0
1	B	314	MET	CB	332.17	22.22 – 43.61	139.9
1	B	332	TRP	NE1	428.54	118.53 – 139.98	139.5
1	B	335	LYS	CA	357.51	46.18 – 67.77	139.2
1	B	342	LYS	CA	356.88	46.18 – 67.77	138.9
1	B	304	LYS	CA	353.98	46.18 – 67.77	137.6
1	B	337	ASN	ND2	412.80	101.55 – 123.95	133.9
1	B	310	ARG	CA	358.12	45.44 – 68.13	132.8
1	B	318	ARG	CA	355.45	45.44 – 68.13	131.6
1	B	324	ARG	CA	354.96	45.44 – 68.13	131.4
1	B	323	HIS	CA	355.08	45.04 – 67.94	130.4
1	B	332	TRP	CA	362.10	45.21 – 70.26	121.5
1	B	302	TYR	CA	357.68	45.75 – 70.63	120.4
1	B	319	TRP	CA	357.80	45.21 – 70.26	119.8
1	B	328	PHE	CA	363.62	45.38 – 70.89	119.8
1	B	333	PHE	CA	362.09	45.38 – 70.89	119.2
1	B	311	PHE	CA	356.35	45.38 – 70.89	116.9
1	B	313	ILE	CA	362.18	48.30 – 75.08	112.2
1	B	339	ILE	CA	361.77	48.30 – 75.08	112.1
1	B	322	VAL	CA	362.06	48.38 – 76.73	105.6
1	B	314	MET	N	428.25	102.99 – 137.21	90.0
1	B	308	GLU	N	422.04	103.74 – 137.78	88.5
1	B	341	GLU	N	421.84	103.74 – 137.78	88.5
1	B	329	GLU	N	421.56	103.74 – 137.78	88.4
1	B	338	GLU	N	420.25	103.74 – 137.78	88.0
1	B	317	SER	N	416.96	99.14 – 133.45	87.6
1	B	306	ALA	N	424.92	106.13 – 140.55	87.6

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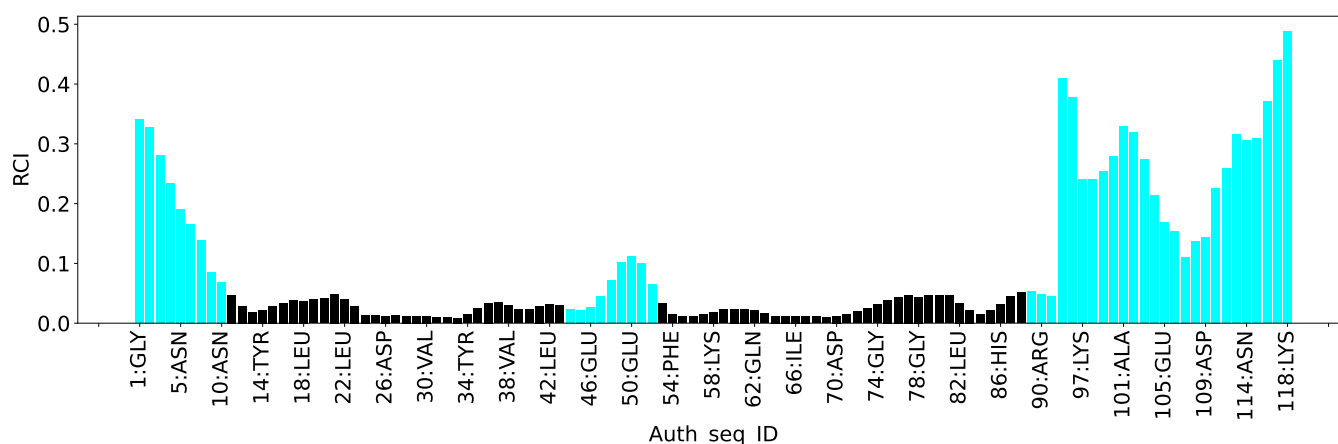
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	325	SER	N	415.69	99.14 – 133.45	87.3
1	B	324	ARG	N	433.81	102.91 – 138.82	87.2
1	B	312	ALA	N	422.65	106.13 – 140.55	87.0
1	B	330	GLU	N	416.36	103.74 – 137.78	86.8
1	B	334	ALA	N	421.89	106.13 – 140.55	86.7
1	B	336	GLN	N	418.06	102.61 – 137.42	85.6
1	B	342	LYS	N	427.25	102.74 – 139.42	83.5
1	B	316	GLY	N	409.11	91.59 – 127.52	83.4
1	B	310	ARG	N	419.97	102.91 – 138.82	83.3
1	B	327	GLY	N	408.56	91.59 – 127.52	83.2
1	B	318	ARG	N	418.30	102.91 – 138.82	82.8
1	B	320	ASP	N	428.09	102.08 – 139.36	82.5
1	B	304	LYS	N	421.44	102.74 – 139.42	81.9
1	B	331	LYS	N	420.46	102.74 – 139.42	81.6
1	B	335	LYS	N	417.95	102.74 – 139.42	80.9
1	B	303	ASP	N	421.49	102.08 – 139.36	80.7
1	B	326	ASN	N	426.31	99.66 – 138.23	79.7
1	B	340	ASN	N	421.97	99.66 – 138.23	78.6
1	B	337	ASN	N	416.92	99.66 – 138.23	77.3
1	B	309	ASN	N	415.31	99.66 – 138.23	76.8
1	B	323	HIS	N	427.15	99.59 – 139.87	76.3
1	B	332	TRP	N	423.16	101.51 – 141.60	75.2
1	B	319	TRP	N	419.29	101.51 – 141.60	74.3
1	B	328	PHE	N	422.84	99.93 – 140.82	74.0
1	B	311	PHE	N	417.48	99.93 – 140.82	72.7
1	B	333	PHE	N	417.43	99.93 – 140.82	72.7
1	B	339	ILE	N	419.95	100.55 – 142.30	71.5
1	B	313	ILE	N	419.57	100.55 – 142.30	71.4
1	B	322	VAL	N	422.05	99.23 – 142.92	68.9
1	B	321	GLY	HA2	0.60	2.15 – 5.77	-9.3
1	A	33	GLU	HG2	0.52	1.24 – 3.30	-8.5
1	A	33	GLU	HG3	0.48	1.20 – 3.30	-8.4
1	B	310	ARG	HD3	1.03	1.81 – 4.39	-8.1
1	B	310	ARG	HG3	-0.41	0.15 – 2.94	-7.0
1	A	70	ASP	HB2	0.99	1.41 – 4.01	-6.6
1	B	324	ARG	HB3	0.01	0.43 – 3.11	-6.5
1	A	58	LYS	HB2	0.22	0.58 – 2.97	-6.5
1	B	310	ARG	HG2	-0.08	0.26 – 2.87	-6.3
1	B	321	GLY	H	4.58	5.23 – 11.42	-6.1
1	B	310	ARG	HB3	0.22	0.43 – 3.11	-5.8
1	B	310	ARG	HB2	0.35	0.52 – 3.08	-5.6

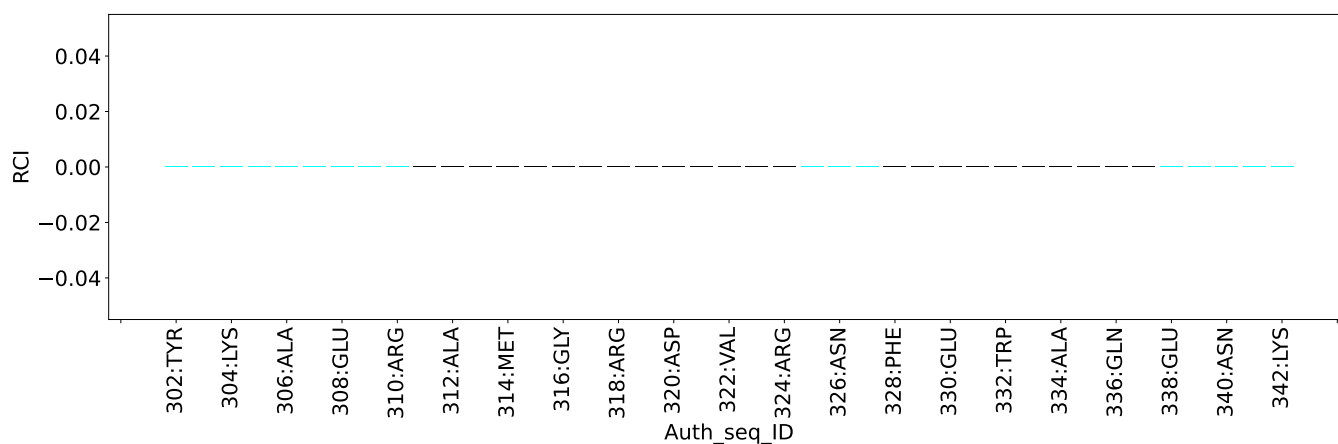
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



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	1459
Intra-residue ($ i-j =0$)	353
Sequential ($ i-j =1$)	301
Medium range ($ i-j >1$ and $ i-j <5$)	231
Long range ($ i-j \geq 5$)	457
Inter-chain	77
Hydrogen bond restraints	40
Disulfide bond restraints	0
Total dihedral-angle restraints	192
Number of unmapped restraints	0
Number of restraints per residue	10.4
Number of long range restraints per residue ¹	3.0

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 [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)	27.9	0.2
0.2-0.5 (Medium)	18.9	0.5
>0.5 (Large)	6.9	1.97

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)	14.8	7.51
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

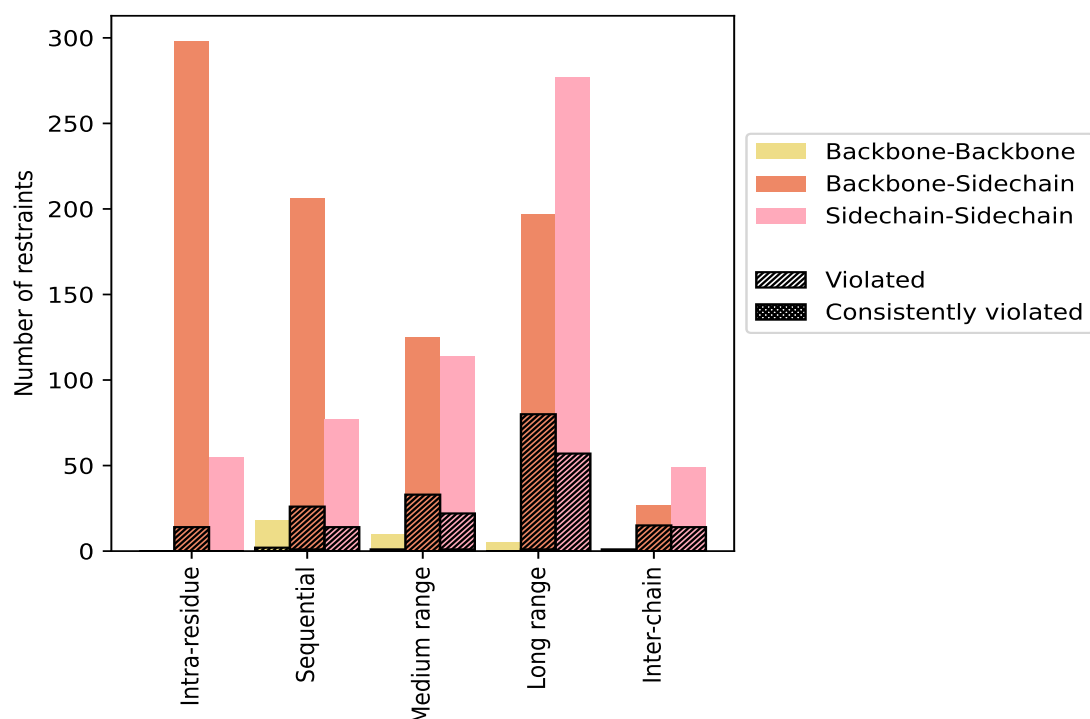
9.1 Summary of distance violations ⓘ

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)	353	24.2	14	4.0	1.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	298	20.4	14	4.7	1.0	0	0.0	0.0
Sidechain-Sidechain	55	3.8	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	301	20.6	42	14.0	2.9	1	0.3	0.1
Backbone-Backbone	18	1.2	2	11.1	0.1	0	0.0	0.0
Backbone-Sidechain	206	14.1	26	12.6	1.8	1	0.5	0.1
Sidechain-Sidechain	77	5.3	14	18.2	1.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	231	15.8	47	20.3	3.2	1	0.4	0.1
Backbone-Backbone	10	0.7	1	10.0	0.1	0	0.0	0.0
Backbone-Sidechain	107	7.3	24	22.4	1.6	0	0.0	0.0
Sidechain-Sidechain	114	7.8	22	19.3	1.5	1	0.9	0.1
Long range (i-j ≥5)	457	31.3	117	25.6	8.0	0	0.0	0.0
Backbone-Backbone	5	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	175	12.0	60	34.3	4.1	0	0.0	0.0
Sidechain-Sidechain	277	19.0	57	20.6	3.9	0	0.0	0.0
Inter-chain	77	5.3	30	39.0	2.1	0	0.0	0.0
Backbone-Backbone	1	0.1	1	100.0	0.1	0	0.0	0.0
Backbone-Sidechain	27	1.9	15	55.6	1.0	0	0.0	0.0
Sidechain-Sidechain	49	3.4	14	28.6	1.0	0	0.0	0.0
Hydrogen bond	40	2.7	29	72.5	2.0	1	2.5	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1459	100.0	279	19.1	19.1	3	0.2	0.2
Backbone-Backbone	34	2.3	4	11.8	0.3	0	0.0	0.0
Backbone-Sidechain	853	58.5	168	19.7	11.5	2	0.2	0.1
Sidechain-Sidechain	572	39.2	107	18.7	7.3	1	0.2	0.1

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 disulfide 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	6	12	30	5	53	0.32	1.26	0.29	0.18
2	2	3	9	31	8	53	0.37	1.33	0.3	0.25
3	0	7	10	13	8	38	0.35	1.81	0.36	0.22
4	2	7	7	27	8	51	0.28	1.27	0.24	0.2
5	4	10	12	30	7	63	0.28	1.7	0.29	0.2
6	2	3	6	30	12	53	0.26	0.97	0.23	0.18
7	5	7	12	29	10	63	0.3	1.57	0.32	0.19
8	0	5	15	29	9	58	0.29	1.97	0.32	0.18
9	1	12	16	36	8	73	0.31	1.34	0.3	0.19
10	4	5	10	28	7	54	0.29	0.97	0.22	0.19

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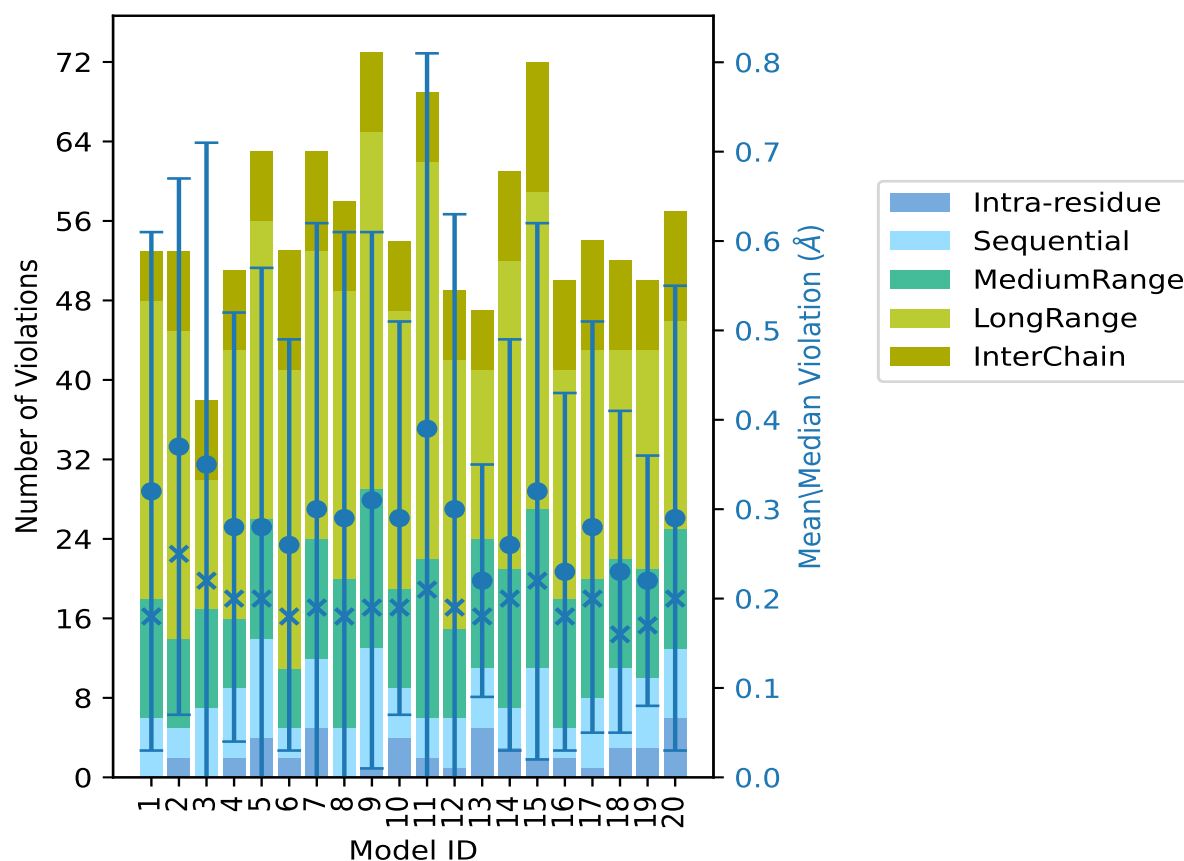
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	2	4	16	40	7	69	0.39	1.92	0.42	0.21
12	1	5	9	27	7	49	0.3	1.51	0.33	0.19
13	5	6	13	17	6	47	0.22	0.74	0.13	0.18
14	3	4	14	31	9	61	0.26	1.29	0.23	0.2
15	2	9	16	32	13	72	0.32	1.54	0.3	0.22
16	2	3	13	23	9	50	0.23	1.24	0.2	0.18
17	1	7	12	23	11	54	0.28	1.16	0.23	0.2
18	3	8	11	21	9	52	0.23	0.99	0.18	0.16
19	3	7	11	22	7	50	0.22	0.88	0.14	0.17
20	6	7	12	21	11	57	0.29	1.42	0.26	0.2

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

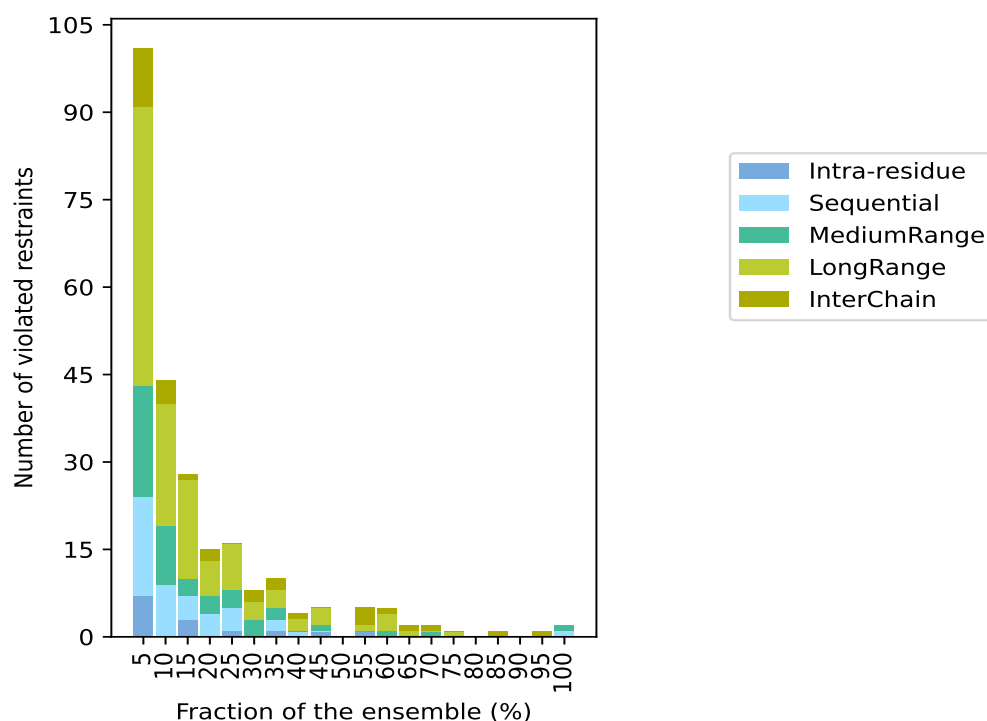
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1169(IR:339, SQ:259, MR:184, LR:340, IC:47) restraints are 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	%
7	17	19	48	10	101	1	5.0
0	9	10	21	4	44	2	10.0
3	4	3	17	1	28	3	15.0
0	4	3	6	2	15	4	20.0
1	4	3	8	0	16	5	25.0
0	0	3	3	2	8	6	30.0
1	2	2	3	2	10	7	35.0
0	1	0	2	1	4	8	40.0
1	0	1	3	0	5	9	45.0
0	0	0	0	0	0	10	50.0
1	0	0	1	3	5	11	55.0
0	0	1	3	1	5	12	60.0
0	0	0	1	1	2	13	65.0
0	0	1	0	1	2	14	70.0
0	0	0	1	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	1	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	1	1	19	95.0
0	1	1	0	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

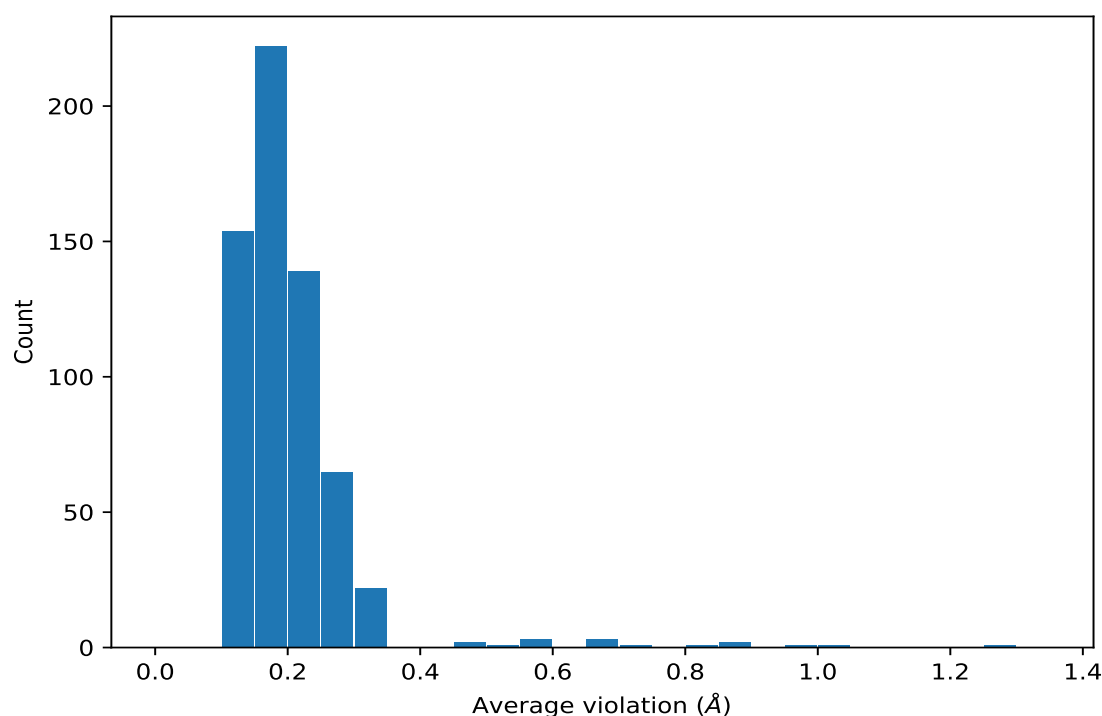
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 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)
(2,13)	1:39:A:ASP:H	1:58:A:LYS:O	20	0.8	0.34	0.89
(1,1049)	1:27:A:ILE:HB	1:30:A:VAL:HG11	20	0.32	0.05	0.32
(1,1049)	1:27:A:ILE:HB	1:30:A:VAL:HG12	20	0.32	0.05	0.32
(1,1049)	1:27:A:ILE:HB	1:30:A:VAL:HG13	20	0.32	0.05	0.32
(1,1049)	1:27:A:ILE:HB	1:30:A:VAL:HG21	20	0.32	0.05	0.32
(1,1049)	1:27:A:ILE:HB	1:30:A:VAL:HG22	20	0.32	0.05	0.32
(1,1049)	1:27:A:ILE:HB	1:30:A:VAL:HG23	20	0.32	0.05	0.32
(1,773)	2:319:B:TRP:HD1	2:320:B:ASP:H	20	0.27	0.06	0.26
(1,921)	1:29:A:THR:HG21	2:319:B:TRP:HZ2	19	0.24	0.1	0.26
(1,921)	1:29:A:THR:HG22	2:319:B:TRP:HZ2	19	0.24	0.1	0.26
(1,921)	1:29:A:THR:HG23	2:319:B:TRP:HZ2	19	0.24	0.1	0.26
(2,14)	1:39:A:ASP:N	1:58:A:LYS:O	18	0.7	0.28	0.74
(2,30)	1:28:A:LEU:O	1:32:A:SER:N	18	0.23	0.05	0.24
(1,1237)	1:72:A:LEU:HD11	2:324:B:ARG:HA	17	0.26	0.06	0.27
(1,1237)	1:72:A:LEU:HD12	2:324:B:ARG:HA	17	0.26	0.06	0.27
(1,1237)	1:72:A:LEU:HD13	2:324:B:ARG:HA	17	0.26	0.06	0.27

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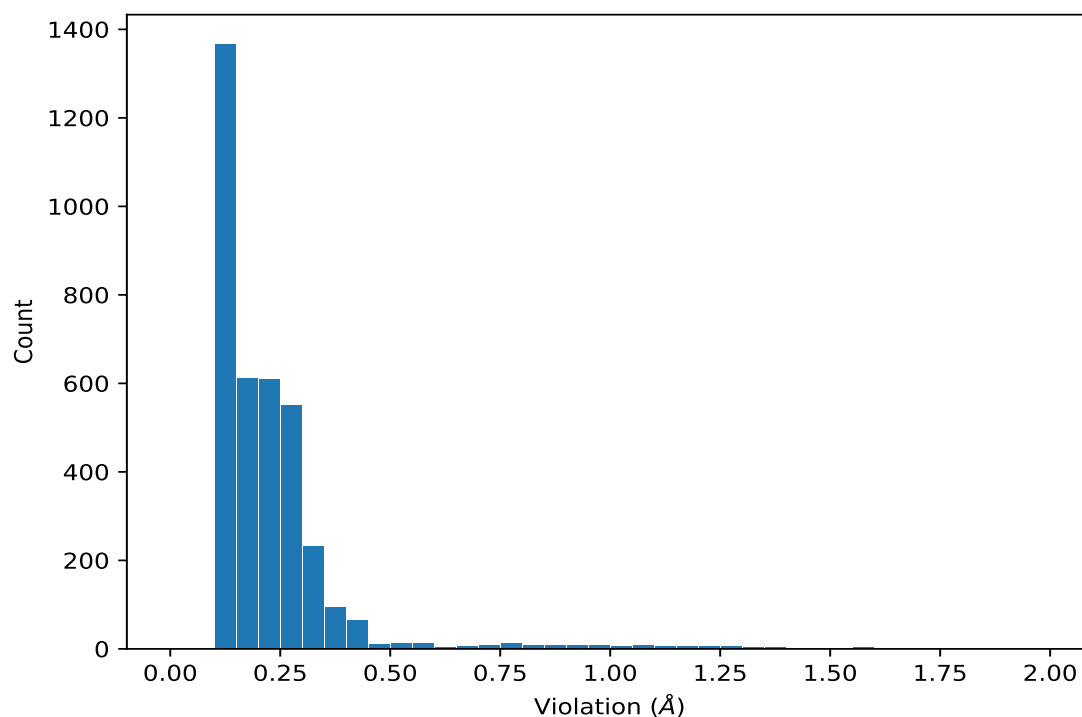
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1237)	1:72:A:LEU:HD21	2:324:B:ARG:HA	17	0.26	0.06	0.27
(1,1237)	1:72:A:LEU:HD22	2:324:B:ARG:HA	17	0.26	0.06	0.27
(1,1237)	1:72:A:LEU:HD23	2:324:B:ARG:HA	17	0.26	0.06	0.27
(2,21)	1:43:A:SER:H	1:54:A:PHE:O	16	1.28	0.46	1.25
(2,31)	1:63:A:ARG:O	1:67:A:LEU:H	16	0.98	0.31	1.03
(2,32)	1:63:A:ARG:O	1:67:A:LEU:N	16	0.73	0.27	0.79

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 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)
(2,21)	1:43:A:SER:H	1:54:A:PHE:O	8	1.97
(2,21)	1:43:A:SER:H	1:54:A:PHE:O	11	1.92
(2,21)	1:43:A:SER:H	1:54:A:PHE:O	3	1.81
(2,21)	1:43:A:SER:H	1:54:A:PHE:O	5	1.7
(2,3)	1:13:A:ILE:O	1:57:A:LEU:H	11	1.58
(2,22)	1:43:A:SER:N	1:54:A:PHE:O	11	1.57
(2,21)	1:43:A:SER:H	1:54:A:PHE:O	7	1.57
(2,21)	1:43:A:SER:H	1:54:A:PHE:O	15	1.54
(2,31)	1:63:A:ARG:O	1:67:A:LEU:H	12	1.51
(2,21)	1:43:A:SER:H	1:54:A:PHE:O	12	1.44

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

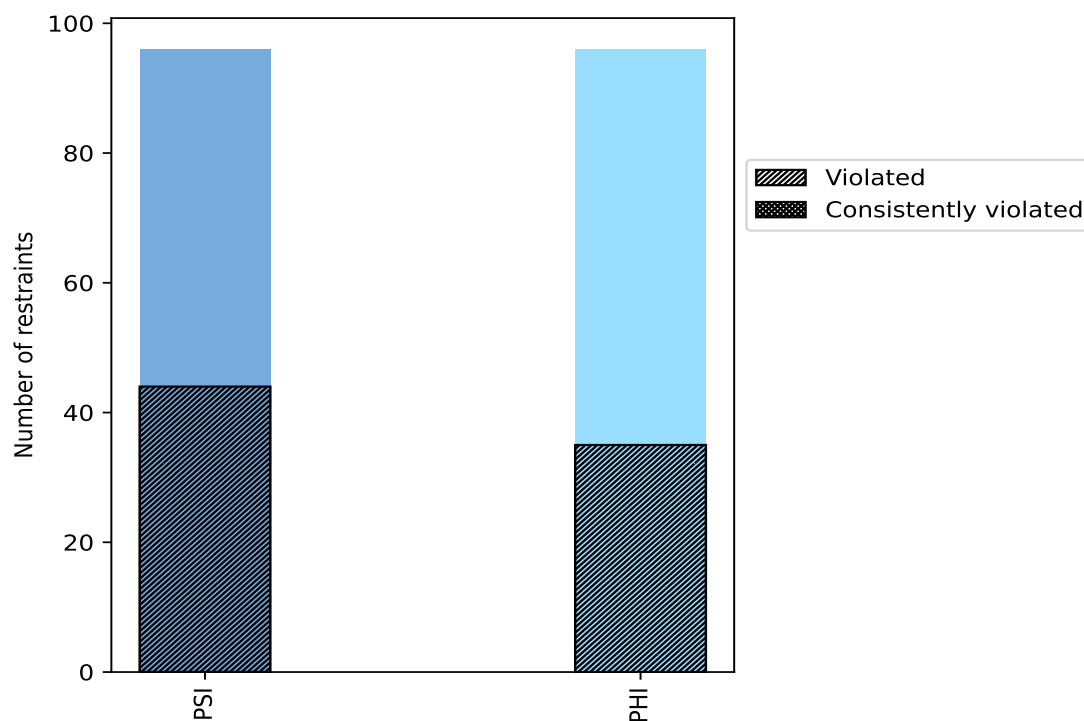
10.1 Summary of dihedral-angle violations [i](#)

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	96	50.0	44	45.8	22.9	0	0.0	0.0
PHI	96	50.0	35	36.5	18.2	0	0.0	0.0
Total	192	100.0	79	41.1	41.1	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 [i](#)



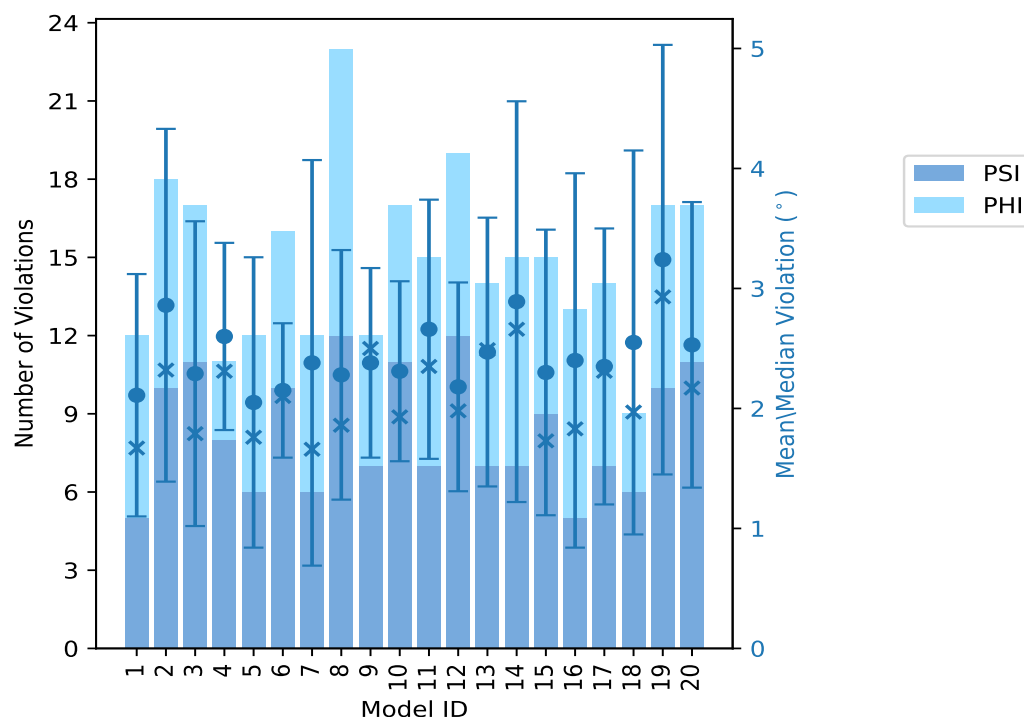
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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 (°)
	PSI	PHI	Total				
1	5	7	12	2.11	4.14	1.01	1.67
2	10	8	18	2.86	6.11	1.47	2.32
3	11	6	17	2.29	6.15	1.27	1.79
4	8	3	11	2.6	4.05	0.78	2.31
5	6	6	12	2.05	5.23	1.21	1.76
6	10	6	16	2.15	3.1	0.56	2.1
7	6	6	12	2.38	7.32	1.69	1.66
8	12	11	23	2.28	4.65	1.04	1.86
9	7	5	12	2.38	3.65	0.79	2.5
10	11	6	17	2.31	3.9	0.75	1.93
11	7	8	15	2.66	4.89	1.08	2.35
12	12	7	19	2.18	5.23	0.87	1.98
13	7	7	14	2.47	4.33	1.12	2.49
14	7	8	15	2.89	7.51	1.67	2.66
15	9	6	15	2.3	5.18	1.19	1.73
16	5	8	13	2.4	5.98	1.56	1.83
17	7	7	14	2.35	5.1	1.15	2.31
18	6	3	9	2.55	5.66	1.6	1.97
19	10	7	17	3.24	7.22	1.79	2.93
20	11	6	17	2.53	5.41	1.19	2.17

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	
PSI	PHI	Total	Count ¹	%
13	9	22	1	5.0
9	6	15	2	10.0
7	6	13	3	15.0
4	2	6	4	20.0
3	4	7	5	25.0
2	3	5	6	30.0
1	0	1	7	35.0
0	1	1	8	40.0
0	3	3	9	45.0
1	0	1	10	50.0
1	1	2	11	55.0

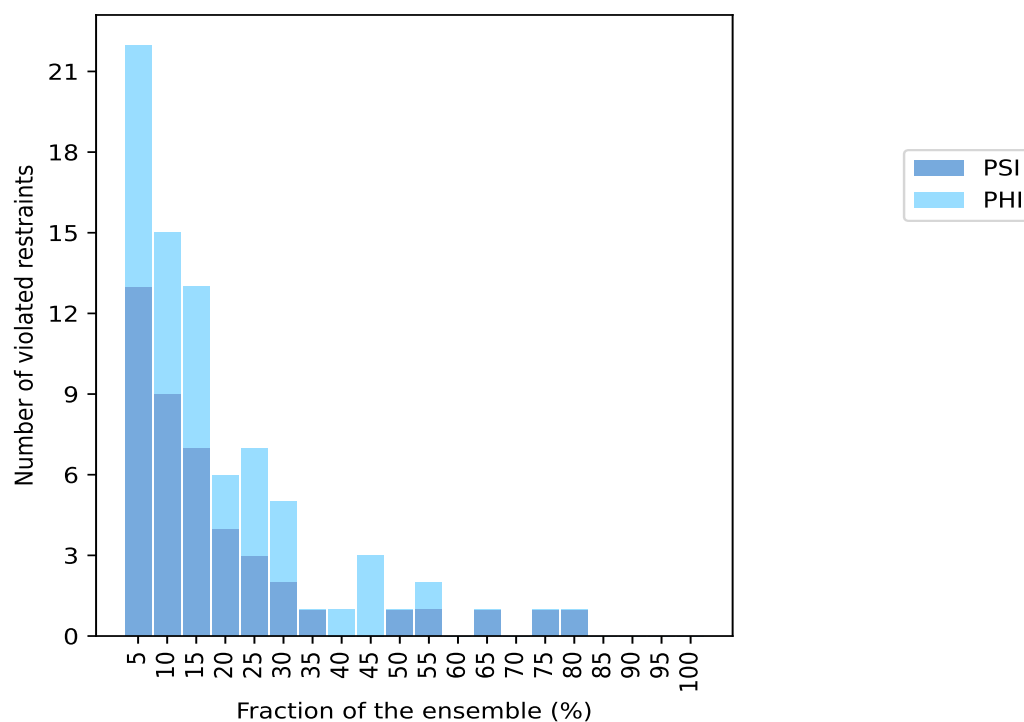
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
1	0	1	13	65.0
0	0	0	14	70.0
1	0	1	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

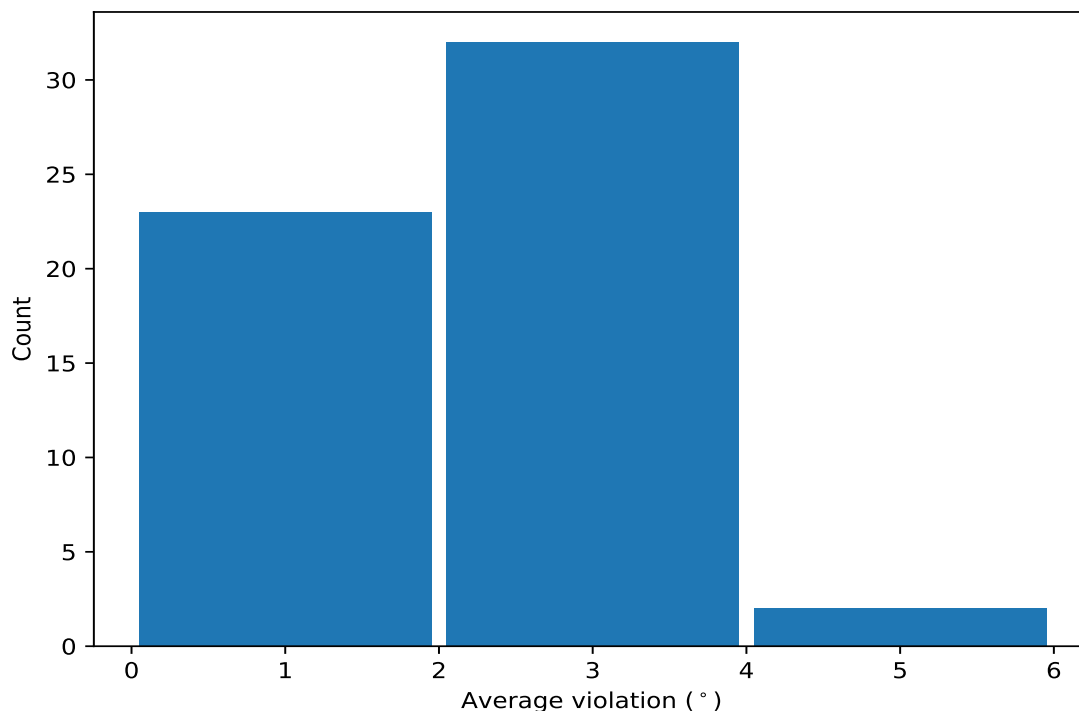


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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 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.

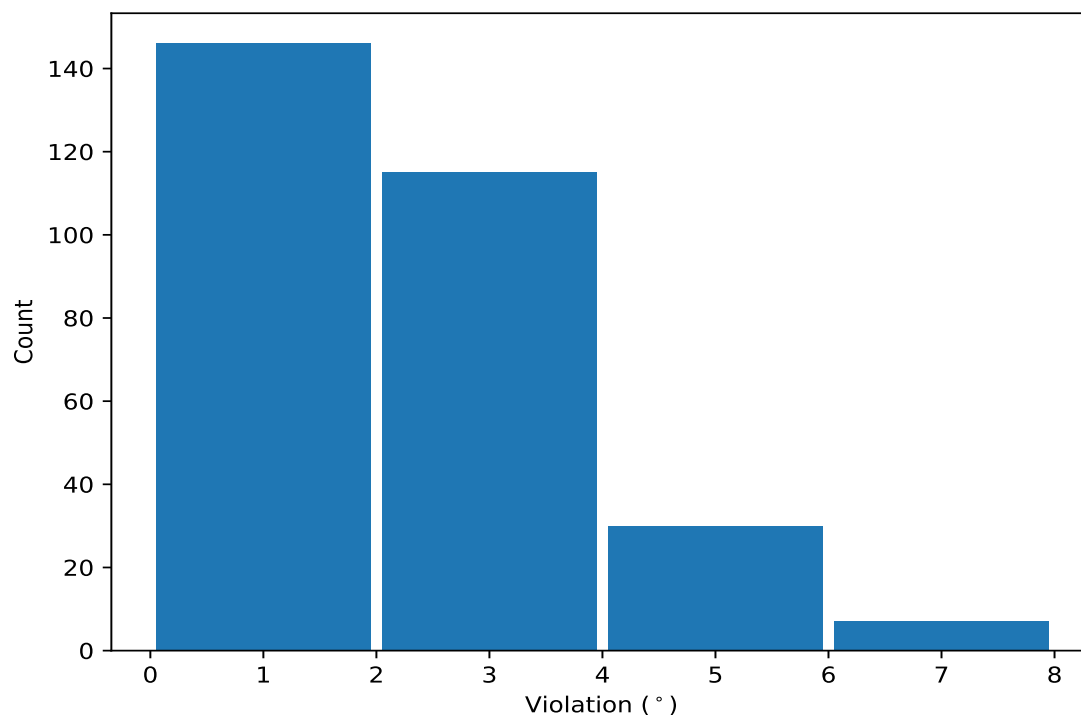
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,176)	2:329:B:GLU:N	2:329:B:GLU:CA	2:329:B:GLU:C	2:330:B:GLU:N	16	2.91	0.82	2.81
(1,42)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:GLU:N	15	3.1	1.67	2.53
(1,46)	1:37:A:PRO:N	1:37:A:PRO:CA	1:37:A:PRO:C	1:38:A:VAL:N	13	3.0	1.25	2.67
(1,102)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ASP:N	11	3.98	1.44	4.18
(1,47)	1:37:A:PRO:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	11	2.32	1.15	1.9
(1,22)	1:21:A:GLU:N	1:21:A:GLU:CA	1:21:A:GLU:C	1:22:A:LEU:N	10	2.15	0.93	2.0
(1,15)	1:17:A:ASN:C	1:18:A:LEU:N	1:18:A:LEU:CA	1:18:A:LEU:C	9	2.51	0.66	2.42
(1,169)	2:323:B:HIS:C	2:324:B:ARG:N	2:324:B:ARG:CA	2:324:B:ARG:C	9	2.34	0.88	2.08
(1,65)	1:46:A:GLU:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	9	2.06	0.61	1.98
(1,161)	2:318:B:ARG:C	2:319:B:TRP:N	2:319:B:TRP:CA	2:319:B:TRP:C	8	1.92	0.51	1.82

¹ Number of violated models, ²Standard 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 [i](#)

The following table provides the list of violations for 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,81)	1:58:A:LYS:C	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:C	14	7.51
(1,42)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:GLU:N	7	7.32
(1,109)	1:72:A:LEU:C	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	19	7.22
(1,147)	2:309:B:ASN:C	2:310:B:ARG:N	2:310:B:ARG:CA	2:310:B:ARG:C	3	6.15
(1,109)	1:72:A:LEU:C	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	2	6.11
(1,102)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ASP:N	19	6.08
(1,103)	1:69:A:VAL:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	2	6.01
(1,102)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ASP:N	16	5.98
(1,102)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ASP:N	18	5.66
(1,104)	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	1:71:A:ASN:N	20	5.41