W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB NMR Structure Validation Summary Report (i)

Jun 6, 2023 – 05:48 pm BST

PDB ID	:	4BIT
BMRB ID	:	19164
Title	:	solution structure of cerebral dopamine neurotrophic factor (CDNF)
Authors	:	Latge, C.; Cabral, K.M.S.; Raymundo, D.P.; Foguel, D.; Herrmann, T.; Almeida, M.S.
Deposited on	:	2013-04-13

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:

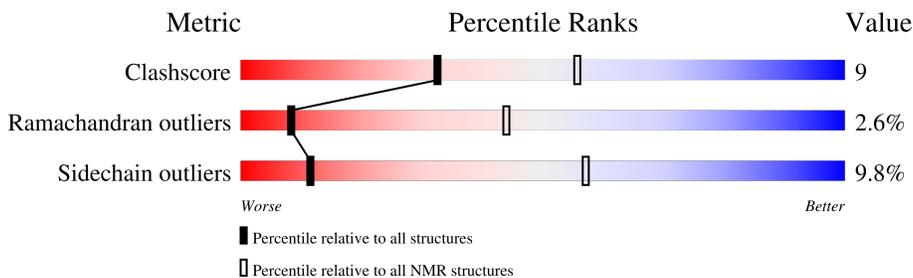|		
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance ⓘ

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

The overall completeness of chemical shifts assignment is 92%.

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	Percentile Ranks	Value
Clashscore		9
Ramachandran outliers		2.6%
Sidechain outliers		9.8%

Worse / Better

▌ Percentile relative to all structures

◫ Percentile relative to all NMR structures

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	161	63% 19% • 18%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:100 (90)	1.43	12
2	A:106-A:130, A:137-A:153 (42)	0.73	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 5 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2580 atoms, of which 1301 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CEREBRAL DOPAMINE NEUROTROPHIC FACTOR.

Mol	Chain	Residues	Atoms						Trace
1	A	161	Total	C	H	N	O	S	0
			2580	806	1301	218	243	12	

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.
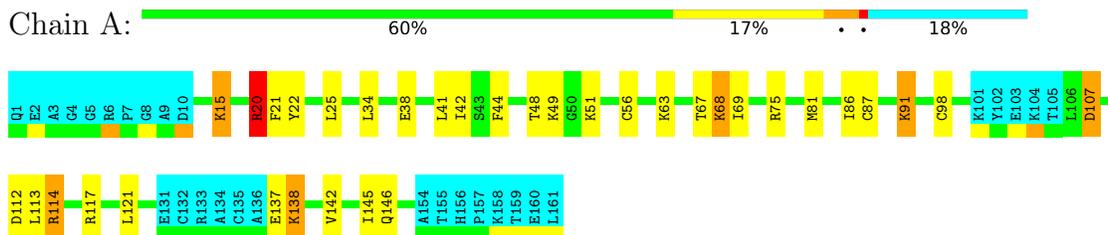
• Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR
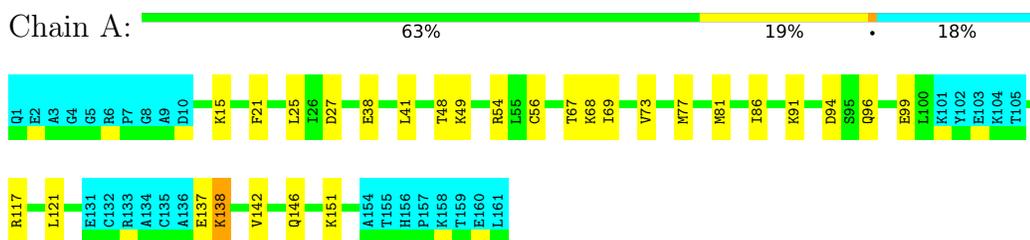
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 12. Colouring as in section 4.1 above.

• Molecule 1: CEREBRAL DOPAMINE NEUROTROPHIC FACTOR

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *CNS USING RECOORD SCRIPTS.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY.*

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

Software name	Classification	Version
CNS	refinement	1.3
UNIO	structure solution	10
CNS	structure solution	1.3

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	2029
Number of shifts mapped to atoms	2029
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.88±0.06	1±1/1078 (0.1± 0.1%)	0.81±0.06	0±1/1448 (0.0± 0.1%)
All	All	0.88	12/21560 (0.1%)	0.81	6/28960 (0.0%)

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	0.1±0.3	0.7±0.6
All	All	2	13

5 of 8 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
1	A	81	MET	N-CA	-6.54	1.33	1.46	3	1
1	A	58	TYR	CB-CG	6.42	1.61	1.51	5	1
1	A	30	VAL	C-N	-6.28	1.19	1.34	4	1
1	A	91	LYS	CA-C	-5.93	1.37	1.52	2	1
1	A	137	GLU	CD-OE2	-5.38	1.19	1.25	1	3

5 of 6 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	96	GLN	CB-CA-C	-6.52	97.36	110.40	5	1
1	A	95	SER	N-CA-C	5.75	126.53	111.00	5	1
1	A	57	TYR	CA-CB-CG	5.70	124.24	113.40	5	1
1	A	91	LYS	N-CA-CB	5.55	120.58	110.60	2	1
1	A	81	MET	N-CA-CB	-5.49	100.71	110.60	3	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	91	LYS	CA	1
1	A	95	SER	CA	1

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	114	ARG	Sidechain	5
1	A	28	ARG	Sidechain	4
1	A	20	ARG	Sidechain	3
1	A	75	ARG	Sidechain	1

6.2　Too-close contacts　ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1062	1094	1094	20±8
All	All	21240	21880	21878	403

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 9.

5 of 239 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:113:LEU:HA	1:A:116:MET:SD	0.81	2.16	10	6
1:A:76:PRO:HG2	1:A:81:MET:SD	0.78	2.18	3	1
1:A:55:LEU:HA	1:A:99:GLU:O	0.78	1.79	5	1
1:A:54:ARG:O	1:A:57:TYR:HB3	0.75	1.82	5	2
1:A:22:TYR:HB3	1:A:28:ARG:HA	0.73	1.60	4	1

6.3   Torsion angles ⓘ

6.3.1   Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	132/161 (82%)	117±5 (89±4%)	12±4 (9±3%)	3±2 (3±2%)	8	44
All	All	2640/3220 (82%)	2338 (89%)	234 (9%)	68 (3%)	8	44

5 of 28 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	69	ILE	9
1	A	15	LYS	7
1	A	68	LYS	6
1	A	73	VAL	6
1	A	108	LEU	5

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	120/141 (85%)	108±2 (90±2%)	12±2 (10±2%)	11	57
All	All	2400/2820 (85%)	2166 (90%)	234 (10%)	11	57

5 of 63 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	138	LYS	20
1	A	113	LEU	16
1	A	49	LYS	14
1	A	41	LEU	13
1	A	117	ARG	12

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	4-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
4	A	30:VAL	C	31:ASN	N	1.19

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_ chem_ shift_ list*

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	2029
Number of shifts mapped to atoms	2029
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

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 0) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	113	LEU	HD11	0.881	.	1
1	A	113	LEU	HD12	0.881	.	1
1	A	113	LEU	HD13	0.881	.	1
1	A	142	VAL	HG21	0.954	.	1
1	A	142	VAL	HG22	0.954	.	1
1	A	142	VAL	HG23	0.954	.	1
1	A	144	LEU	HD11	1.080	.	1
1	A	144	LEU	HD12	1.080	.	1
1	A	144	LEU	HD13	1.080	.	1
1	A	161	LEU	HD11	0.911	.	1
1	A	161	LEU	HD12	0.911	.	1
1	A	161	LEU	HD13	0.911	.	1
1	A	106	LEU	HD11	0.896	.	1
1	A	106	LEU	HD12	0.896	.	1
1	A	106	LEU	HD13	0.896	.	1

7.1.2   Chemical shift referencing   ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	159	-0.24 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_\beta$	152	0.39 ± 0.05	None needed (< 0.5 ppm)
$^{13}C'$	136	-0.19 ± 0.08	None needed (< 0.5 ppm)
^{15}N	139	0.82 ± 0.32	Should be applied

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 92%, i.e. 1712 atoms were assigned a chemical shift out of a possible 1867. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|	Total	^1H	^{13}C	^{15}N
Backbone	617/658 (94%)	254/265 (96%)	246/264 (93%)	117/129 (91%)
Sidechain	1003/1098 (91%)	683/713 (96%)	312/345 (90%)	8/40 (20%)
Aromatic	92/111 (83%)	46/54 (85%)	45/54 (83%)	1/3 (33%)
Overall	1712/1867 (92%)	983/1032 (95%)	603/663 (91%)	126/172 (73%)

7.1.4   Statistically unusual chemical shifts   ⓘ

There are no statistically unusual chemical shifts.

7.1.5   Random Coil Index (RCI) plots   ⓘ

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

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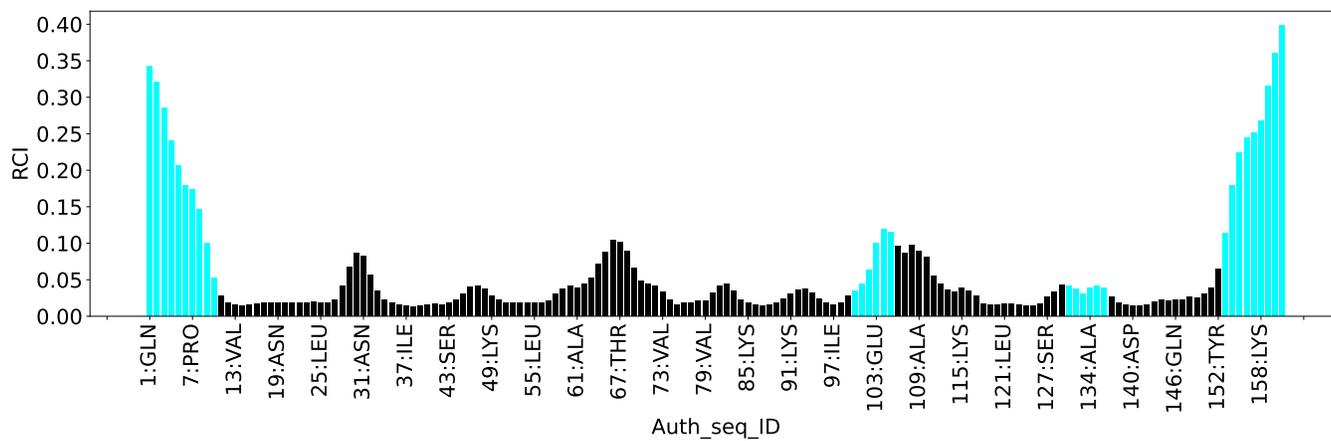
8　NMR restraints analysis ⓘ

8.1　Conformationally restricting restraints ⓘ

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

Description	Value
Total distance restraints	2017
Intra-residue ($|i\text{-}j|$=0)	746
Sequential ($|i\text{-}j|$=1)	551
Medium range ($|i\text{-}j|$>1 and $|i\text{-}j|$<5)	387
Long range ($|i\text{-}j|$≥5)	333
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	12.5
Number of long range restraints per residue[1]	2.1

[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)	65.7	0.2
0.2-0.5 (Medium)	113.9	0.5
>0.5 (Large)	164.1	5.75

8.2.2 Average number of dihedral-angle violations per model ⓘ

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

9 Distance violation analysis (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)	746	37.0	264	35.4	13.1	20	2.7	1.0
Backbone-Backbone	3	0.1	1	33.3	0.0	0	0.0	0.0
Backbone-Sidechain	577	28.6	188	32.6	9.3	17	2.9	0.8
Sidechain-Sidechain	166	8.2	75	45.2	3.7	3	1.8	0.1
Sequential (|i-j|=1)	551	27.3	197	35.8	9.8	27	4.9	1.3
Backbone-Backbone	162	8.0	27	16.7	1.3	2	1.2	0.1
Backbone-Sidechain	322	16.0	119	37.0	5.9	14	4.3	0.7
Sidechain-Sidechain	67	3.3	51	76.1	2.5	11	16.4	0.5
Medium range (|i-j|>1 & |i-j|<5)	387	19.2	170	43.9	8.4	30	7.8	1.5
Backbone-Backbone	105	5.2	17	16.2	0.8	0	0.0	0.0
Backbone-Sidechain	188	9.3	89	47.3	4.4	13	6.9	0.6
Sidechain-Sidechain	94	4.7	64	68.1	3.2	17	18.1	0.8
Long range (|i-j|≥5)	333	16.5	139	41.7	6.9	16	4.8	0.8
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	116	5.8	42	36.2	2.1	5	4.3	0.2
Sidechain-Sidechain	216	10.7	97	44.9	4.8	11	5.1	0.5
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	2017	100.0	770	38.2	38.2	93	4.6	4.6
Backbone-Backbone	271	13.4	45	16.6	2.2	2	0.7	0.1
Backbone-Sidechain	1203	59.6	438	36.4	21.7	49	4.1	2.4
Sidechain-Sidechain	543	26.9	287	52.9	14.2	42	7.7	2.1

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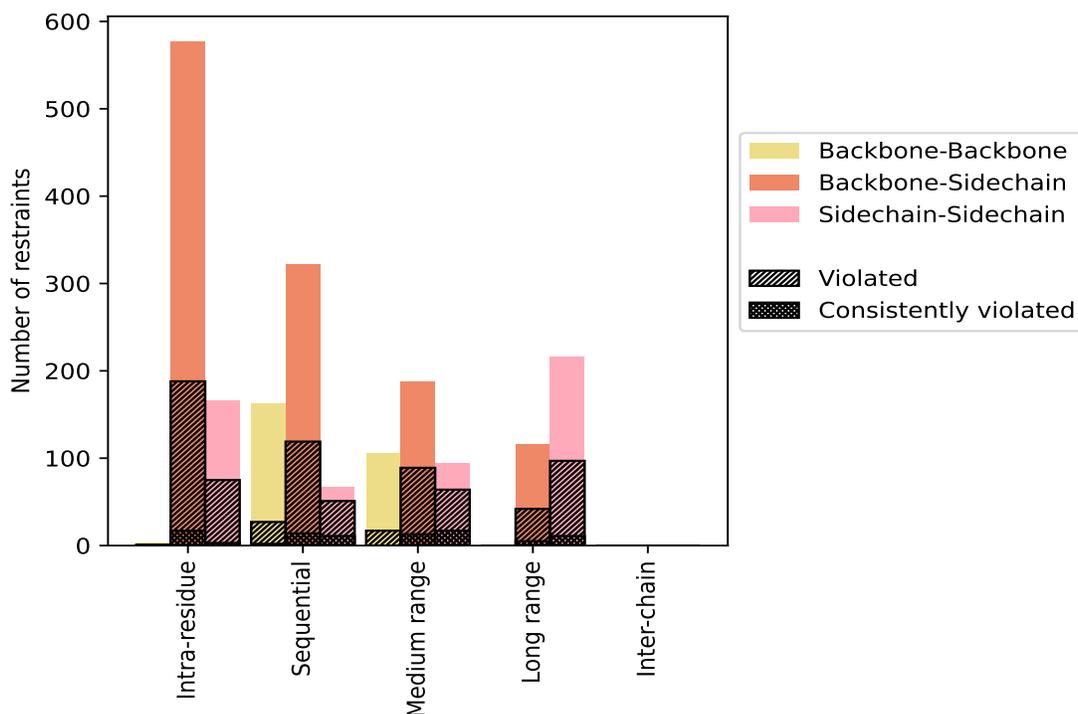
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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	102	103	89	56	0	350	0.7	3.18	0.62	0.47
2	100	95	89	55	0	339	0.7	3.23	0.61	0.48
3	106	95	93	72	0	366	0.78	5.75	0.79	0.48
4	106	103	101	58	0	368	0.69	4.67	0.66	0.44
5	106	103	98	60	0	367	0.72	5.04	0.65	0.47
6	102	104	77	51	0	334	0.65	3.05	0.54	0.48
7	105	94	84	55	0	338	0.69	3.33	0.6	0.49
8	100	89	81	53	0	323	0.68	3.2	0.56	0.49
9	104	97	87	59	0	347	0.71	3.28	0.59	0.53
10	116	97	91	51	0	355	0.68	3.56	0.62	0.46
11	103	86	86	46	0	321	0.69	3.09	0.59	0.48

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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD[6] (Å) | Median (Å) |
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	101	93	82	44	0	320	0.68	3.18	0.59	0.45
13	104	106	87	48	0	345	0.69	3.56	0.63	0.44
14	105	98	86	55	0	344	0.71	3.67	0.65	0.49
15	110	102	85	48	0	345	0.66	3.11	0.56	0.47
16	112	98	86	51	0	347	0.68	3.17	0.59	0.5
17	106	101	84	54	0	345	0.64	3.42	0.55	0.48
18	112	99	79	50	0	340	0.69	3.0	0.59	0.48
19	116	95	83	49	0	343	0.67	3.35	0.6	0.44
20	107	90	87	52	0	336	0.68	3.63	0.59	0.47

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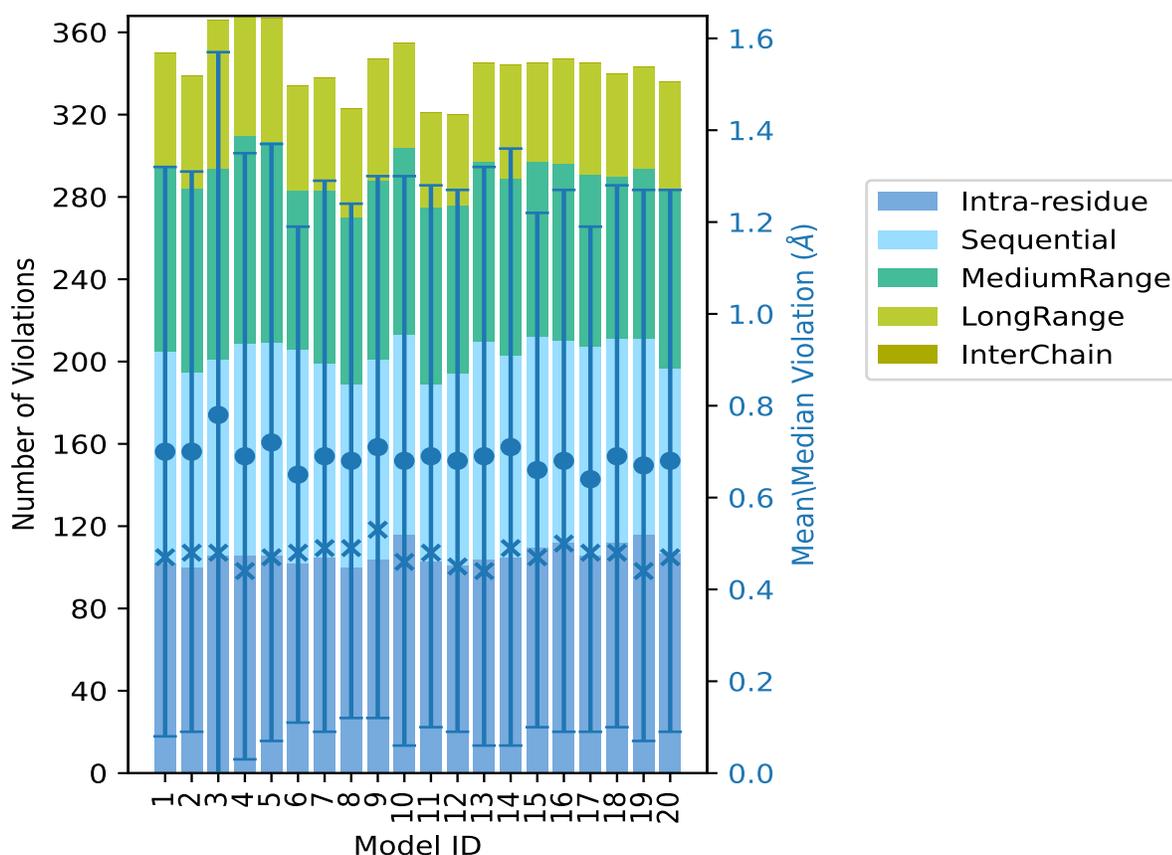
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis
on the right

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, 1247(IR:482, SQ:354, MR:217, LR:194, 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]	%
61	28	37	33	0	159	1	5.0
18	16	13	19	0	66	2	10.0
19	9	6	6	0	40	3	15.0
10	6	7	11	0	34	4	20.0
10	10	7	6	0	33	5	25.0
8	11	4	4	0	27	6	30.0
12	6	3	5	0	26	7	35.0
17	11	5	3	0	36	8	40.0
8	6	4	4	0	22	9	45.0
11	8	2	1	0	22	10	50.0
8	5	2	4	0	19	11	55.0
12	6	3	4	0	25	12	60.0
12	6	5	5	0	28	13	65.0
4	5	3	3	0	15	14	70.0
5	9	4	5	0	23	15	75.0
5	1	5	0	0	11	16	80.0
9	7	8	2	0	26	17	85.0
8	8	9	5	0	30	18	90.0
7	12	13	3	0	35	19	95.0
20	27	30	16	0	93	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ
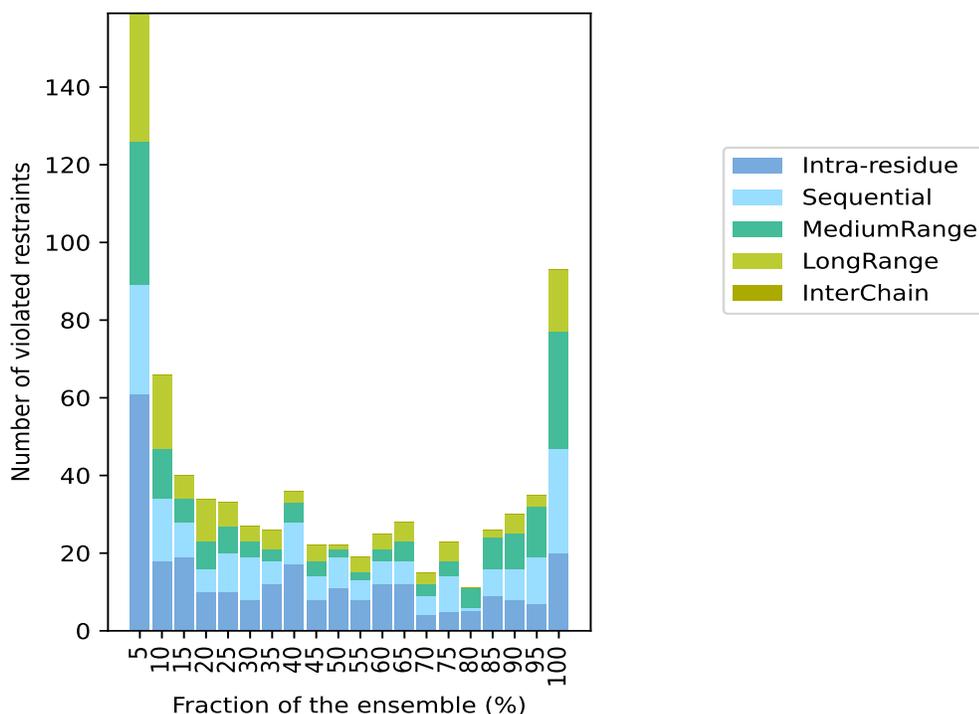
9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble
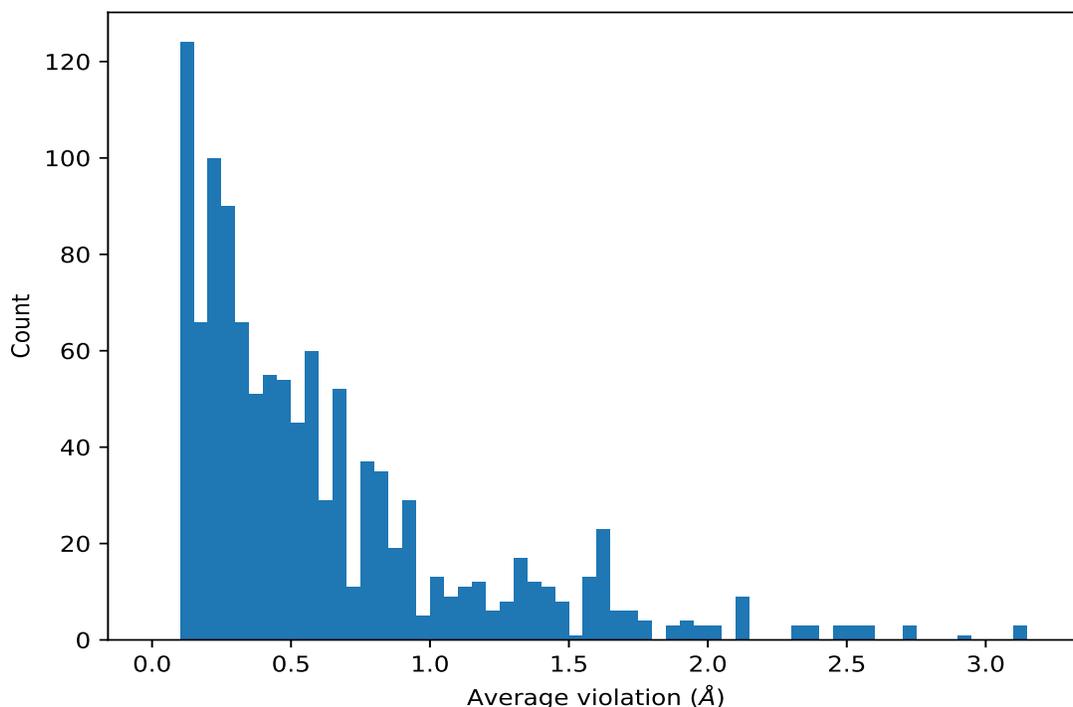
9.4.2 Table: Most violated distance restraints ⓘ

The following table provides the mean and the standard deviation of the 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)
(1,851)	1:A:122:LYS:HD3	1:A:118:VAL:HG11	20	3.11	0.29	3.14
(1,851)	1:A:122:LYS:HD3	1:A:118:VAL:HG12	20	3.11	0.29	3.14
(1,851)	1:A:122:LYS:HD3	1:A:118:VAL:HG13	20	3.11	0.29	3.14
(1,75)	1:A:107:ASP:HB3	1:A:111:VAL:HG21	20	2.73	0.54	2.9
(1,75)	1:A:107:ASP:HB3	1:A:111:VAL:HG22	20	2.73	0.54	2.9
(1,75)	1:A:107:ASP:HB3	1:A:111:VAL:HG23	20	2.73	0.54	2.9
(1,52)	1:A:118:VAL:HG21	1:A:138:LYS:HE2	20	2.57	0.86	2.87
(1,52)	1:A:118:VAL:HG22	1:A:138:LYS:HE2	20	2.57	0.86	2.87
(1,52)	1:A:118:VAL:HG23	1:A:138:LYS:HE2	20	2.57	0.86	2.87
(1,845)	1:A:118:VAL:HG11	1:A:122:LYS:HG2	20	2.55	0.25	2.51
(1,845)	1:A:118:VAL:HG12	1:A:122:LYS:HG2	20	2.55	0.25	2.51
(1,845)	1:A:118:VAL:HG13	1:A:122:LYS:HG2	20	2.55	0.25	2.51
(1,53)	1:A:138:LYS:HE3	1:A:118:VAL:HG21	20	2.47	0.4	2.5
(1,53)	1:A:138:LYS:HE3	1:A:118:VAL:HG22	20	2.47	0.4	2.5
(1,53)	1:A:138:LYS:HE3	1:A:118:VAL:HG23	20	2.47	0.4	2.5
(1,858)	1:A:111:VAL:HG21	1:A:107:ASP:HA	20	2.39	0.38	2.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,858)	1:A:111:VAL:HG22	1:A:107:ASP:HA	20	2.39	0.38	2.5
(1,858)	1:A:111:VAL:HG23	1:A:107:ASP:HA	20	2.39	0.38	2.5
(1,947)	1:A:79:VAL:HG21	1:A:76:PRO:HB3	20	2.32	0.33	2.34
(1,947)	1:A:79:VAL:HG22	1:A:76:PRO:HB3	20	2.32	0.33	2.34
(1,947)	1:A:79:VAL:HG23	1:A:76:PRO:HB3	20	2.32	0.33	2.34
(1,850)	1:A:118:VAL:HG11	1:A:122:LYS:HD2	20	2.14	0.36	2.17
(1,850)	1:A:118:VAL:HG12	1:A:122:LYS:HD2	20	2.14	0.36	2.17
(1,850)	1:A:118:VAL:HG13	1:A:122:LYS:HD2	20	2.14	0.36	2.17
(1,772)	1:A:31:ASN:HB2	1:A:30:VAL:HG21	20	1.97	0.36	2.02
(1,772)	1:A:31:ASN:HB2	1:A:30:VAL:HG22	20	1.97	0.36	2.02
(1,772)	1:A:31:ASN:HB2	1:A:30:VAL:HG23	20	1.97	0.36	2.02
(1,549)	1:A:34:LEU:HB3	1:A:33:SER:HB3	20	1.95	0.41	1.96

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

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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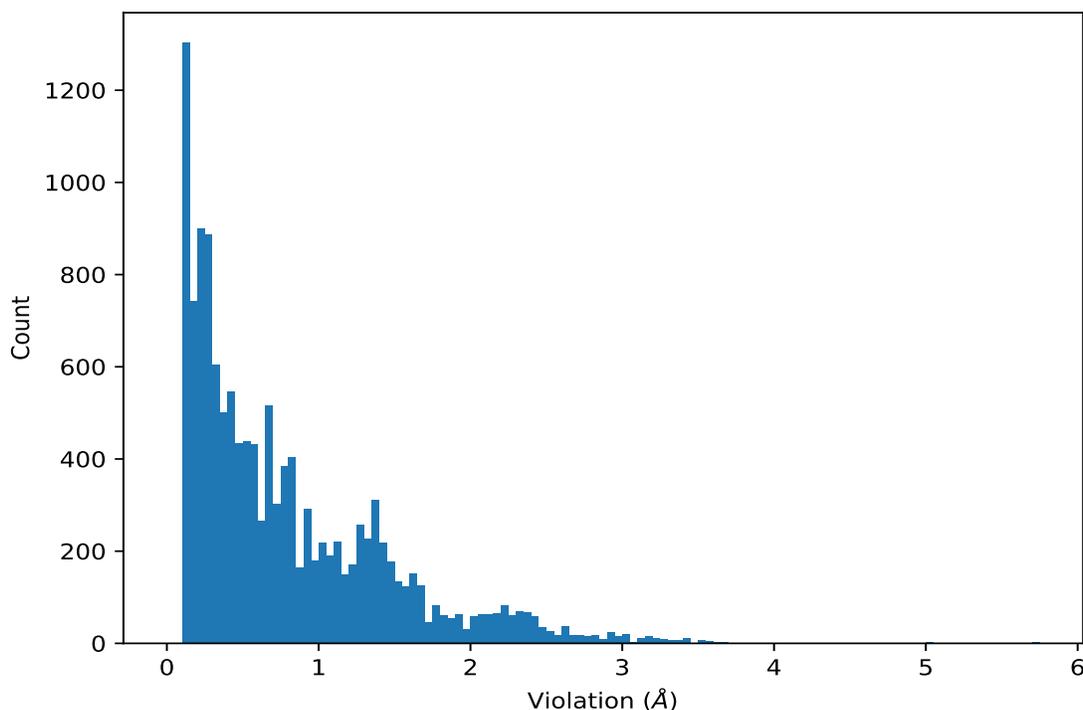
9.5.2 Table : All distance violations ⓘ

The following table 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)
(1,445)	1:A:90:LEU:HD11	1:A:73:VAL:H	3	5.75
(1,445)	1:A:90:LEU:HD12	1:A:73:VAL:H	3	5.75
(1,445)	1:A:90:LEU:HD13	1:A:73:VAL:H	3	5.75
(1,244)	1:A:85:LYS:HB3	1:A:81:MET:HG2	3	5.31
(1,1163)	1:A:13:VAL:HG11	1:A:101:LYS:HA	5	5.04
(1,1163)	1:A:13:VAL:HG12	1:A:101:LYS:HA	5	5.04
(1,1163)	1:A:13:VAL:HG13	1:A:101:LYS:HA	5	5.04
(1,809)	1:A:27:ASP:HB2	1:A:24:SER:HA	4	4.67
(1,245)	1:A:81:MET:HG3	1:A:85:LYS:HB3	3	4.56
(1,846)	1:A:122:LYS:HG3	1:A:118:VAL:HG11	14	3.67
(1,846)	1:A:122:LYS:HG3	1:A:118:VAL:HG12	14	3.67
(1,846)	1:A:122:LYS:HG3	1:A:118:VAL:HG13	14	3.67
(1,851)	1:A:122:LYS:HD3	1:A:118:VAL:HG11	20	3.63
(1,851)	1:A:122:LYS:HD3	1:A:118:VAL:HG12	20	3.63
(1,851)	1:A:122:LYS:HD3	1:A:118:VAL:HG13	20	3.63
(1,75)	1:A:107:ASP:HB3	1:A:111:VAL:HG21	10	3.56
(1,75)	1:A:107:ASP:HB3	1:A:111:VAL:HG22	10	3.56
(1,75)	1:A:107:ASP:HB3	1:A:111:VAL:HG23	10	3.56
(1,75)	1:A:107:ASP:HB3	1:A:111:VAL:HG21	13	3.56
(1,75)	1:A:107:ASP:HB3	1:A:111:VAL:HG22	13	3.56
(1,75)	1:A:107:ASP:HB3	1:A:111:VAL:HG23	13	3.56
(1,851)	1:A:122:LYS:HD3	1:A:118:VAL:HG11	13	3.52

10   Dihedral-angle violation analysis ⓘ

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value