wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	6BER
BMRB ID	:	30360
Title	:	Solution structure of de novo macrocycle design10.2
Authors	:	Shortridge, M.D.; Hosseinzadeh, P.; Pardo-Avila, F.; Varani, G.; Baker, D.
Deposited on	:	2017-10-25

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 (1)) were used in the production of this report:

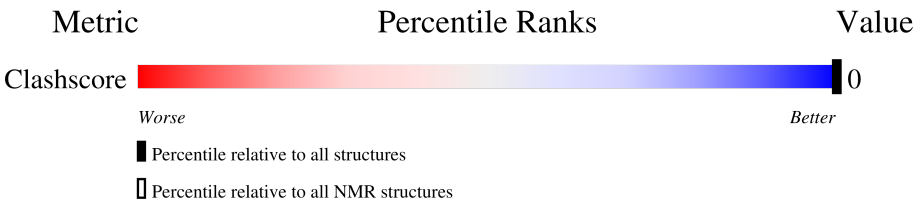
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 49%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864

Molprobity failed to run

2 Ensemble composition and analysis (i)

This entry contains 20 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 142 atoms, of which 65 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein (with D amino acids) called E(DVA)DP(DGL)(DHI)(DPR)N(DAL)(DPR).

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	10	142	47	65	13	17	0

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.

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

The representative model is number 1. Colouring as in section 4.1 above.

5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
GROMACS	refinement	2016.1
X-PLOR NIH	structure calculation	

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	48
Number of shifts mapped to atoms	47
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	49%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DGL, DPR, DVA, DAL, DHI

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	0.55±0.04	0±0/30 (0.0± 0.0%)	1.77±0.34	0±1/37 (1.4± 2.3%)
All	All	0.56	0/600 (0.0%)	1.81	10/740 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	2

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	1	GLU	OE1-CD-OE2	-8.06	113.62	123.30	1	3
1	A	3	ASP	CB-CG-OD2	-6.99	112.01	118.30	5	2
1	A	4	PRO	N-CA-CB	6.54	111.15	103.30	1	3
1	A	3	ASP	CB-CG-OD1	5.62	123.36	118.30	6	1
1	A	4	PRO	CA-N-CD	-5.28	104.11	111.50	1	1

There are no chirality outliers.

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	7	DPR	Mainchain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	1	GLU	Peptide	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	1540	1300	1224	-

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is -.

There are no clashes.

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

There are no protein molecules in this entry.

6.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides 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 49% for the well-defined parts and 49% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *marie_bmrb.txt*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	48
Number of shifts mapped to atoms	47
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	DAL	HB	1.347	0.00	.

7.1.2 Chemical shift referencing (i)

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

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 49%, i.e. 22 atoms were assigned a chemical shift out of a possible 45. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	6/18 (33%)	6/7 (86%)	0/8 (0%)	0/3 (0%)
Sidechain	16/27 (59%)	16/16 (100%)	0/10 (0%)	0/1 (0%)
Overall	22/45 (49%)	22/23 (96%)	0/18 (0%)	0/4 (0%)

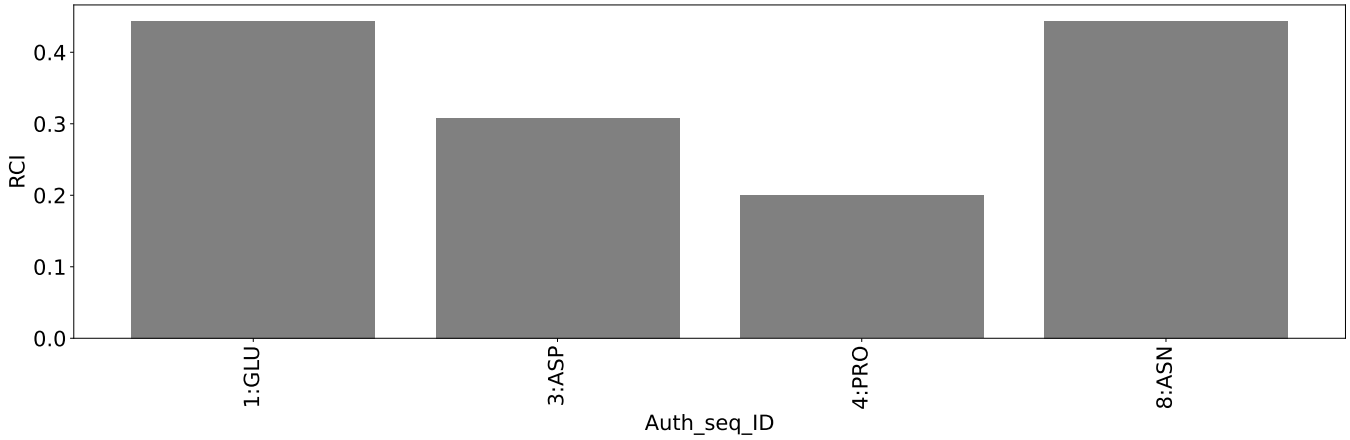
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	202
Intra-residue (|i-j|=0)	68
Sequential (|i-j|=1)	89
Medium range (|i-j|>1 and |i-j|<5)	32
Long range (|i-j|≥5)	13
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	7
Number of restraints per residue	20.2
Number of long range restraints per residue[1]	1.3

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	7.5	0.2
0.2-0.5 (Medium)	10.8	0.5
>0.5 (Large)	3.2	1.16

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

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

9 Distance violation analysis (i)

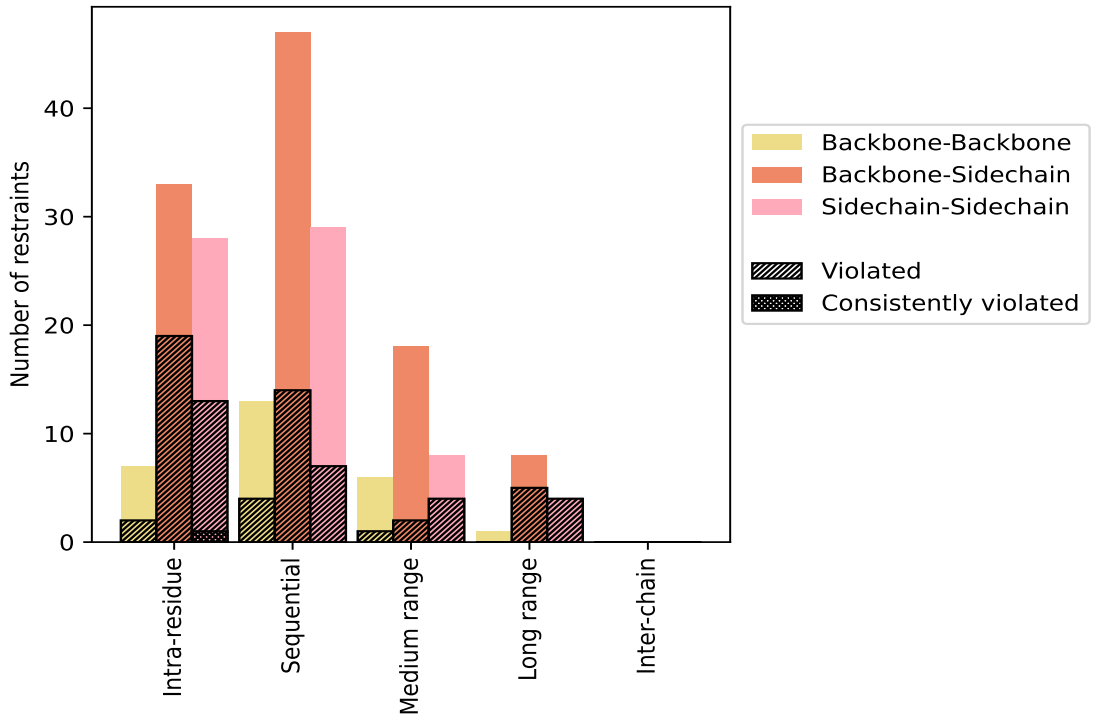
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	68	33.7	34	50.0	16.8	1	1.5	0.5
Backbone-Backbone	7	3.5	2	28.6	1.0	0	0.0	0.0
Backbone-Sidechain	33	16.3	19	57.6	9.4	0	0.0	0.0
Sidechain-Sidechain	28	13.9	13	46.4	6.4	1	3.6	0.5
Sequential (|i-j|=1)	89	44.1	25	28.1	12.4	0	0.0	0.0
Backbone-Backbone	13	6.4	4	30.8	2.0	0	0.0	0.0
Backbone-Sidechain	47	23.3	14	29.8	6.9	0	0.0	0.0
Sidechain-Sidechain	29	14.4	7	24.1	3.5	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	32	15.8	7	21.9	3.5	0	0.0	0.0
Backbone-Backbone	6	3.0	1	16.7	0.5	0	0.0	0.0
Backbone-Sidechain	18	8.9	2	11.1	1.0	0	0.0	0.0
Sidechain-Sidechain	8	4.0	4	50.0	2.0	0	0.0	0.0
Long range (|i-j|≥5)	13	6.4	9	69.2	4.5	0	0.0	0.0
Backbone-Backbone	1	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	4.0	5	62.5	2.5	0	0.0	0.0
Sidechain-Sidechain	4	2.0	4	100.0	2.0	0	0.0	0.0
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	202	100.0	75	37.1	37.1	1	0.5	0.5
Backbone-Backbone	27	13.4	7	25.9	3.5	0	0.0	0.0
Backbone-Sidechain	106	52.5	40	37.7	19.8	0	0.0	0.0
Sidechain-Sidechain	69	34.2	28	40.6	13.9	1	1.4	0.5

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	13	9	1	4	0	27	0.26	0.57	0.14	0.23
2	11	8	2	1	0	22	0.29	0.62	0.14	0.29
3	9	5	2	4	0	20	0.44	0.82	0.22	0.35
4	12	9	1	1	0	23	0.33	1.02	0.21	0.25
5	11	8	1	1	0	21	0.35	0.99	0.2	0.34
6	12	6	3	1	0	22	0.34	0.86	0.22	0.24
7	11	9	3	1	0	24	0.27	0.93	0.18	0.2
8	9	5	1	3	0	18	0.39	1.16	0.27	0.24
9	9	4	1	2	0	16	0.32	0.74	0.18	0.26
10	13	7	2	0	0	22	0.3	0.59	0.13	0.3
11	10	4	3	0	0	17	0.37	0.88	0.19	0.39

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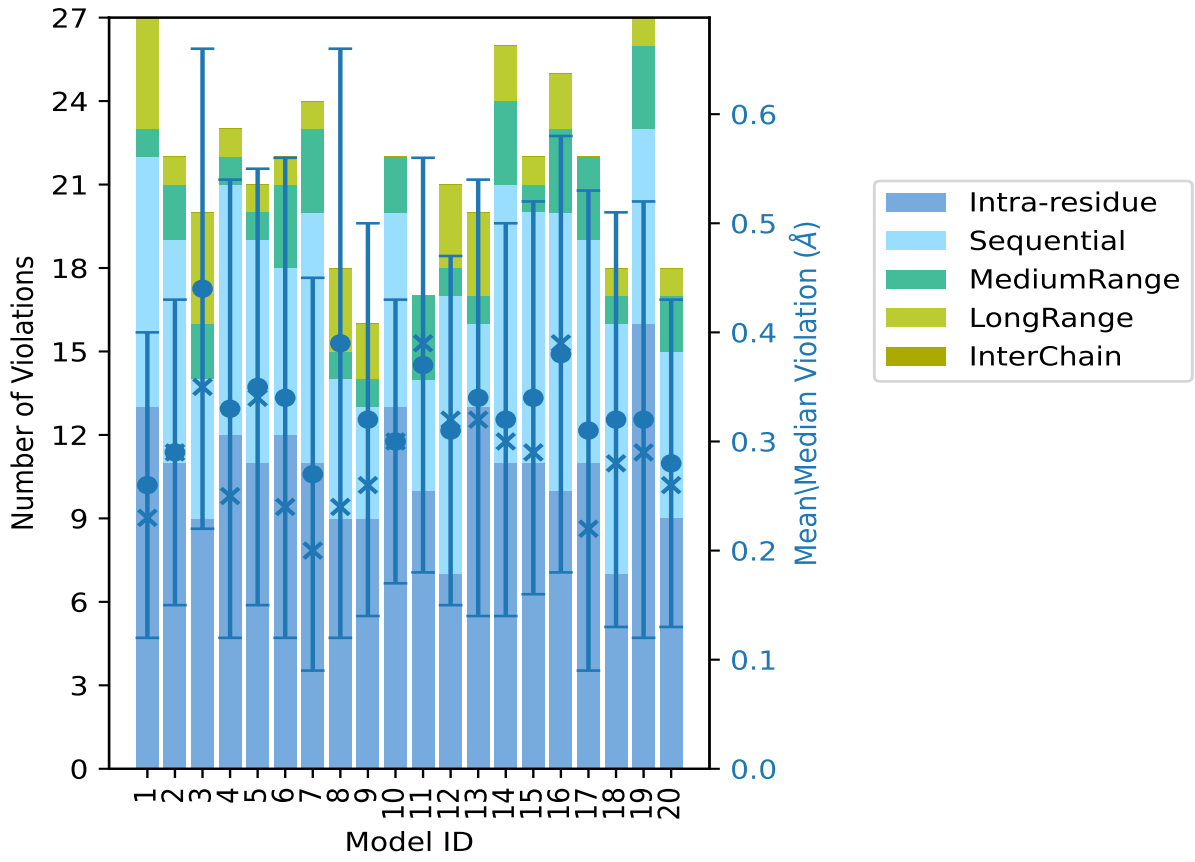
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	7	10	1	3	0	21	0.31	0.82	0.16	0.32
13	13	3	1	3	0	20	0.34	0.8	0.2	0.32
14	11	10	3	2	0	26	0.32	0.82	0.18	0.3
15	11	9	1	1	0	22	0.34	0.66	0.18	0.29
16	10	10	3	2	0	25	0.38	0.91	0.2	0.39
17	11	8	3	0	0	22	0.31	1.03	0.22	0.22
18	7	9	1	1	0	18	0.32	0.94	0.19	0.28
19	16	7	3	1	0	27	0.32	1.03	0.2	0.29
20	9	6	2	1	0	18	0.28	0.65	0.15	0.26

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

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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

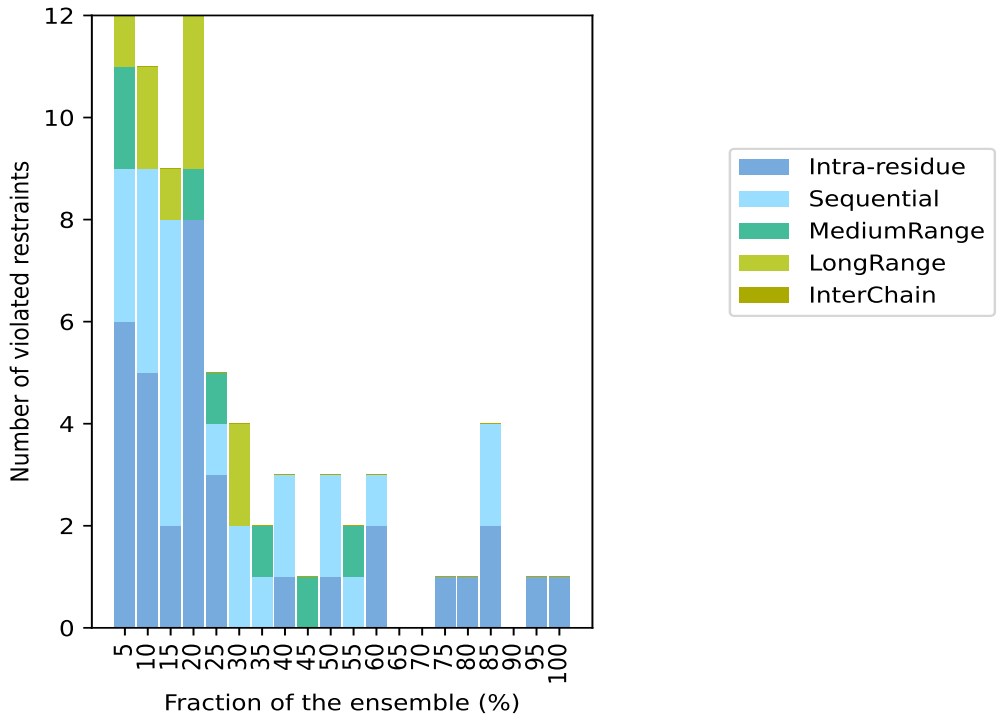
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 127(IR:34, SQ:64, MR:25, LR:4, 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]	%
6	3	2	1	0	12	1	5.0
5	4	0	2	0	11	2	10.0
2	6	0	1	0	9	3	15.0
8	0	1	3	0	12	4	20.0
3	1	1	0	0	5	5	25.0
0	2	0	2	0	4	6	30.0
0	1	1	0	0	2	7	35.0
1	2	0	0	0	3	8	40.0
0	0	1	0	0	1	9	45.0
1	2	0	0	0	3	10	50.0
0	1	1	0	0	2	11	55.0
2	1	0	0	0	3	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
1	0	0	0	0	1	15	75.0
1	0	0	0	0	1	16	80.0
2	2	0	0	0	4	17	85.0
0	0	0	0	0	0	18	90.0
1	0	0	0	0	1	19	95.0
1	0	0	0	0	1	20	100.0

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

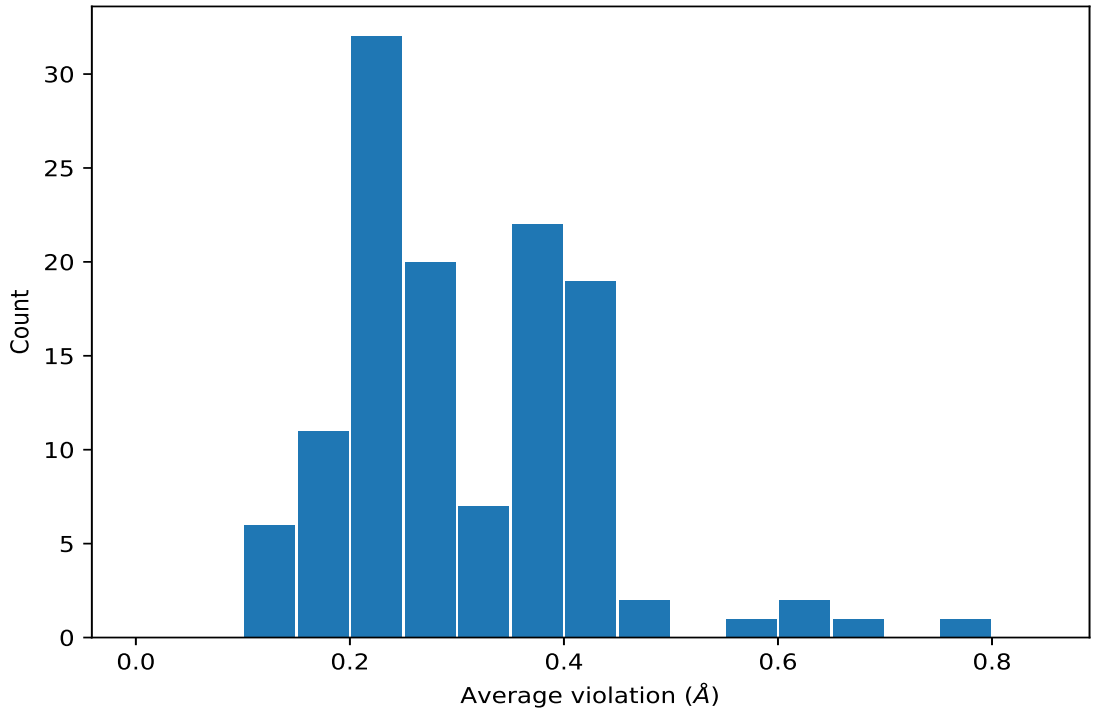
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,40)	1:A:2:DVA:HG11	1:A:2:DVA:HB	20	0.41	0.04	0.41
(1,40)	1:A:2:DVA:HG12	1:A:2:DVA:HB	20	0.41	0.04	0.41
(1,40)	1:A:2:DVA:HG13	1:A:2:DVA:HB	20	0.41	0.04	0.41
(1,40)	1:A:2:DVA:HG21	1:A:2:DVA:HB	20	0.41	0.04	0.41
(1,40)	1:A:2:DVA:HG22	1:A:2:DVA:HB	20	0.41	0.04	0.41
(1,40)	1:A:2:DVA:HG23	1:A:2:DVA:HB	20	0.41	0.04	0.41
(1,61)	1:A:3:ASP:HB2	1:A:3:ASP:H	19	0.4	0.18	0.38
(1,202)	1:A:10:DPR:HG3	1:A:9:DAL:H	17	0.77	0.29	0.82
(1,164)	1:A:8:ASN:HB3	1:A:8:ASN:HA	17	0.41	0.13	0.4
(1,15)	1:A:7:DPR:HA	1:A:8:ASN:H	17	0.22	0.07	0.21
(1,172)	1:A:9:DAL:HB1	1:A:9:DAL:HA	17	0.2	0.04	0.2
(1,172)	1:A:9:DAL:HB2	1:A:9:DAL:HA	17	0.2	0.04	0.2
(1,172)	1:A:9:DAL:HB3	1:A:9:DAL:HA	17	0.2	0.04	0.2
(1,160)	1:A:8:ASN:HB2	1:A:8:ASN:HD21	16	0.56	0.15	0.62
(1,39)	1:A:2:DVA:HG11	1:A:2:DVA:HA	15	0.2	0.06	0.19
(1,39)	1:A:2:DVA:HG12	1:A:2:DVA:HA	15	0.2	0.06	0.19

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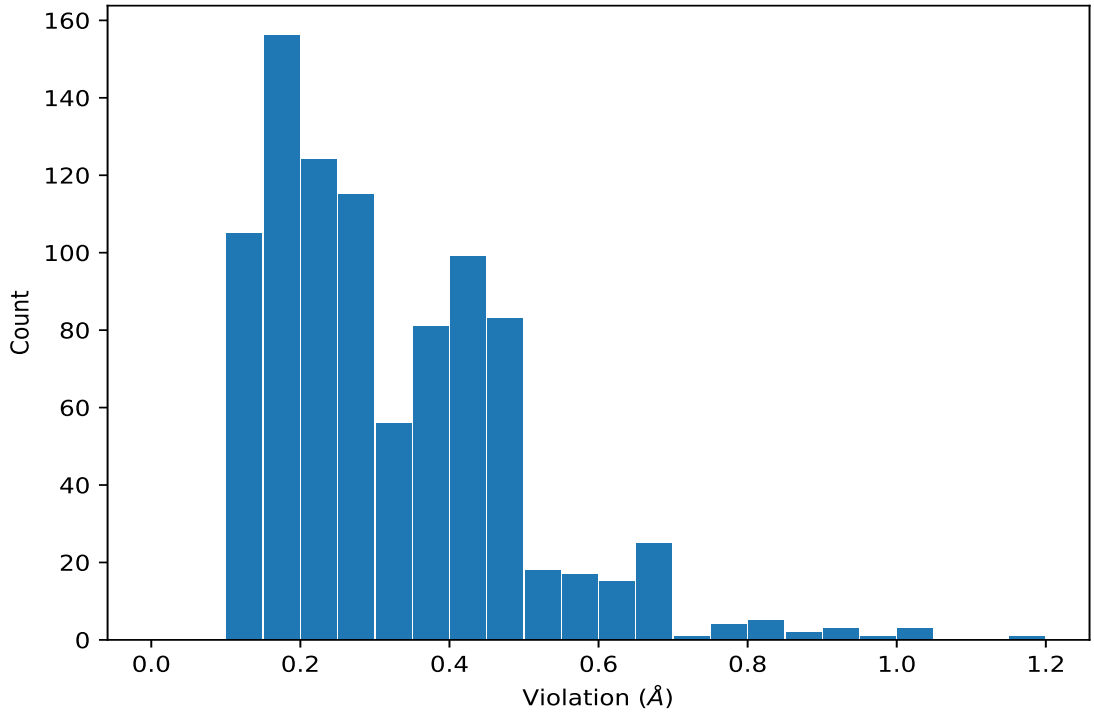
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,39)	1:A:2:DVA:HG13	1:A:2:DVA:HA	15	0.2	0.06	0.19
(1,39)	1:A:2:DVA:HG21	1:A:2:DVA:HA	15	0.2	0.06	0.19
(1,39)	1:A:2:DVA:HG22	1:A:2:DVA:HA	15	0.2	0.06	0.19
(1,39)	1:A:2:DVA:HG23	1:A:2:DVA:HA	15	0.2	0.06	0.19
(1,33)	1:A:1:GLU:HB3	1:A:1:GLU:HA	12	0.42	0.07	0.42
(1,7)	1:A:4:PRO:HA	1:A:5:DGL:H	12	0.21	0.07	0.18

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

The following table provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:A:10:DPR:HG3	1:A:9:DAL:H	8	1.16
(1,202)	1:A:10:DPR:HG3	1:A:9:DAL:H	17	1.03
(1,202)	1:A:10:DPR:HG3	1:A:9:DAL:H	19	1.03
(1,202)	1:A:10:DPR:HG3	1:A:9:DAL:H	4	1.02
(1,202)	1:A:10:DPR:HG3	1:A:9:DAL:H	5	0.99
(1,202)	1:A:10:DPR:HG3	1:A:9:DAL:H	18	0.94
(1,202)	1:A:10:DPR:HG3	1:A:9:DAL:H	7	0.93
(1,129)	1:A:7:DPR:HB3	1:A:8:ASN:HD21	16	0.91
(1,160)	1:A:8:ASN:HB2	1:A:8:ASN:HD21	11	0.88
(1,202)	1:A:10:DPR:HG3	1:A:9:DAL:H	6	0.86

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found