



Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 06:38 pm BST

PDB ID : 6ZX6
BMRB ID : 34542
Title : Antiparallel basket-type G-quadruplex DNA structure formed in human Bcl-2 promoter containing 8-oxoG
Authors : Bielskute, S.; Plavec, J.; Podbevsek, P.
Deposited on : 2020-07-29

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 ⓘ 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
Mogul : 1.8.4, CSD as541be (2020)
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

2 Ensemble composition and analysis

This entry contains 12 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

There is only 1 type of molecule in this entry. The entry contains 809 atoms, of which 277 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called bcl2ex-oxoG19.

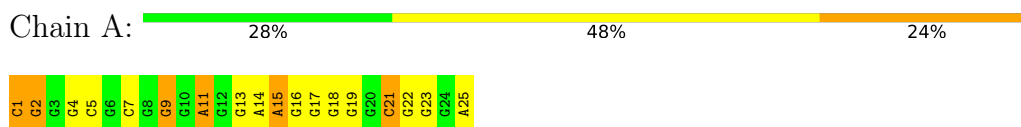
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	25	809	246	277	117	145	24	0

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: bcl2ex-oxoG19



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

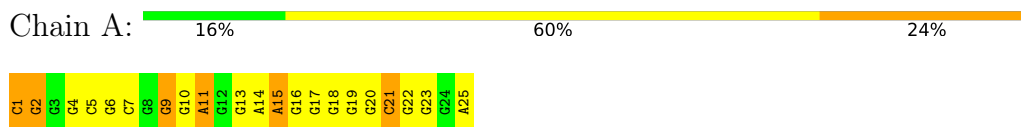
4.2.1 Score per residue for model 1

- Molecule 1: bcl2ex-oxoG19



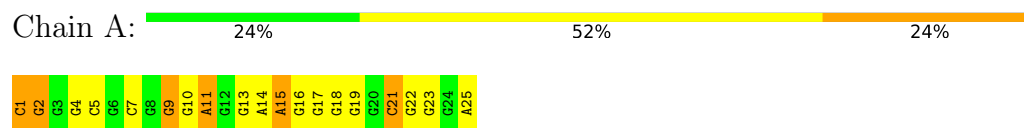
4.2.2 Score per residue for model 2

- Molecule 1: bcl2ex-oxoG19



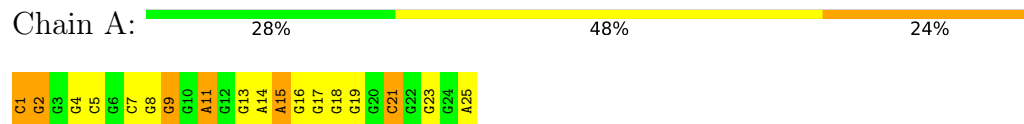
4.2.3 Score per residue for model 3

- Molecule 1: bcl2ex-oxoG19



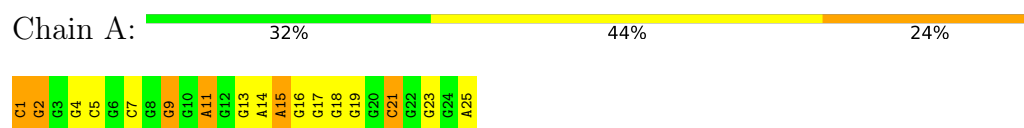
4.2.4 Score per residue for model 4

- Molecule 1: bcl2ex-oxoG19



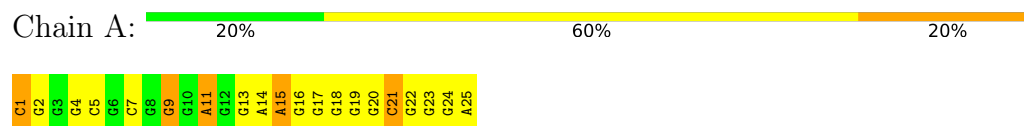
4.2.5 Score per residue for model 5

- Molecule 1: bcl2ex-oxoG19



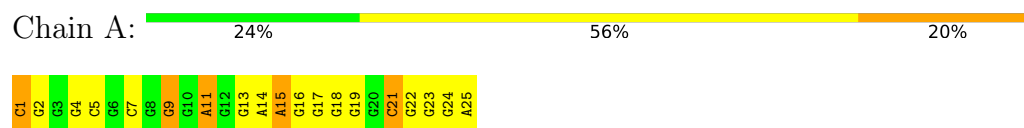
4.2.6 Score per residue for model 6

- Molecule 1: bcl2ex-oxoG19



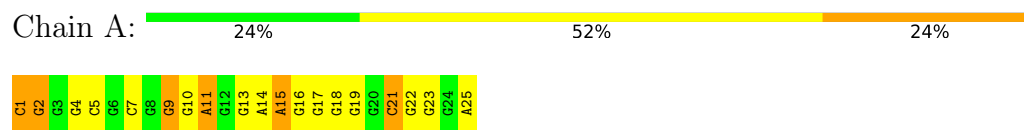
4.2.7 Score per residue for model 7

- Molecule 1: bcl2ex-oxoG19



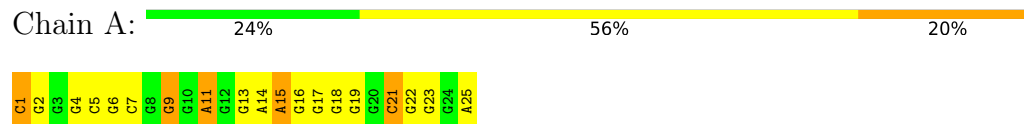
4.2.8 Score per residue for model 8

- Molecule 1: bcl2ex-oxoG19



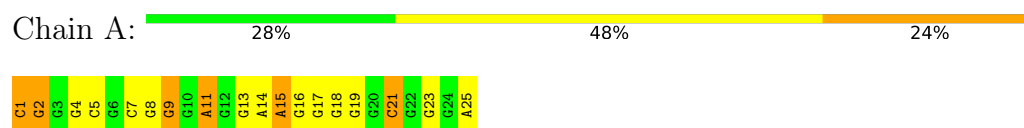
4.2.9 Score per residue for model 9

- Molecule 1: bcl2ex-oxoG19



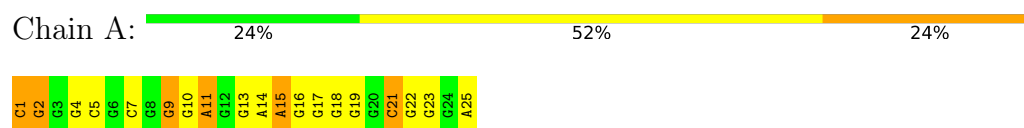
4.2.10 Score per residue for model 10

- Molecule 1: bcl2ex-oxoG19



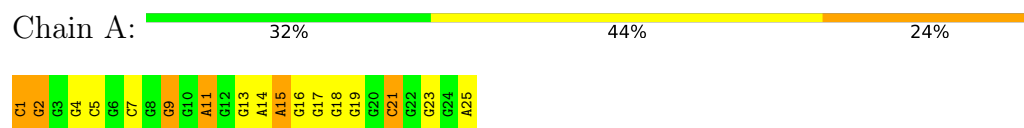
4.2.11 Score per residue for model 11

- Molecule 1: bcl2ex-oxoG19



4.2.12 Score per residue for model 12

- Molecule 1: bcl2ex-oxoG19



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 12 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
Amber	structure calculation	

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	180
Number of shifts mapped to atoms	180
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	35%

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: 8OG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.64±0.00	0±0/575 (0.0± 0.0%)	2.46±0.01	38±2/888 (4.3± 0.2%)
All	All	1.64	0/6900 (0.0%)	2.46	460/10656 (4.3%)

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	6.2±0.4
All	All	0	75

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	DA	N1-C6-N6	-11.53	111.68	118.60	3	12
1	A	16	DG	O4'-C1'-N9	10.83	115.58	108.00	4	12
1	A	23	DG	O4'-C1'-N9	10.39	115.27	108.00	7	12
1	A	11	DA	N1-C6-N6	-10.08	112.56	118.60	3	12
1	A	21	DC	N3-C2-O2	-9.46	115.28	121.90	4	12
1	A	25	DA	N1-C6-N6	-9.37	112.97	118.60	6	12
1	A	18	DG	O4'-C1'-N9	9.33	114.53	108.00	6	12
1	A	15	DA	N1-C6-N6	-9.32	113.01	118.60	6	12
1	A	1	DC	O4'-C1'-N1	9.04	114.33	108.00	11	12
1	A	13	DG	O4'-C1'-N9	8.93	114.25	108.00	11	12
1	A	21	DC	N1-C2-O2	8.75	124.15	118.90	10	12
1	A	9	DG	O4'-C1'-N9	8.61	114.03	108.00	8	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	15	DA	O4'-C1'-N9	8.22	113.75	108.00	3	12
1	A	11	DA	C5-C6-N1	7.70	121.55	117.70	3	12
1	A	1	DC	N3-C2-O2	-7.52	116.64	121.90	5	12
1	A	15	DA	C5-C6-N1	7.51	121.46	117.70	2	12
1	A	25	DA	C5-C6-N1	7.46	121.43	117.70	1	12
1	A	14	DA	C5-C6-N1	7.34	121.37	117.70	10	12
1	A	14	DA	C4-C5-C6	-6.95	113.53	117.00	3	12
1	A	11	DA	C4-C5-C6	-6.86	113.57	117.00	3	12
1	A	25	DA	C4-C5-C6	-6.84	113.58	117.00	1	12
1	A	7	DC	N3-C2-O2	-6.79	117.15	121.90	5	12
1	A	5	DC	N3-C2-O2	-6.70	117.21	121.90	2	12
1	A	15	DA	C4-C5-C6	-6.50	113.75	117.00	11	12
1	A	21	DC	O4'-C1'-N1	6.48	112.54	108.00	4	12
1	A	17	DG	O4'-C1'-N9	6.26	112.39	108.00	1	12
1	A	21	DC	N3-C4-C5	6.16	124.36	121.90	12	12
1	A	4	DG	N3-C4-C5	-6.06	125.57	128.60	12	12
1	A	1	DC	N1-C2-O2	5.85	122.41	118.90	5	12
1	A	9	DG	N3-C4-C5	-5.49	125.86	128.60	3	12
1	A	7	DC	N3-C4-C5	5.48	124.09	121.90	2	12
1	A	22	DG	O4'-C1'-N9	5.47	111.83	108.00	7	7
1	A	16	DG	C5-C6-N1	5.47	114.23	111.50	10	11
1	A	2	DG	N3-C4-C5	-5.43	125.89	128.60	11	9
1	A	10	DG	N3-C2-N2	-5.34	116.16	119.90	3	4
1	A	4	DG	C5-C6-N1	5.33	114.17	111.50	9	12
1	A	18	DG	N3-C4-C5	-5.30	125.95	128.60	4	12
1	A	24	DG	O4'-C1'-N9	5.25	111.68	108.00	6	2
1	A	5	DC	N1-C2-O2	5.25	122.05	118.90	2	12
1	A	5	DC	O4'-C1'-N1	5.19	111.64	108.00	1	6
1	A	10	DG	O4'-C1'-N9	5.19	111.63	108.00	3	1
1	A	7	DC	N1-C2-O2	5.10	121.96	118.90	5	1
1	A	20	DG	C5-C6-N1	5.10	114.05	111.50	2	2
1	A	17	DG	C5-C6-N1	5.05	114.03	111.50	6	3
1	A	10	DG	C5-C6-N1	5.05	114.03	111.50	2	2
1	A	6	DG	N1-C6-O6	-5.03	116.88	119.90	2	2
1	A	5	DC	N3-C4-C5	5.01	123.90	121.90	11	1
1	A	23	DG	N3-C4-C5	-5.00	126.10	128.60	9	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	1	DC	Sidechain	12
1	A	2	DG	Sidechain	12
1	A	9	DG	Sidechain	12
1	A	11	DA	Sidechain	12
1	A	15	DA	Sidechain	12
1	A	21	DC	Sidechain	12
1	A	8	DG	Sidechain	3

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	6384	3324	3324	-

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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	8OG	A	19	1	22,25,26	1.28±0.01	1±0 (4±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	8OG	A	19	1	30,37,40	2.25±0.11	6±1 (19±3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	8OG	A	19	1	-	0±0,7,21,22	0±0,3,3,3

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	19	8OG	C8-N7	4.76	1.29	1.38	4	12

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	8OG	N7-C8-N9	7.69	115.70	106.58	8	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	8OG	O4'-C1'-N9	6.34	114.67	108.29	5	12
1	A	19	8OG	C5-N7-C8	4.11	103.56	109.47	9	12
1	A	19	8OG	C2'-C1'-N9	4.02	111.26	116.01	5	5
1	A	19	8OG	O8-C8-N7	3.49	120.31	126.64	9	12
1	A	19	8OG	C4-C5-N7	2.15	110.23	106.08	4	12
1	A	19	8OG	O5'-C5'-C4'	2.08	116.07	108.99	4	5

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

The completeness of assignment taking into account all chemical shift lists is 35% for the well-defined parts and 35% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `starch_output`

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	180
Number of shifts mapped to atoms	180
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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

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 35%, i.e. 173 atoms were assigned a chemical shift out of a possible 496. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	93/288 (32%)	93/168 (55%)	0/120 (0%)	0/0 (—%)
Base	80/208 (38%)	52/136 (38%)	28/32 (88%)	0/40 (0%)
Overall	173/496 (35%)	145/304 (48%)	28/152 (18%)	0/40 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 35%, i.e. 173 atoms were assigned a chemical shift out of a possible 496. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Sugar	93/288 (32%)	93/168 (55%)	0/120 (0%)	0/0 (—%)
Base	80/208 (38%)	52/136 (38%)	28/32 (88%)	0/40 (0%)
Overall	173/496 (35%)	145/304 (48%)	28/152 (18%)	0/40 (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](#)

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

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	278
Intra-residue ($ i-j =0$)	122
Sequential ($ i-j =1$)	70
Medium range ($ i-j >1$ and $ i-j <5$)	21
Long range ($ i-j \geq 5$)	65
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	11.1
Number of long range restraints per residue ¹	2.6

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

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)	None	None
0.2-0.5 (Medium)	1.0	0.29
>0.5 (Large)	None	None

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](#)

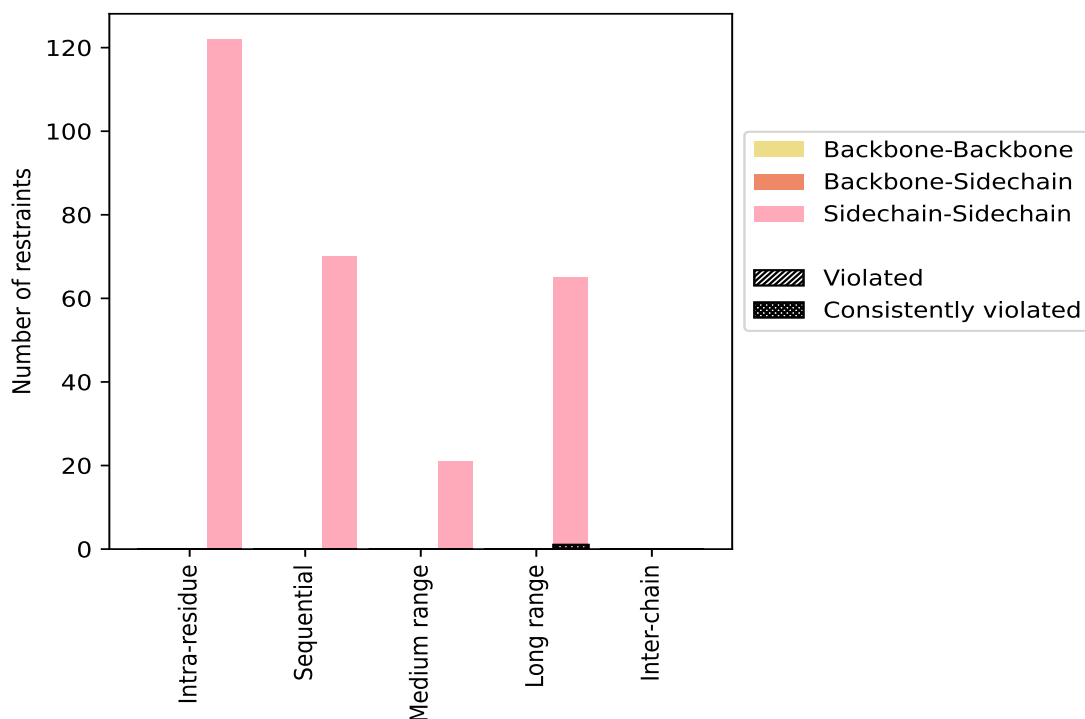
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	122	43.9	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	122	43.9	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	70	25.2	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	70	25.2	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	21	7.6	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	21	7.6	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	65	23.4	1	1.5	0.4	1	1.5	0.4
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	65	23.4	1	1.5	0.4	1	1.5	0.4
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	278	100.0	1	0.4	0.4	1	0.4	0.4
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	278	100.0	1	0.4	0.4	1	0.4	0.4

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 disulfid bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	1	0	1	0.26	0.26	0.0	0.26
2	0	0	0	1	0	1	0.26	0.26	0.0	0.26
3	0	0	0	1	0	1	0.26	0.26	0.0	0.26
4	0	0	0	1	0	1	0.25	0.25	0.0	0.25
5	0	0	0	1	0	1	0.29	0.29	0.0	0.29
6	0	0	0	1	0	1	0.26	0.26	0.0	0.26
7	0	0	0	1	0	1	0.26	0.26	0.0	0.26
8	0	0	0	1	0	1	0.25	0.25	0.0	0.25
9	0	0	0	1	0	1	0.27	0.27	0.0	0.27
10	0	0	0	1	0	1	0.26	0.26	0.0	0.26
11	0	0	0	1	0	1	0.26	0.26	0.0	0.26

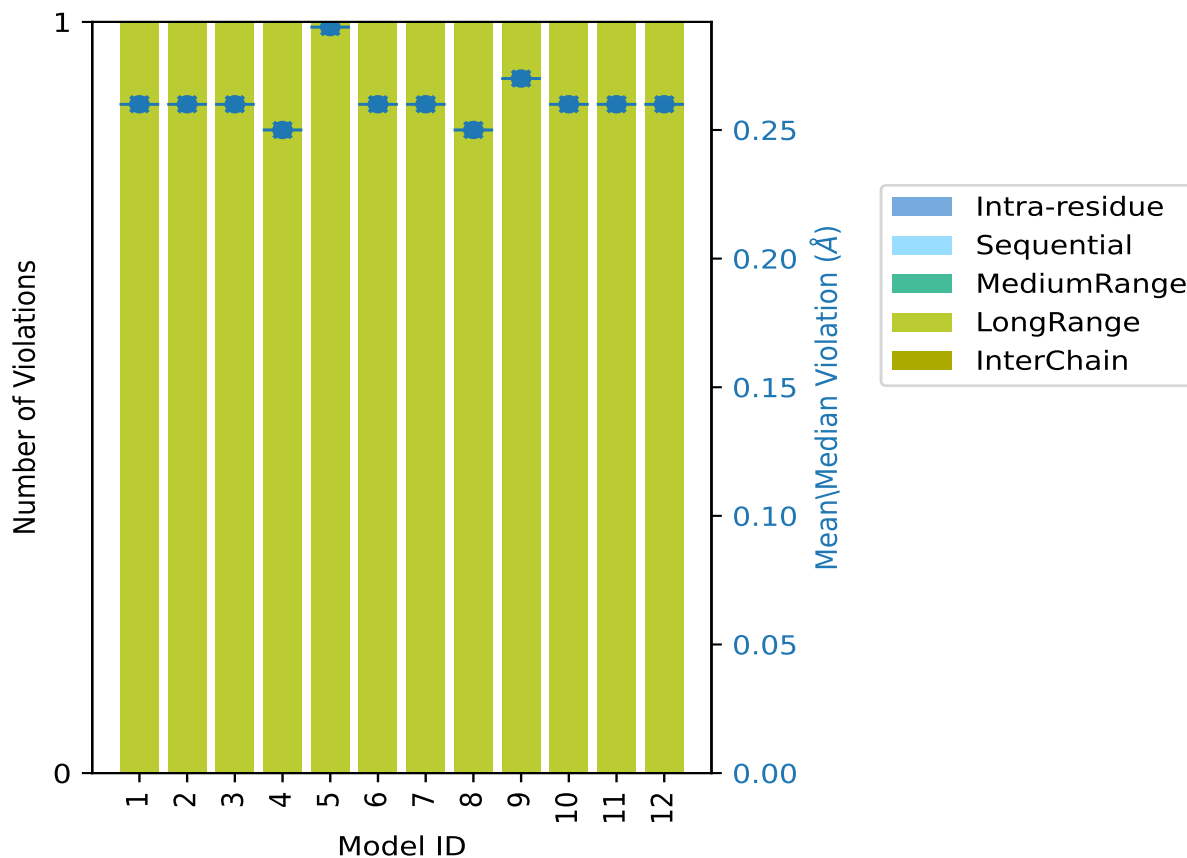
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	0	0	0	1	0	1	0.26	0.26	0.0	0.26

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 [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](#)

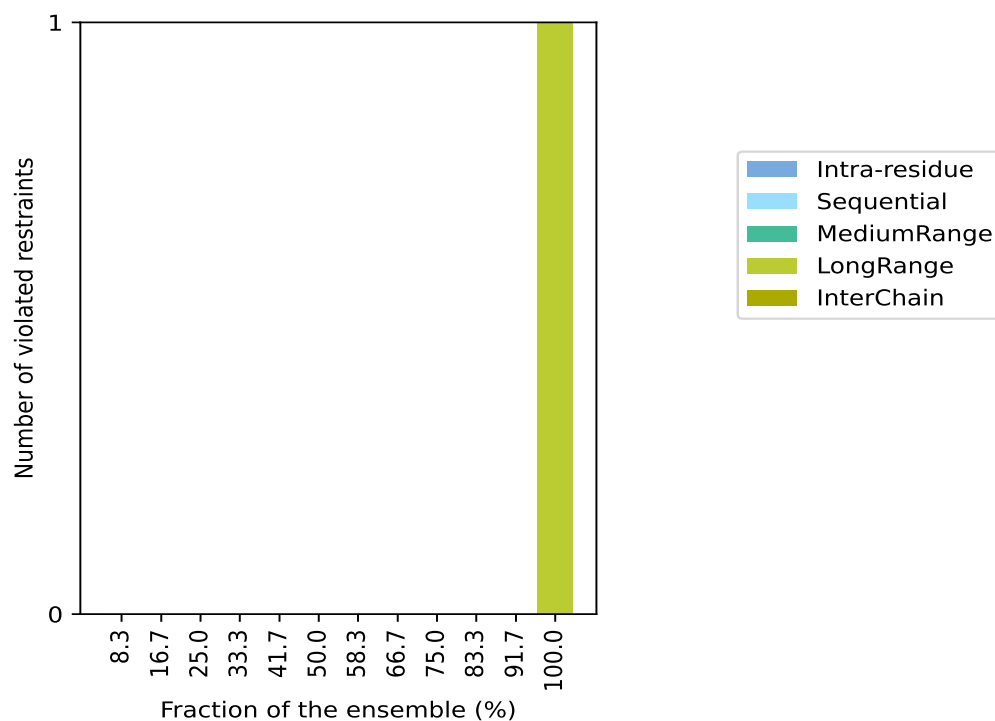
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 277(IR:122, SQ:70, MR:21, LR:64, IC:0) restraints are not 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	0	0	0	0	0	1	8.3
0	0	0	0	0	0	2	16.7
0	0	0	0	0	0	3	25.0
0	0	0	0	0	0	4	33.3
0	0	0	0	0	0	5	41.7
0	0	0	0	0	0	6	50.0
0	0	0	0	0	0	7	58.3
0	0	0	0	0	0	8	66.7
0	0	0	0	0	0	9	75.0
0	0	0	0	0	0	10	83.3
0	0	0	0	0	0	11	91.7
0	0	0	1	0	1	12	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

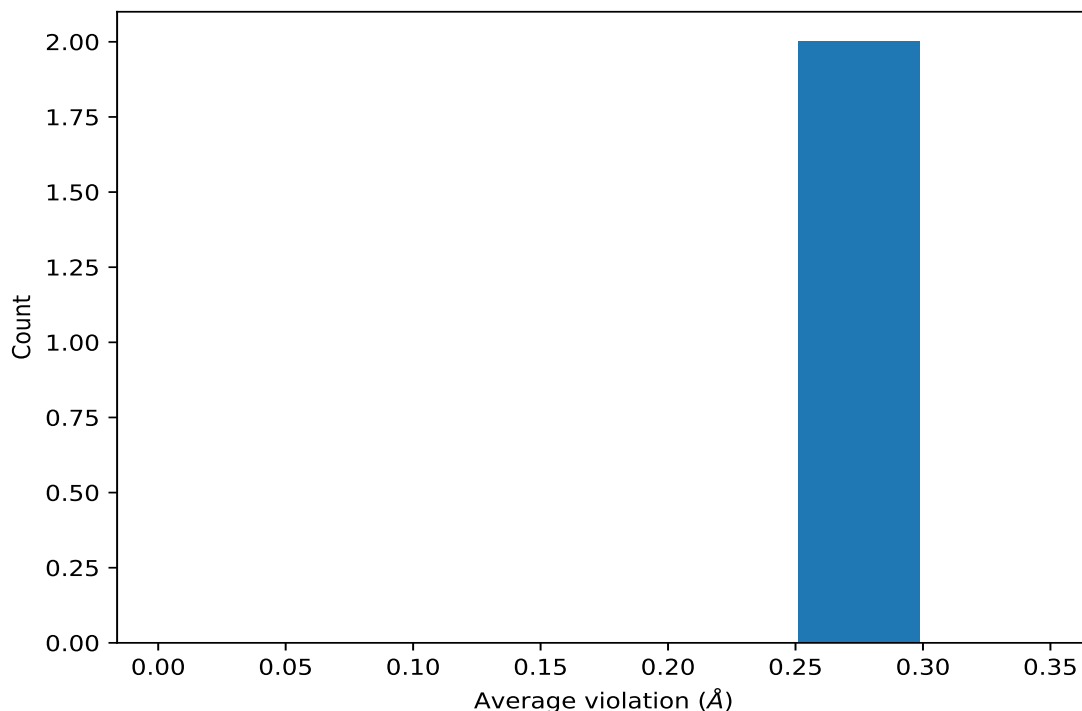
9.3.1 Bar graph : Distance violation statistics for the ensemble [\(i\)](#)



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 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. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

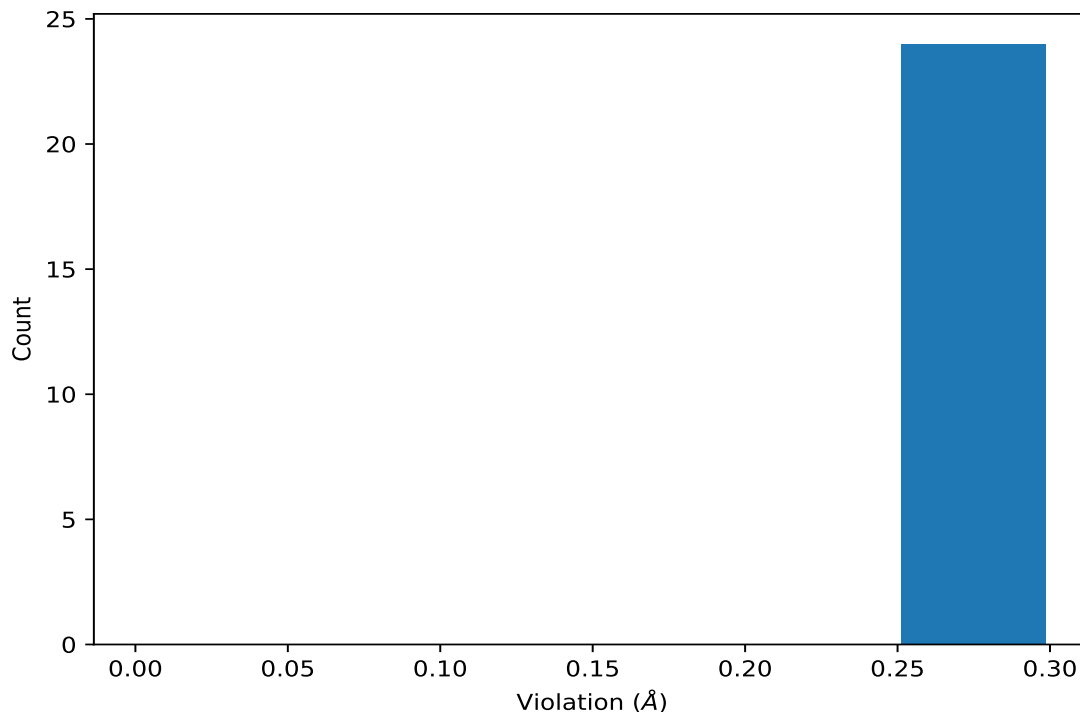
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	12	0.26	0.01	0.26
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	12	0.26	0.01	0.26

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 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)
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	5	0.29
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	5	0.29
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	9	0.27
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	9	0.27
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	1	0.26
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	1	0.26
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	2	0.26
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	2	0.26
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	3	0.26
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	6	0.26
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	6	0.26
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	7	0.26
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	7	0.26
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	10	0.26
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	10	0.26
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	11	0.26
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	11	0.26
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	12	0.26
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	12	0.26
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	4	0.25
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	4	0.25
(2,126)	1:A:21:DC:H41	1:A:6:DG:H22	8	0.25
(2,126)	1:A:21:DC:H42	1:A:6:DG:H22	8	0.25

10 Dihedral-angle violation analysis

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