



wwPDB NMR Structure Validation Summary Report ⓘ

Jun 6, 2023 – 08:05 pm BST

PDB ID : 4BY9
BMRB ID : 19400
Title : The structure of the Box CD enzyme reveals regulation of rRNA methylation
Authors : Lapinaite, A.; Simon, B.; Skjaerven, L.; Rakwalska-Bange, M.; Gabel, F.; Carlomagno, T.
Deposited on : 2013-07-18

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 : 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

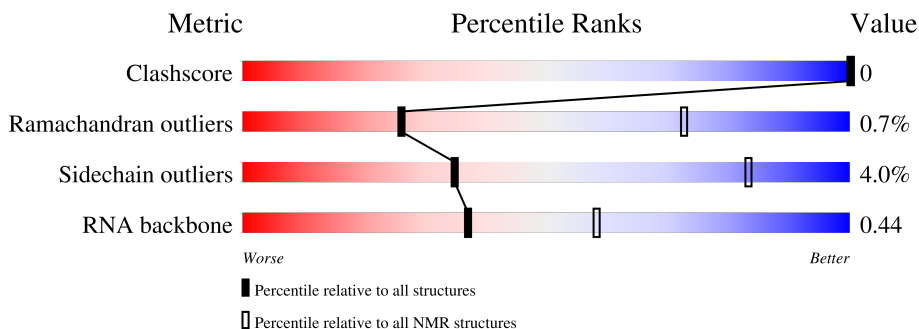
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 1%.

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
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428
RNA backbone	4643	676

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	72	21% 53% 24% .
1	B	72	14% 58% 24% .
2	C	366	91% 8% .
2	F	366	91% 8% .
2	I	366	90% 9% .
2	L	366	90% 9% .
3	D	121	90% 10%

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Mol	Chain	Length	Quality of chain
3	G	121	 93% 7%
3	J	121	 92% 7%
3	M	121	 93% 7%
4	E	227	 89% 10%
4	H	227	 92% 7%
4	K	227	 94% 6%
4	N	227	 93% 6%
5	W	11	 9% 64% 27%
5	X	11	 73% 27%
5	Y	11	 9% 73% 18%
5	Z	11	 9% 73% 18%

2 Ensemble composition and analysis

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 52476 atoms, of which 25544 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called SSR26.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	72	2342	696	782	300	493	71	0
1	B	72	2342	696	782	300	493	71	0

- Molecule 2 is a protein called NOP5/NOP56 RELATED PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	C	366	6006	1903	3025	518	553	7	0
2	F	366	6006	1903	3025	518	553	7	0
2	I	366	6006	1903	3025	518	553	7	0
2	L	366	6006	1903	3025	518	553	7	0

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
3	D	121	1906	591	980	153	179	3	0
3	G	121	1906	591	980	153	179	3	0
3	J	121	1906	591	980	153	179	3	0
3	M	121	1906	591	980	153	179	3	0

- Molecule 4 is a protein called FIBRILLARIN-LIKE RRNA/TRNA 2'-O-METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
4	E	227	3691	1174	1869	312	334	2	0
4	H	227	3691	1174	1869	312	334	2	0

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Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
4	K	227	Total	C	H	N	O	S	0
			3691	1174	1869	312	334	2	
4	N	227	Total	C	H	N	O	S	0
			3691	1174	1869	312	334	2	

- Molecule 5 is a RNA chain called 5'-R(*UP*CP*GP*CP*CP*CP*AP*UP*CP*AP*CP)-3'.

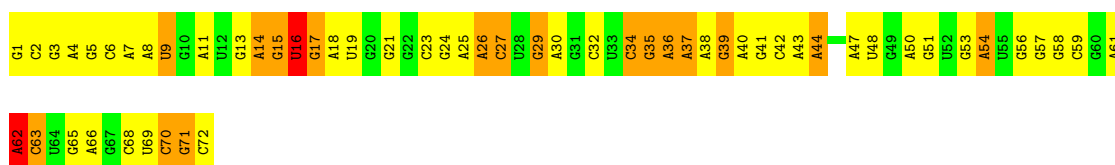
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
5	W	11	Total	C	H	N	O	P	0
			345	102	121	37	75	10	
5	X	11	Total	C	H	N	O	P	0
			345	102	121	37	75	10	
5	Y	11	Total	C	H	N	O	P	0
			345	102	121	37	75	10	
5	Z	11	Total	C	H	N	O	P	0
			345	102	121	37	75	10	

4 Residue-property plots [i](#)

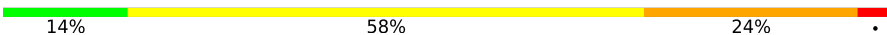
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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.

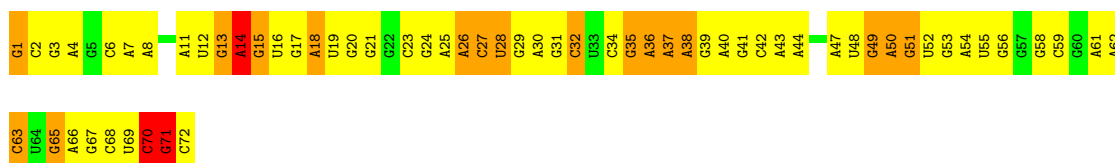
- Molecule 1: SSR26

Chain A: 




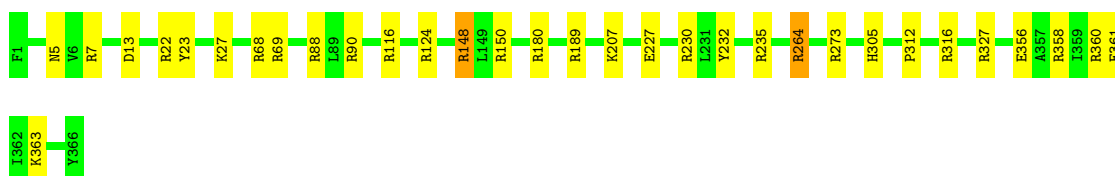
- Molecule 1: SSR26

Chain B: 



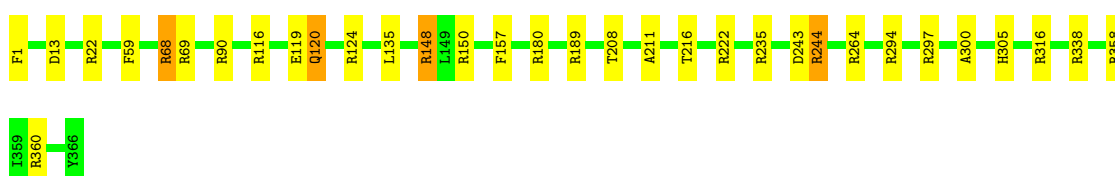
- Molecule 2: NOP5/NOP56 RELATED PROTEIN

Chain C: 

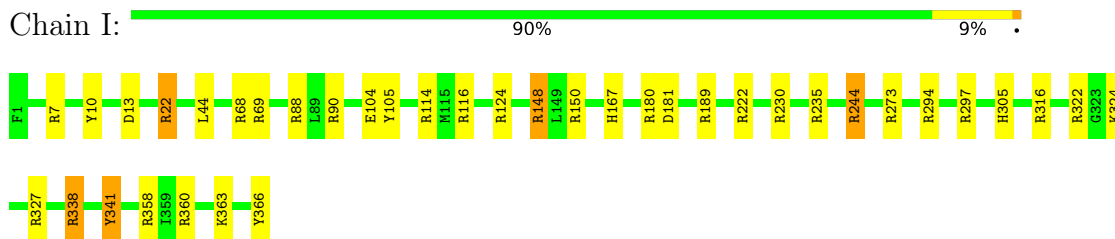


- Molecule 2: NOP5/NOP56 RELATED PROTEIN

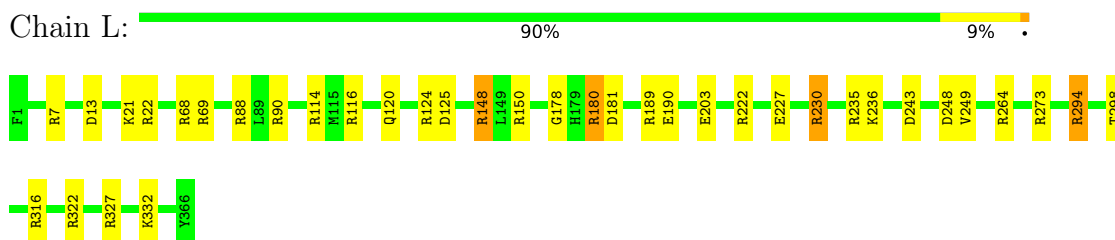
Chain F: 



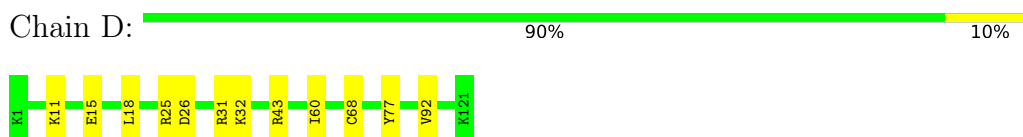
- Molecule 2: NOP5/NOP56 RELATED PROTEIN



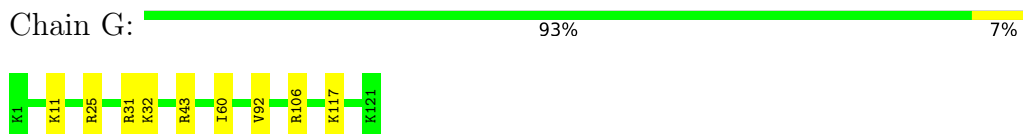
- Molecule 2: NOP5/NOP56 RELATED PROTEIN



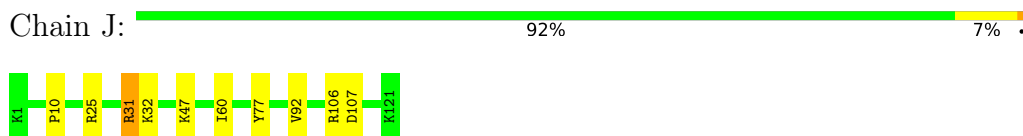
- Molecule 3: 50S RIBOSOMAL PROTEIN L7AE



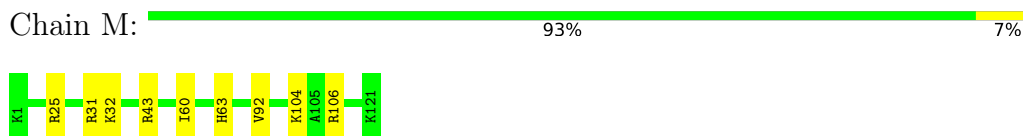
- Molecule 3: 50S RIBOSOMAL PROTEIN L7AE



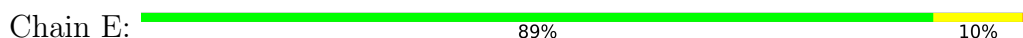
- Molecule 3: 50S RIBOSOMAL PROTEIN L7AE

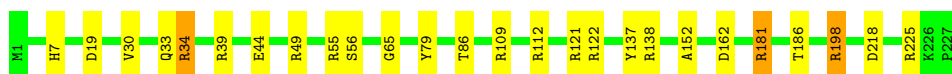


- Molecule 3: 50S RIBOSOMAL PROTEIN L7AE



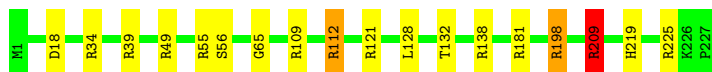
- Molecule 4: FIBRILLARIN-LIKE RRNA/TRNA 2'-O-METHYLTRANSFERASE





- Molecule 4: FIBRILLARIN-LIKE RRNA/TRNA 2'-O-METHYLTRANSFERASE

Chain H: 92% 7%



- Molecule 4: FIBRILLARIN-LIKE RRNA/TRNA 2'-O-METHYLTRANSFERASE

Chain K: 94% 6%



- Molecule 4: FIBRILLARIN-LIKE RRNA/TRNA 2'-O-METHYLTRANSFERASE

Chain N: 93% 6%



- Molecule 5: 5'-R(*UP*CP*GP*CP*CP*CP*AP*UP*CP*AP*CP)-3'

Chain W: 9% 64% 27%



- Molecule 5: 5'-R(*UP*CP*GP*CP*CP*CP*AP*UP*CP*AP*CP)-3'

Chain X: 73% 27%



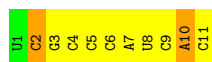
- Molecule 5: 5'-R(*UP*CP*GP*CP*CP*CP*AP*UP*CP*AP*CP)-3'

Chain Y: 9% 73% 18%



- Molecule 5: 5'-R(*UP*CP*GP*CP*CP*CP*AP*UP*CP*AP*CP)-3'

Chain Z: 9% 73% 18%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *ARIA*.

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
CNS	refinement	1.2
NMRView	structure solution	

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	319
Number of shifts mapped to atoms	319
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

6 Model quality i

6.1 Standard geometry i

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	1.43	0/1751 (0.0%)	2.35	131/2734 (4.8%)
1	B	1.44	0/1751 (0.0%)	2.35	140/2734 (5.1%)
2	C	0.75	0/3036 (0.0%)	1.13	24/4085 (0.6%)
2	F	0.75	0/3036 (0.0%)	1.13	20/4085 (0.5%)
2	I	0.75	0/3036 (0.0%)	1.17	30/4085 (0.7%)
2	L	0.75	0/3036 (0.0%)	1.15	27/4085 (0.7%)
3	D	0.67	0/938 (0.0%)	1.06	4/1264 (0.3%)
3	G	0.67	0/938 (0.0%)	1.05	4/1264 (0.3%)
3	J	0.68	0/938 (0.0%)	1.00	3/1264 (0.2%)
3	M	0.67	0/938 (0.0%)	1.06	4/1264 (0.3%)
4	E	0.74	0/1861 (0.0%)	1.12	15/2515 (0.6%)
4	H	0.75	0/1861 (0.0%)	1.13	14/2515 (0.6%)
4	K	0.75	0/1861 (0.0%)	1.10	9/2515 (0.4%)
4	N	0.75	0/1861 (0.0%)	1.11	11/2515 (0.4%)
5	W	1.44	0/248 (0.0%)	2.29	20/383 (5.2%)
5	X	1.40	0/248 (0.0%)	2.23	21/383 (5.5%)
5	Y	1.39	0/248 (0.0%)	2.25	21/383 (5.5%)
5	Z	1.43	0/248 (0.0%)	2.38	21/383 (5.5%)
All	All	0.89	0/27834 (0.0%)	1.42	519/38456 (1.3%)

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	12
1	B	0	13
2	F	0	4
2	I	0	3
2	L	0	2
3	J	0	1
4	H	0	4

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Mol	Chain	Chirality	Planarity
4	K	0	3
4	N	0	2
5	W	0	3
5	X	0	3
5	Y	0	2
5	Z	0	1
All	All	0	53

There are no bond-length outliers.

5 of 519 angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	22	ARG	NE-CZ-NH1	13.29	126.94	120.30
2	C	358	ARG	NE-CZ-NH1	11.90	126.25	120.30
1	B	63	C	O4'-C1'-N1	11.60	117.48	108.20
2	L	116	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	A	44	A	N1-C6-N6	-10.87	112.08	118.60

There are no chirality outliers.

5 of 53 planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	9	U	Sidechain
1	A	16	U	Sidechain
1	A	17	G	Sidechain
1	A	29	G	Sidechain
1	A	34	C	Sidechain

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
2	I	2981	3025	3025	1
All	All	26932	25544	25544	1

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:I:324:LYS:HE2	2:I:366:TYR:CE1	0.41	2.49

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
2	C	364/366 (99%)	338 (93%)	25 (7%)	1 (0%)	44 80
2	F	364/366 (99%)	338 (93%)	22 (6%)	4 (1%)	18 66
2	I	364/366 (99%)	351 (96%)	13 (4%)	0 (0%)	100 100
2	L	364/366 (99%)	343 (94%)	18 (5%)	3 (1%)	24 71
3	D	119/121 (98%)	113 (95%)	4 (3%)	2 (2%)	13 56
3	G	119/121 (98%)	110 (92%)	8 (7%)	1 (1%)	24 71
3	J	119/121 (98%)	110 (92%)	7 (6%)	2 (2%)	13 56
3	M	119/121 (98%)	114 (96%)	4 (3%)	1 (1%)	24 71
4	E	225/227 (99%)	211 (94%)	11 (5%)	3 (1%)	16 63
4	H	225/227 (99%)	212 (94%)	12 (5%)	1 (0%)	38 78
4	K	225/227 (99%)	210 (93%)	14 (6%)	1 (0%)	38 78
4	N	225/227 (99%)	211 (94%)	14 (6%)	0 (0%)	100 100
All	All	2832/2856 (99%)	2661 (94%)	152 (5%)	19 (1%)	26 73

5 of 19 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	C	312	PRO
3	D	11	LYS
3	D	92	VAL
4	E	44	GLU
4	E	65	GLY

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	312/312 (100%)	300 (96%)	12 (4%)	36	84
2	F	312/312 (100%)	301 (96%)	11 (4%)	39	86
2	I	312/312 (100%)	301 (96%)	11 (4%)	39	86
2	L	312/312 (100%)	298 (96%)	14 (4%)	31	80
3	D	98/98 (100%)	91 (93%)	7 (7%)	18	67
3	G	98/98 (100%)	94 (96%)	4 (4%)	34	82
3	J	98/98 (100%)	93 (95%)	5 (5%)	27	77
3	M	98/98 (100%)	94 (96%)	4 (4%)	34	82
4	E	197/197 (100%)	185 (94%)	12 (6%)	22	71
4	H	197/197 (100%)	191 (97%)	6 (3%)	44	89
4	K	197/197 (100%)	193 (98%)	4 (2%)	57	93
4	N	197/197 (100%)	190 (96%)	7 (4%)	38	86
All	All	2428/2428 (100%)	2331 (96%)	97 (4%)	35	83

5 of 97 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	C	5	ASN
2	C	13	ASP
2	C	27	LYS
2	C	148	ARG
2	C	207	LYS

6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	71/72 (99%)	10 (14%)	4 (6%)	0.44
1	B	71/72 (99%)	12 (17%)	6 (8%)	0.45
5	W	10/11 (91%)	0 (0%)	0 (0%)	0.40
5	X	10/11 (91%)	0 (0%)	0 (0%)	0.46

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
5	Y	10/11 (91%)	0 (0%)	0 (0%)	0.48
5	Z	10/11 (91%)	1 (10%)	0 (0%)	0.35
All	All	182/188 (97%)	23 (13%)	10 (5%)	0.44

The overall RNA backbone suiteness is 0.44.

5 of 23 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	14	A
1	A	15	G
1	A	16	U
1	A	26	A
1	A	27	C

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	14	A
1	A	15	G
1	A	29	G
1	A	70	C
1	B	15	G

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 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

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 1% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_0*

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	319
Number of shifts mapped to atoms	319
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 [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 1%, i.e. 319 atoms were assigned a chemical shift out of a possible 44070. 0 out of 496 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/14184 (0%)	0/5752 (0%)	0/5712 (0%)	0/2720 (0%)
Sidechain	319/23816 (1%)	240/15440 (2%)	79/7420 (1%)	0/956 (0%)
Aromatic	0/2504 (0%)	0/1220 (0%)	0/1208 (0%)	0/76 (0%)
Sugar	0/2068 (0%)	0/1128 (0%)	0/940 (0%)	0/0 (—%)
Base	0/1498 (0%)	0/934 (0%)	0/318 (0%)	0/246 (0%)
Overall	319/44070 (1%)	240/24474 (1%)	79/15598 (1%)	0/3998 (0%)

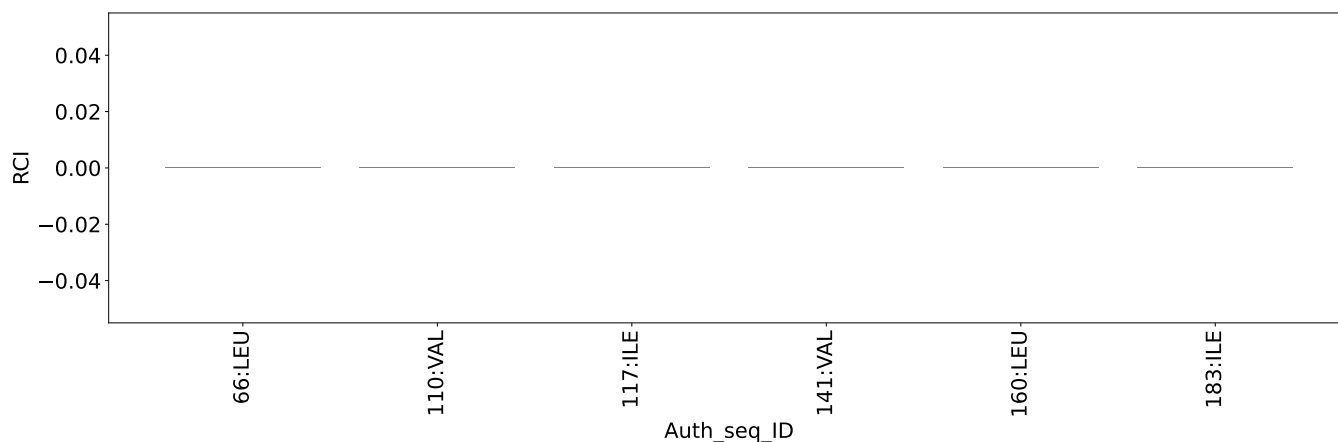
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

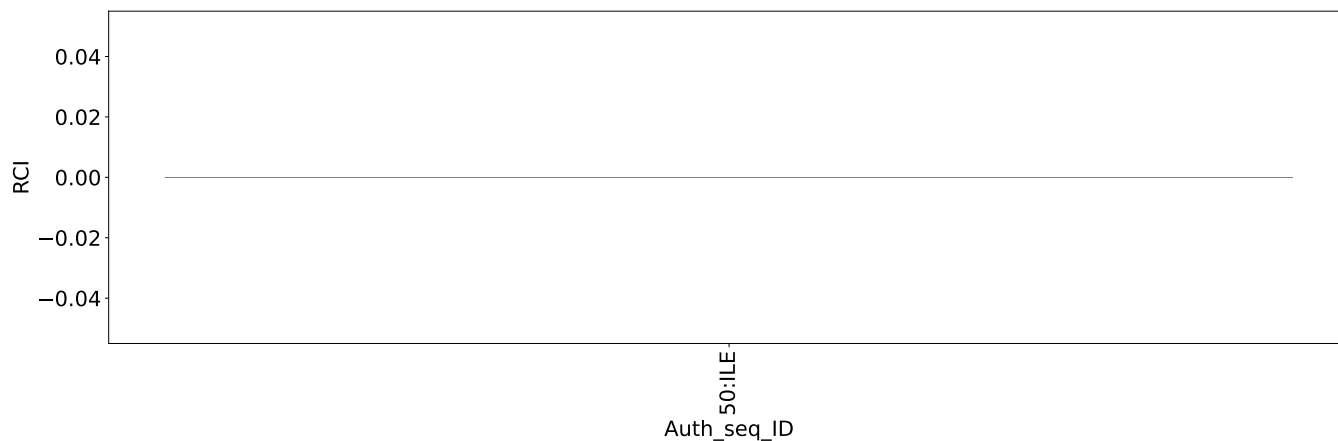
7.1.5 Random Coil Index (RCI) plots [i](#)

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.

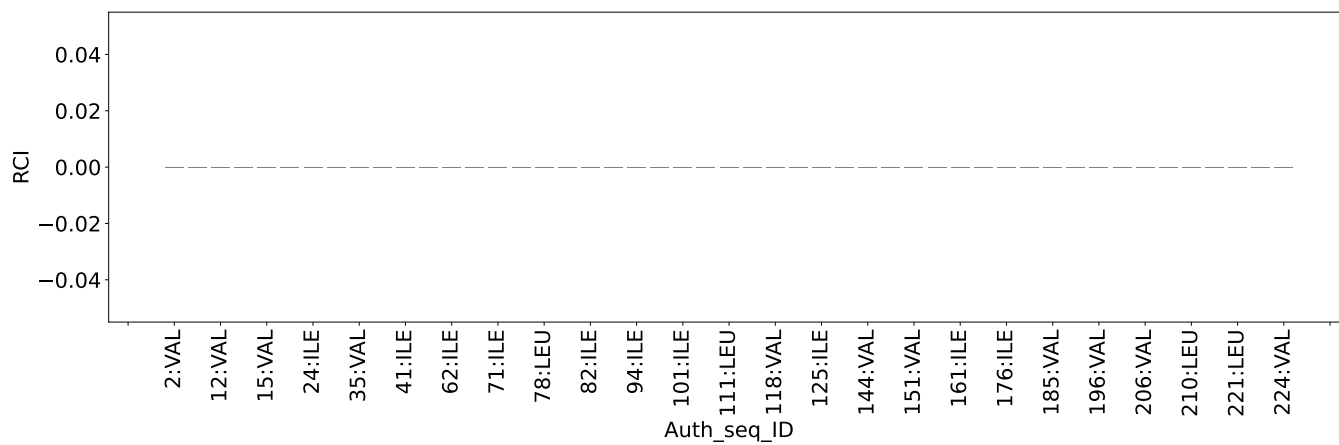
Random coil index (RCI) for chain C:



Random coil index (RCI) for chain D:



Random coil index (RCI) for chain E:



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	514
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	514
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.2
Number of long range restraints per residue ¹	0.0

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

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	4.0	0.18
0.2-0.5 (Medium)	7.0	0.39
>0.5 (Large)	151.0	17.43

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

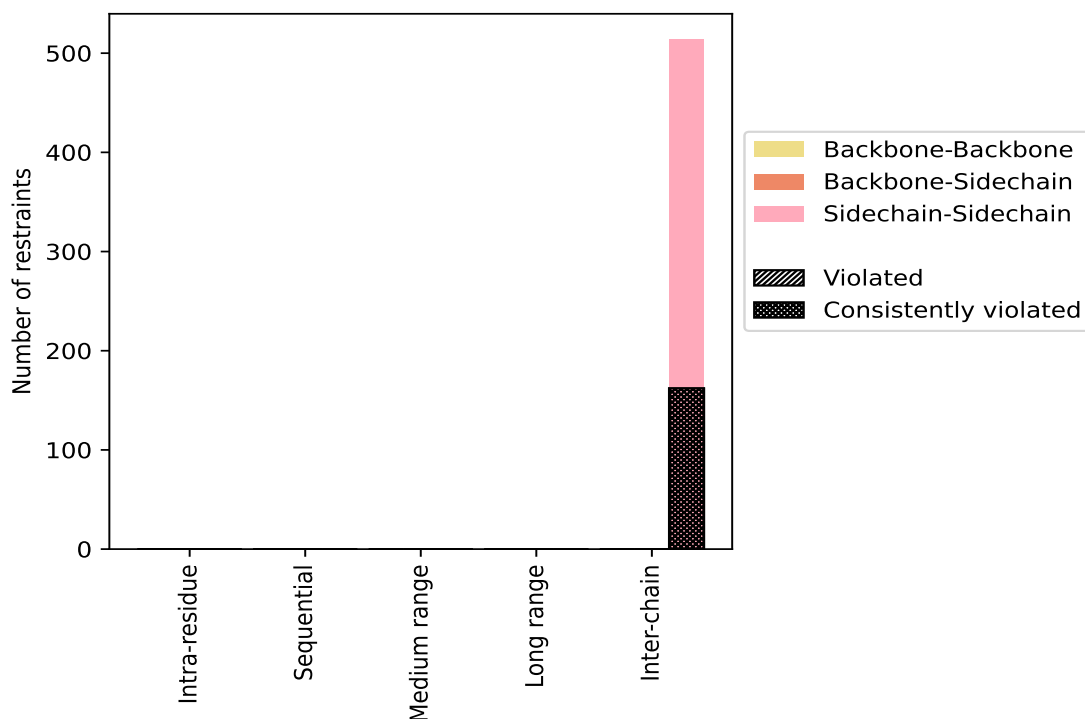
9.1 Summary of distance violations

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)	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
Sequential (i-j =1)	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
Medium range (i-j >1 & i-j <5)	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
Long range (i-j ≥5)	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
Inter-chain	514	100.0	162	31.5	31.5	162	31.5	31.5
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	514	100.0	162	31.5	31.5	162	31.5	31.5
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	514	100.0	162	31.5	31.5	162	31.5	31.5
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	514	100.0	162	31.5	31.5	162	31.5	31.5

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

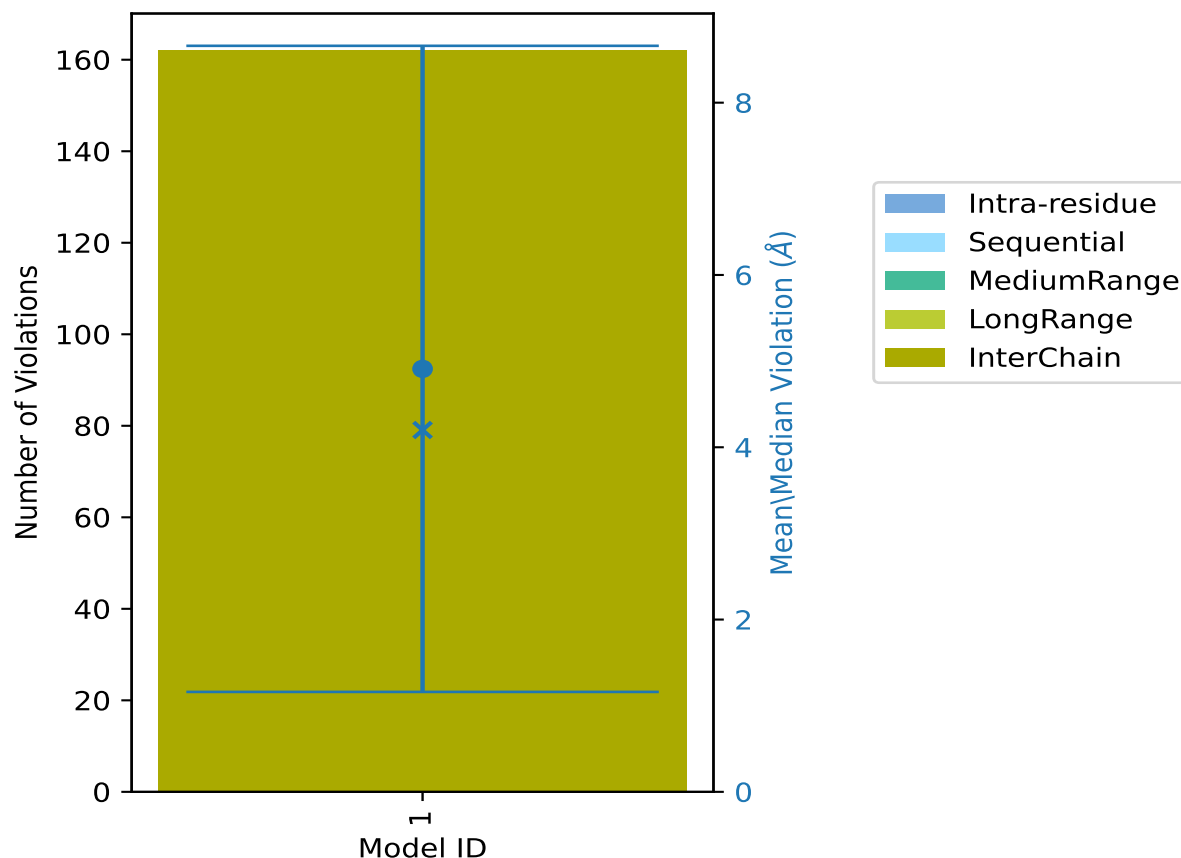
9.2 Distance violation statistics for each model [i](#)

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	0	162	162	4.91	17.43	3.75	4.2

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 [i](#)



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

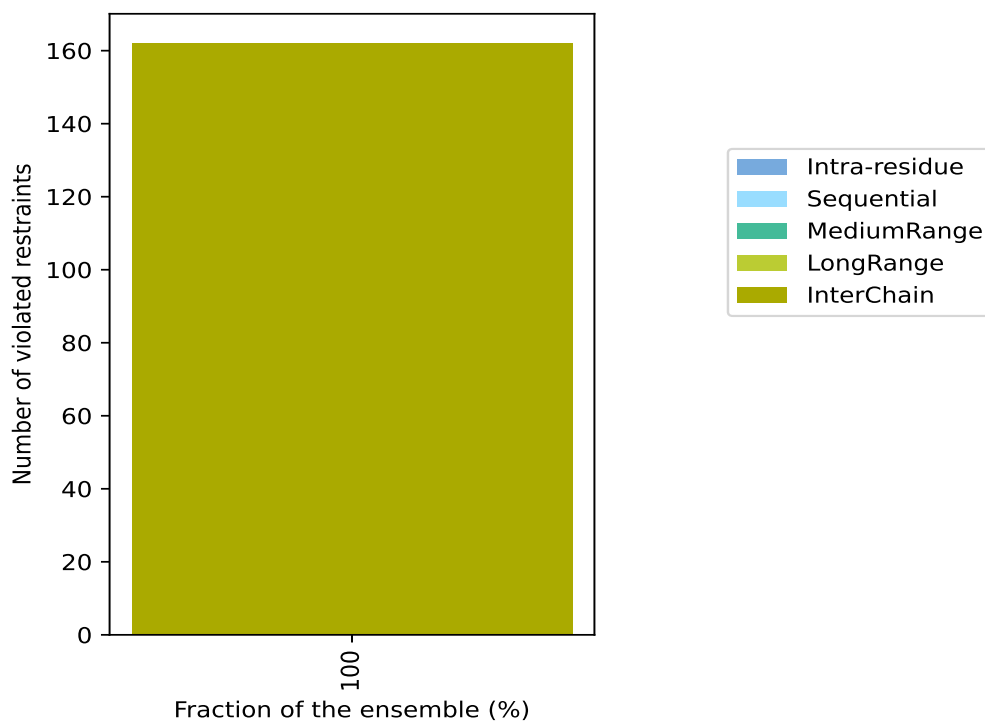
9.3 Distance violation statistics for the ensemble [i](#)

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, 352(IR:0, SQ:0, MR:0, LR:0, IC:352) 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	162	162	1	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](#)



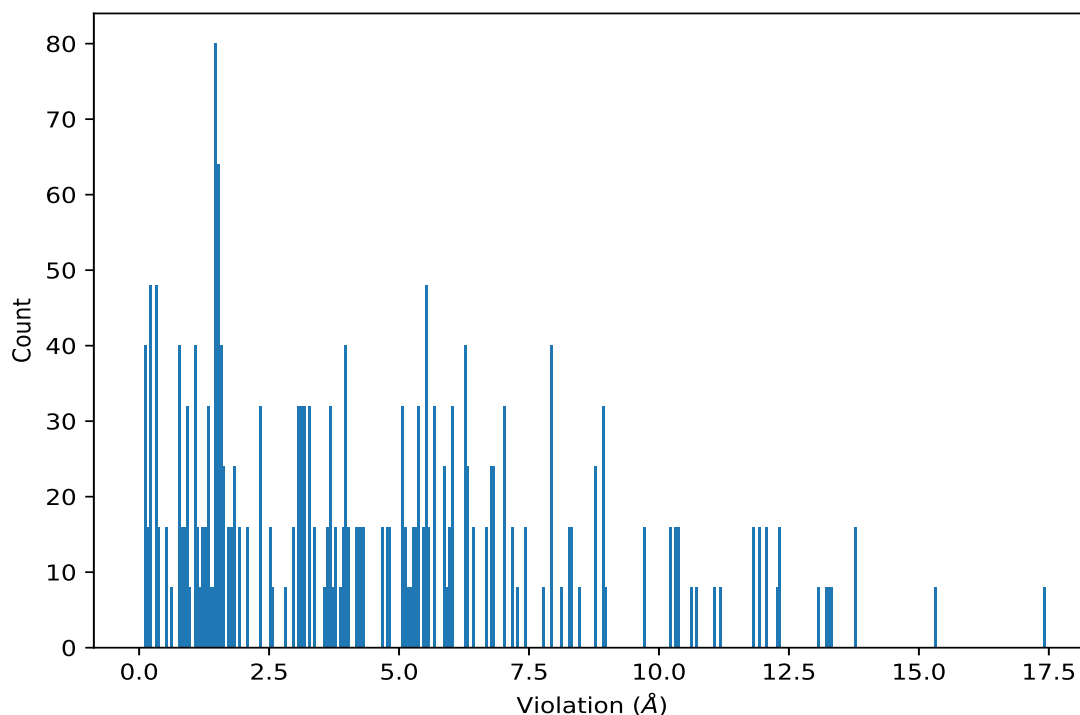
9.4 Most violated distance restraints in the ensemble [i](#)

No violations found

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)
(1,29)	2:C:196:GLU:OE2	4:E:125:ILE:CD1	1	17.43
(1,29)	2:C:196:GLU:OE2	4:H:125:ILE:CD1	1	17.43
(1,29)	2:F:196:GLU:OE2	4:E:125:ILE:CD1	1	17.43
(1,29)	2:F:196:GLU:OE2	4:H:125:ILE:CD1	1	17.43
(1,29)	2:I:196:GLU:OE2	4:E:125:ILE:CD1	1	17.43
(1,29)	2:I:196:GLU:OE2	4:H:125:ILE:CD1	1	17.43
(1,29)	2:L:196:GLU:OE2	4:E:125:ILE:CD1	1	17.43
(1,29)	2:L:196:GLU:OE2	4:H:125:ILE:CD1	1	17.43
(1,212)	2:C:247:ASP:OD2	4:K:176:ILE:CD1	1	15.31
(1,212)	2:C:247:ASP:OD2	4:N:176:ILE:CD1	1	15.31
(1,212)	2:F:247:ASP:OD2	4:K:176:ILE:CD1	1	15.31
(1,212)	2:F:247:ASP:OD2	4:N:176:ILE:CD1	1	15.31
(1,212)	2:I:247:ASP:OD2	4:K:176:ILE:CD1	1	15.31
(1,212)	2:I:247:ASP:OD2	4:N:176:ILE:CD1	1	15.31
(1,212)	2:L:247:ASP:OD2	4:K:176:ILE:CD1	1	15.31
(1,212)	2:L:247:ASP:OD2	4:N:176:ILE:CD1	1	15.31
(1,270)	3:D:45:GLN:NE2	4:E:185:VAL:CG1	1	13.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	3:D:45:GLN:NE2	4:E:185:VAL:CG2	1	13.77
(1,270)	3:D:45:GLN:NE2	4:H:185:VAL:CG1	1	13.77
(1,270)	3:D:45:GLN:NE2	4:H:185:VAL:CG2	1	13.77
(1,270)	3:G:45:GLN:NE2	4:E:185:VAL:CG1	1	13.77
(1,270)	3:G:45:GLN:NE2	4:E:185:VAL:CG2	1	13.77
(1,270)	3:G:45:GLN:NE2	4:H:185:VAL:CG1	1	13.77
(1,270)	3:G:45:GLN:NE2	4:H:185:VAL:CG2	1	13.77
(1,270)	3:J:45:GLN:NE2	4:E:185:VAL:CG1	1	13.77
(1,270)	3:J:45:GLN:NE2	4:E:185:VAL:CG2	1	13.77
(1,270)	3:J:45:GLN:NE2	4:H:185:VAL:CG1	1	13.77
(1,270)	3:J:45:GLN:NE2	4:H:185:VAL:CG2	1	13.77
(1,270)	3:M:45:GLN:NE2	4:E:185:VAL:CG1	1	13.77
(1,270)	3:M:45:GLN:NE2	4:E:185:VAL:CG2	1	13.77
(1,270)	3:M:45:GLN:NE2	4:H:185:VAL:CG1	1	13.77
(1,270)	3:M:45:GLN:NE2	4:H:185:VAL:CG2	1	13.77
(1,424)	3:D:71:LYS:NZ	4:E:94:ILE:CD1	1	13.32
(1,424)	3:D:71:LYS:NZ	4:H:94:ILE:CD1	1	13.32
(1,424)	3:G:71:LYS:NZ	4:E:94:ILE:CD1	1	13.32
(1,424)	3:G:71:LYS:NZ	4:H:94:ILE:CD1	1	13.32
(1,424)	3:J:71:LYS:NZ	4:E:94:ILE:CD1	1	13.32
(1,424)	3:J:71:LYS:NZ	4:H:94:ILE:CD1	1	13.32
(1,424)	3:M:71:LYS:NZ	4:E:94:ILE:CD1	1	13.32
(1,424)	3:M:71:LYS:NZ	4:H:94:ILE:CD1	1	13.32
(1,433)	3:D:71:LYS:NZ	4:E:117:ILE:CD1	1	13.26
(1,433)	3:D:71:LYS:NZ	4:H:117:ILE:CD1	1	13.26
(1,433)	3:G:71:LYS:NZ	4:E:117:ILE:CD1	1	13.26
(1,433)	3:G:71:LYS:NZ	4:H:117:ILE:CD1	1	13.26
(1,433)	3:J:71:LYS:NZ	4:E:117:ILE:CD1	1	13.26
(1,433)	3:J:71:LYS:NZ	4:H:117:ILE:CD1	1	13.26
(1,433)	3:M:71:LYS:NZ	4:E:117:ILE:CD1	1	13.26
(1,433)	3:M:71:LYS:NZ	4:H:117:ILE:CD1	1	13.26
(1,85)	2:C:196:GLU:OE2	4:K:125:ILE:CD1	1	13.2
(1,85)	2:C:196:GLU:OE2	4:N:125:ILE:CD1	1	13.2
(1,85)	2:F:196:GLU:OE2	4:K:125:ILE:CD1	1	13.2
(1,85)	2:F:196:GLU:OE2	4:N:125:ILE:CD1	1	13.2
(1,85)	2:I:196:GLU:OE2	4:K:125:ILE:CD1	1	13.2
(1,85)	2:I:196:GLU:OE2	4:N:125:ILE:CD1	1	13.2
(1,85)	2:L:196:GLU:OE2	4:K:125:ILE:CD1	1	13.2
(1,85)	2:L:196:GLU:OE2	4:N:125:ILE:CD1	1	13.2
(1,156)	2:C:247:ASP:OD2	4:E:176:ILE:CD1	1	13.05
(1,156)	2:C:247:ASP:OD2	4:H:176:ILE:CD1	1	13.05
(1,156)	2:F:247:ASP:OD2	4:E:176:ILE:CD1	1	13.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	2:F:247:ASP:OD2	4:H:176:ILE:CD1	1	13.05
(1,156)	2:I:247:ASP:OD2	4:E:176:ILE:CD1	1	13.05
(1,156)	2:I:247:ASP:OD2	4:H:176:ILE:CD1	1	13.05
(1,156)	2:L:247:ASP:OD2	4:E:176:ILE:CD1	1	13.05
(1,156)	2:L:247:ASP:OD2	4:H:176:ILE:CD1	1	13.05
(1,214)	2:C:247:ASP:OD2	4:K:183:ILE:CD1	1	12.33
(1,214)	2:C:247:ASP:OD2	4:N:183:ILE:CD1	1	12.33
(1,214)	2:F:247:ASP:OD2	4:K:183:ILE:CD1	1	12.33
(1,214)	2:F:247:ASP:OD2	4:N:183:ILE:CD1	1	12.33
(1,214)	2:I:247:ASP:OD2	4:K:183:ILE:CD1	1	12.33
(1,214)	2:I:247:ASP:OD2	4:N:183:ILE:CD1	1	12.33
(1,214)	2:L:247:ASP:OD2	4:K:183:ILE:CD1	1	12.33
(1,214)	2:L:247:ASP:OD2	4:N:183:ILE:CD1	1	12.33
(1,487)	3:D:71:LYS:NZ	4:K:117:ILE:CD1	1	12.3
(1,487)	3:D:71:LYS:NZ	4:N:117:ILE:CD1	1	12.3
(1,487)	3:G:71:LYS:NZ	4:K:117:ILE:CD1	1	12.3
(1,487)	3:G:71:LYS:NZ	4:N:117:ILE:CD1	1	12.3
(1,487)	3:J:71:LYS:NZ	4:K:117:ILE:CD1	1	12.3
(1,487)	3:J:71:LYS:NZ	4:N:117:ILE:CD1	1	12.3
(1,487)	3:M:71:LYS:NZ	4:K:117:ILE:CD1	1	12.3
(1,487)	3:M:71:LYS:NZ	4:N:117:ILE:CD1	1	12.3
(1,478)	3:D:71:LYS:NZ	4:K:94:ILE:CD1	1	12.29

10 Dihedral-angle violation analysis

No dihedral-angle restraints found