

wwPDB NMR Structure Validation Summary Report (i)

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PDB ID : 2L8I BMRB ID : 17409

Title: A biocompatible backbone modification? - Structure and dynamics of a

triazole-linked DNA duplex

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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

Mogul : 1.8.5 (274361), 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

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

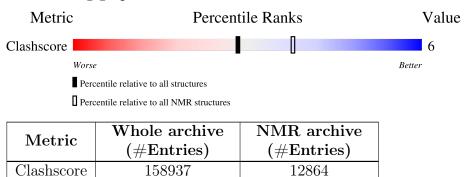
Validation Pipeline (wwPDB-VP) : 2.36.2

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 55%.

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.



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	13	85% 15%							
2	В	12	33%	67%						



2 Ensemble composition and analysis (i)

This entry contains 11 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 are 2 unique types of molecules in this entry. The entry contains 827 atoms, of which 298 are hydrogens and 0 are deuteriums.

• Molecule 1 is a DNA chain called DNA (5'-D(*GP*CP*TP*GP*CP*AP*AP*AP*CP*GP* TP*CP*G)-3').

Mol	Chain	Residues		Atoms						
1	Λ	19	Total	С	Н	N	О	Р	0	
	А	13	411	126	147	51	75	12	0	

• Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*A P*GP*C)-3').

Mol	Chain	Residues		Atoms						
9	D	19	Total	С	Н	N	О	Р	0	
2	D	12	416	129	151	51	74	11	U	

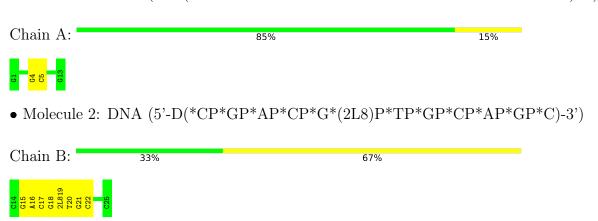


4 Residue-property plots (i)

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.

 \bullet Molecule 1: DNA (5'-D(*GP*CP*TP*GP*CP*AP*AP*AP*CP*GP*TP*CP*G)-3')

Chain A:

There are no outlier residues in this chain.

• Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

Chain B: 75% 25%





Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: torsion angle dynamics.

Of the 100 calculated structures, 11 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
X-PLOR NIH	refinement	2.20
X-PLOR NIH	structure solution	2.20

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	305
Number of shifts mapped to atoms	305
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	55%



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: 2L8

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	
1	A	264	147	147	1±1	
2	В	265	151	151	4±1	
All	All	5819	3278	3278	58	

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 6.

5 of 8 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom 2	Clash(Å)	Distance(Å)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:4:DG:C2	1:A:5:DC:C2	0.52	2.98	8	10	
2:B:20:DT:C2	2:B:21:DG:N7	0.49	2.81	8	10	
2:B:17:DC:C2	2:B:18:DG:C8	0.47	3.02	9	9	
2:B:21:DG:C4	2:B:22:DC:C5	0.47	3.03	9	11	
2:B:15:DG:C6	2:B:16:DA:N6	0.45	2.84	8	8	



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.

Mal	Type	Chain	Res Link Bond lengths				
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	#Z>2
2	2L8	В	19	2	43,46,47	0.57 ± 0.01	2±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.

Mal	Type	Chain	nain Res Link Bond angles				
IVIOI	туре	Chain	rtes	LIIIK	Counts	RMSZ	#Z>2
2	2L8	В	19	2	57,67,70	0.67 ± 0.02	2±0 (3±0%)

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
2	2L8	В	19	2	-	$0\pm0,16,46,47$	$0\pm0,5,5,5$

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

Mol	Chain	nain Res	Type	Atoms	Z	Observed (Å)	$\operatorname{oserved}(\mathring{A}) \mid \operatorname{Ideal}(\mathring{A})$		dels
WIOI	Chain		Type			Observed(A)	ideai(A)	Worst	Total
2	В	19	2L8	C2A-N4A	2.33	1.37	1.34	6	11
2	В	19	2L8	N4A-N5A	2.20	1.30	1.34	4	11

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	${f Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$	Mod	dels
				Atoms		Observed()	Ideal()	Worst	Total
2	В	19	2L8	C3A-C2A-N4A	3.00	106.88	111.34	3	11
2	В	19	2L8	O4'-C4'-C7A	2.18	105.38	108.89	10	10

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 55% for the well-defined parts and 55% for the entire structure.

7.1 Chemical shift list 1

File name: working cs.cif

Chemical shift list name: assigned_chem_shift_list_1

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	305
Number of shifts mapped to atoms	305
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 Re	Dog	Res Type	Atom	Shift Data		
LIST ID		nes			Value	Uncertainty	Ambiguity
1	В	19	2L8	C1'1	86.1		1
1	В	19	2L8	C3'1	74.8		1
1	В	19	2L8	C61	134.9	•	1
1	В	19	2L8	H11'	5.76		1
1	В	19	2L8	H12'	2.77	•	1
1	В	19	2L8	H13'	4.79		1
1	В	19	2L8	H14'	4.17	•	1
1	В	19	2L8	H1C6	7.00		1
1	В	19	2L8	H1C7	4.68	•	1
1	В	19	2L8	H1CA	5.00		1
1	В	19	2L8	H1N3	13.95	•	1
1	В	19	2L8	HC2'	1.94		1



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 55%, i.e. 265 atoms were assigned a chemical shift out of a possible 482. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Sugar	$168/288 \ (58\%)$	$120/168 \ (71\%)$	48/120 (40%)	0/0 (%)
Base	97/194 (50%)	60/122~(49%)	37/40 (92%)	0/32 (0%)
Overall	265/482~(55%)	180/290~(62%)	85/160 (53%)	0/32 (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

