

# Full wwPDB NMR Structure Validation Report (i)

#### Apr 20, 2024 – 11:13 AM EDT

PDB ID	:	1QXB
Title	:	NMR structure determination of the self complementary DNA Dodecamer
		CGCGAATT*CGCG in which a ribose is inserted between the 3'-OH of T8
		and the 5'-phosphate group of C9
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Deposited on	:	2003-09-05

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 (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		
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 was not calculated.

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.

Me	etric	Percent	tile Ranks	Value
Clashsc	ore			6
	Worse	2		Better
	Perc	centile relative to all structures		
	Pero	centile relative to all NMR structures		
		Whole archive	NMR archive	]
Me	tric	(#Entries)	(#Entries)	

	( // ====== )	(// =====)		
Clashscore	158937	12864		
			-	
The table be	low summarises the g	geometric issues obse	erved across the p	polym
fit to the ext	perimental data The	e red orange vellov	v and green segn	nents

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	А	12	33%	33%	33%		
1	В	12	25%	33%	42%		



### 2 Ensemble composition and analysis (i)

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



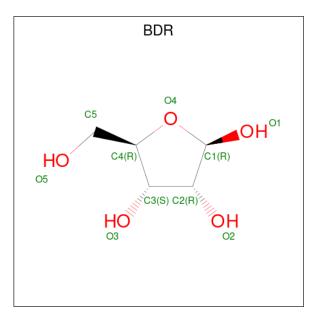
# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 791 atoms, of which 287 are hydrogens and 0 are deuteriums.

• Molecule 1 is a DNA chain called 5'-d(CpGpCpGpApApTpTpCpGpCpG)-3'.

Mol	Chain	Residues		Atoms					Trace	
1	Λ	19	Total	С	Η	Ν	0	Р	0	
		12	378	116	135	46	70	11	0	
1	1 B	D	19	Total	С	Н	Ν	0	Р	0
		12	379	116	136	46	70	11	U	

• Molecule 2 is beta-D-ribofuranose (three-letter code: BDR) (formula:  $C_5H_{10}O_5$ ).



Mol	Chain	Residues	Atoms			
9	Λ	1	Total	С	Η	Ο
	A	T	17	5	8	4
0	р	1	Total	С	Η	Ο
	D	1	17	5	8	4



# 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: 5'-d(CpGpCpGpApApTpTpCpGpCpG)-3'

Chain A:	33%	33%	33%						
C1 C3 C3 C3 C3 C3 C3 C3 C3 C3 C10 C11 C11 C11 C12 C12 C12 C12 C12 C12 C12	62 64 64 610 611 612 612								
• Molecule 1: 5 <sup>7</sup>	• Molecule 1: 5'-d(CpGpCpGpApApTpTpCpGpCpG)-3'								
Chain B:	25%	33%	42%						
C13 614 615 616 716 719 719 719 719 720 721 622 622 623									



### 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: torsion angle dynamics followed by a molecular dynamics refinement.

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
X-PLOR	structure solution	3.851
X-PLOR	refinement	3.851

No chemical shift data was provided.



# 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: BDR

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	Bor	nd lengths	Bond angles		
		RMSZ	#Z > 5	RMSZ	#Z > 5	
1	А	1.09	2/271 ( $0.7%)$	2.21	20/414 ( $4.8%$ )	
1	В	1.07	1/271~(~0.4%)	2.21	20/414 ( $4.8%$ )	
All	All	1.08	3/542 ( $0.6%)$	2.21	40/828 ( $4.8%$ )	

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	8	DT	C5-C7	5.12	1.53	1.50
1	В	20	DT	C5-C7	5.07	1.53	1.50
1	А	7	DT	C5-C7	5.01	1.53	1.50

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	22	DG	N7-C8-N9	9.11	117.66	113.10
1	В	14	DG	N7-C8-N9	9.09	117.64	113.10
1	А	2	DG	N7-C8-N9	9.05	117.63	113.10
1	В	16	DG	N7-C8-N9	9.05	117.62	113.10
1	А	4	DG	N7-C8-N9	9.03	117.62	113.10
1	А	10	DG	N7-C8-N9	8.97	117.58	113.10
1	А	12	DG	N7-C8-N9	8.95	117.58	113.10
1	В	24	DG	N7-C8-N9	8.88	117.54	113.10
1	А	6	DA	N7-C8-N9	7.76	117.68	113.80
1	В	18	DA	N7-C8-N9	7.64	117.62	113.80
1	В	17	DA	N7-C8-N9	7.63	117.61	113.80
1	А	5	DA	N7-C8-N9	7.56	117.58	113.80
1	А	12	DG	C8-N9-C4	-6.94	103.62	106.40
1	В	22	DG	C8-N9-C4	-6.84	103.66	106.40
1	В	24	DG	C8-N9-C4	-6.57	103.77	106.40
1	А	10	DG	C8-N9-C4	-6.56	103.78	106.40

All angle outliers are listed below. They are sorted according to the Z-score.

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	14	DG	C8-N9-C4	-6.55	103.78	106.40
1	В	16	DG	C8-N9-C4	-6.54	103.79	106.40
1	А	2	DG	C8-N9-C4	-6.53	103.79	106.40
1	А	4	DG	C8-N9-C4	-6.46	103.81	106.40
1	В	17	DA	C8-N9-C4	-5.77	103.49	105.80
1	В	19	DT	C6-C5-C7	-5.74	119.45	122.90
1	А	6	DA	C8-N9-C4	-5.69	103.52	105.80
1	А	5	DA	C8-N9-C4	-5.67	103.53	105.80
1	А	7	DT	C6-C5-C7	-5.65	119.51	122.90
1	В	18	DA	C8-N9-C4	-5.58	103.57	105.80
1	А	8	DT	C6-C5-C7	-5.53	119.58	122.90
1	А	2	DG	C5-N7-C8	-5.42	101.59	104.30
1	В	16	DG	C5-N7-C8	-5.39	101.60	104.30
1	В	20	DT	C6-C5-C7	-5.38	119.67	122.90
1	В	14	DG	C5-N7-C8	-5.35	101.63	104.30
1	А	4	DG	C5-N7-C8	-5.32	101.64	104.30
1	В	19	DT	C4-C5-C6	5.26	121.15	118.00
1	В	22	DG	C5-N7-C8	-5.24	101.68	104.30
1	А	8	DT	C4-C5-C6	5.18	121.11	118.00
1	А	10	DG	C5-N7-C8	-5.14	101.73	104.30
1	В	20	DT	C4-C5-C6	5.13	121.08	118.00
1	А	7	DT	C4-C5-C6	5.13	121.08	118.00
1	В	24	DG	C5-N7-C8	-5.10	101.75	104.30
1	А	12	DG	C5-N7-C8	-5.08	101.76	104.30

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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	А	243	135	136	3
1	В	243	136	136	4
All	All	504	287	284	5

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.

Atom-1	Atom-2	$\operatorname{Clash}(\operatorname{\AA})$	Distance(Å)
1:A:12:DG:C2	1:B:14:DG:C2	0.54	2.96
1:B:16:DG:H2"	1:B:17:DA:OP2	0.52	2.05
1:A:4:DG:H2"	1:A:5:DA:OP2	0.46	2.10
1:A:2:DG:C2	1:B:24:DG:C2	0.42	3.07
1:B:20:DT:H2"	1:B:21:DC:O5'	0.41	2.15

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

### 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)

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)

2 ligands are 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	Trune	Chain	Dec	Link	Bond lengths			
	rybe	Chain	nes		Counts	RMSZ	#Z>2	
2	BDR	А	25	-	9,9,10	0.48	0 (0%)	
2	BDR	В	26	-	9,9,10	0.49	0 (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	Turne	Chain	Res Link		B	ond ang	les
10101	туре	Chain	nes	LINK	Counts	RMSZ	#Z>2
2	BDR	А	25	-	10,12,14	2.12	2 (20%)
2	BDR	В	26	-	10,12,14	2.13	2 (20%)

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	BDR	А	25	-	-	0,2,15,18	$0,\!1,\!1,\!1$
2	BDR	В	26	-	-	0,2,15,18	$0,\!1,\!1,\!1$

There are no bond-length outliers.

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	26	BDR	O4-C4-C3	5.44	109.52	104.70
2	А	25	BDR	O4-C4-C3	5.39	109.47	104.70
2	А	25	BDR	C5-C4-C3	3.87	105.76	115.09
2	В	26	BDR	C5-C4-C3	3.83	105.84	115.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



### 6.7 Other polymers (i)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	В	1
1	А	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	В	20:DT	O3'	21:DC	Р	3.93
1	А	8:DT	O3'	9:DC	Р	3.92



# 7 Chemical shift validation (i)

No chemical shift data were provided

