

# wwPDB NMR Structure Validation Summary Report (i)

#### Feb 12, 2022 – 04:47 PM EST

PDB ID	:	1FYI
Title	:	11-MER DNA DUPLEX CONTAINING A 2'-DEOXYARISTEROMYCIN
		8-OXO-GUANINE BASE PAIR;
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Deposited on	:	2000-09-30

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 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)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.26

Clashscore

# 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.

Metric	Percentile Ranks	Value
Clashscore		22
I	Vorse	Better
I	Percentile relative to all structures	
Γ	Percentile relative to all NMR structures	
Motric	Whole archiveNMR archive	

(# Entries)

158937

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%

(#Entries)

12864

Mol	Chain	Length	Quality of chain				
1	А	11	36%	64%			
2	В	11	64%	36%			



## 2 Ensemble composition and analysis (i)

This entry contains 9 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.



#### $1 \mathrm{FYI}$

## 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 700 atoms, of which 252 are hydrogens and 0 are deuteriums.

• Molecule 1 is a DNA chain called 5'-D(\*CP\*AP\*GP\*TP\*GP\*(2AR)P\*GP\*TP\*CP\*AP\*C) -3'.

Mol	Chain	Residues	Atoms						Trace
1	٨	11	Total	С	Н	Ν	0	Р	0
	1 A	11	350	108	127	43	62	10	0

• Molecule 2 is a DNA chain called 5'-D(\*GP\*TP\*GP\*AP\*CP\*(8OG)P\*CP\*AP\*CP\*TP\*G) -3'.

Mol	Chain	Residues		Trace					
0	D	11	Total	С	Η	Ν	Ο	Р	0
	D		350	107	125	43	65	10	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.

• Molecule 1: 5'-D(\*CP\*AP\*GP\*TP\*GP\*(2AR)P\*GP\*TP\*CP\*AP\*C)-3'

Chain A:	36%	64%					
C1 A2 G3 G5 G5 G5 G1 C9 C1 C9 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	4						
• Molecule 2: 5'-D(*GP*TP*GP*AP*CP*(8OG)P*CP*AP*CP*TP*G)-3'							
Chain B:	64%	36%					
G12 G12 G14 G14 G14 C16 G17 C18 C18 C20 C20 C20 C20	4 4 5 5						

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

The representative model is number 4. Colouring as in section 4.1 above.

• Molecule 1: 5'-D(\*CP\*AP\*GP\*TP\*GP\*(2AR)P\*GP\*TP\*CP\*AP\*C)-3'

Chain A:	27%	73%
C1 A2 G3 G5 G5 G5 G5 G5 G7 C1 A10 C11		
• Molecule 2: 5'-	-D(*GP*TP*GP*AP*CP*(8OG)	P*CP*AP*CP*TP*G)-3'
Chain B:	73%	27%
612 713 614 614 617 617 617 719 721 721 721 721		



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

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

Of the 15 calculated structures, 9 were deposited, based on the following criterion: target function.

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

Software name	Classification	Version
X-PLOR	refinement	3.8

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: 8OG,  $2\mathrm{AR}$ 

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		B	ond lengths	Bond angles		
	Unam	RMSZ	$\#Z{>}5$	RMSZ	#Z>5	
1	А	$1.26 {\pm} 0.01$	$2{\pm}1/225$ ( $0.9{\pm}$ $0.3\%)$	$2.23 \pm 0.00$	$16{\pm}1/343~(~4.7{\pm}~0.3\%)$	
2	В	$1.26 {\pm} 0.07$	$2{\pm}1/225~(~0.8{\pm}~0.3\%)$	$2.29 \pm 0.12$	$18{\pm}1/343~(~5.3{\pm}~0.3\%)$	
All	All	1.26	34/4050 ( $0.8%$ )	2.27	309/6174~(~5.0%)	

5 of 6 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Turne	Atoma	Z	Observed(Å)	Ideal(Å)	Models	
	Unam	nes	Type	Atoms		Observed(A)	Ideal(A)	Worst	Total
2	В	13	DT	O3'-P	11.34	1.74	1.61	5	1
2	В	13	DT	C5-C7	5.35	1.53	1.50	8	9
1	А	8	DT	C5-C7	5.30	1.53	1.50	2	8
1	А	4	DT	C5-C7	5.25	1.53	1.50	2	5
1	А	3	DG	N9-C8	-5.21	1.34	1.37	1	5

5 of 41 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(°)	$Ideal(^{o})$	Moo	dels
MOI	Ullalli	nes	туре	Atoms	Z Observed()		Iueai()	Worst	Total
2	В	13	DT	OP1-P-O3'	-18.55	64.40	105.20	5	1
2	В	13	DT	OP2-P-O3'	-12.50	77.69	105.20	5	1
2	В	13	DT	O3'-P-O5'	-11.94	81.32	104.00	5	1
1	А	7	DG	N7-C8-N9	9.88	118.04	113.10	3	9
1	А	3	DG	N7-C8-N9	9.74	117.97	113.10	1	9

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	223	127	127	$14 \pm 3$
2	В	225	125	125	$9{\pm}4$
All	All	4032	2268	2268	140

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 22.

5 of 56 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:11:DC:C2	2:B:12:DG:N2	1.12	2.16	9	2	
1:A:11:DC:N4	2:B:12:DG:C6	1.09	2.20	9	2	
1:A:11:DC:N3	2:B:12:DG:C2	1.03	2.26	9	3	
1:A:11:DC:N3	2:B:12:DG:N1	1.02	2.06	9	3	
1:A:11:DC:C4	2:B:12:DG:N1	1.01	2.28	9	2	

#### 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)

2 non-standard protein/DNA/RNA residues 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	Tinle		Bond len	$\mathbf{gths}$
	туре	Chain	nes	LIIIK	Counts	RMSZ	#Z>2
1	2AR	А	6	1	16,23,24	$0.90{\pm}0.01$	$1\pm0~(6\pm0\%)$
2	80G	В	17	2	18,25,26	$1.90{\pm}0.01$	$2\pm0$ (12 $\pm2\%$ )

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	Trune	Chain	Dec	Timle		Bond ang	gles
10101	туре	Chain	nes	LIIIK	Counts	RMSZ	#Z>2
1	2AR	А	6	1	14,33,36	$1.08 {\pm} 0.01$	$0\pm0~(0\pm2\%)$
2	80G	В	17	2	21,37,40	$2.79 \pm 0.01$	6±0 (28±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	80G	В	17	2	-	$0\pm 0,3,21,22$	$0\pm 0,3,3,3$
1	2AR	А	6	1	-	$0\pm0,3,21,22$	$0\pm 0,3,3,3$

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

Mal	Chain	Dec	Turne	Atoms	Z	Observed(Å)	Ideal(Å)	Moo	dels
	Unam	nes	туре	Atoms		Observed(A)	Iueai(A)	Worst	Total
2	В	17	80G	C8-N7	6.77	1.26	1.34	8	9
2	В	17	80G	C6-N1	3.80	1.39	1.33	8	9
1	А	6	2AR	C8-N7	3.00	1.29	1.34	5	9
2	В	17	80G	C2-N1	2.08	1.39	1.35	7	2



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Mod	dels
	Ullalli		I nes	Type	ype Atoms			Ideal()	Worst
2	В	17	80G	C5-C6-N1	9.01	111.11	123.43	8	9
2	В	17	80G	C2-N1-C6	5.95	125.38	115.93	1	9
2	В	17	80G	C2'-C1'-N9	4.05	111.59	116.01	9	9
2	В	17	80G	C2-N3-C4	3.00	111.93	115.36	7	9
2	В	17	80G	C1'-N9-C4	2.73	132.07	126.99	7	9

5 of 7 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

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)

No chemical shift data were provided

