

# Full wwPDB NMR Structure Validation Report (i)

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PDB ID : 5L06

Title: Solution Structure of a DNA Dodecamer with 5-methylcytosine at the 3rd

Position

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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 following versions of software and data (see references (1)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)

NmrClust : Kelley et al. (1996)

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 : 2.11

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

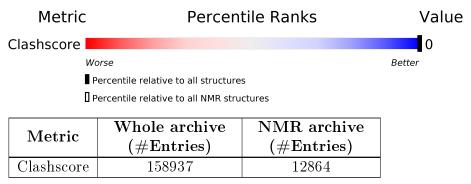
Validation Pipeline (wwPDB-VP) : 2.11

# 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 35%.

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	12	25%	75%	
1	В	12	33%	67%	



# 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.



# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 764 atoms, of which 276 are hydrogens and 0 are deuteriums.

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

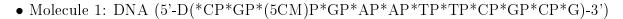
Mol	Chain	Residues		Atoms					Trace	
1	Λ	19	Total	С	Н	N	О	Р	0	
1	A	12	382	117	138	46	70	11		
1	1 B	B 12	12 Tota	Total	С	Н	N	О	Р	0
1			12	382	117	138	46	70	11	U

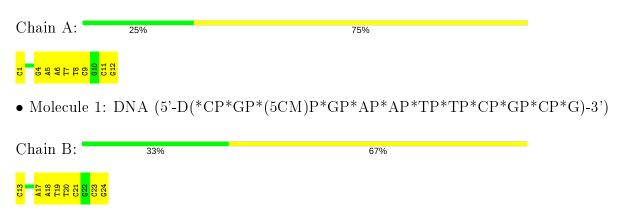


# 4 Residue-property plots (i)

## 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.



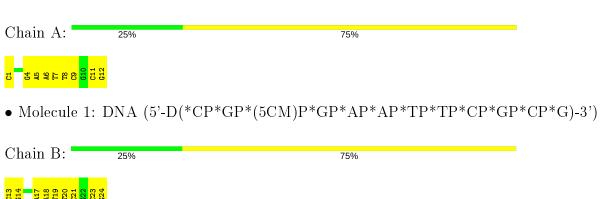


## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

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





#### 4.2.2 Score per residue for model 2

 $\bullet \ \, \text{Molecule 1: DNA (5'-D(*CP*GP*(5CM)P*GP*AP*AP*TP*TP*CP*GP*CP*G)-3')}$ 

Chain A: 25% 75%

C1 G2 A5 A6 T7 T7 T7 C9 C9 C11

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

Chain B: 25% 75%

C13 G14 A17 A18 T19 C21 C21 C23 C23

#### 4.2.3 Score per residue for model 3

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

Chain A: 25% 75%

C1 G2 A5 A6 A6 C9 C9 C11 C11

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

Chain B: 25% 75%

C13 G14 A17 A18 T19 T20 C21 C23 G24

#### 4.2.4 Score per residue for model 4

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

Chain A: 42% 58%

C1
A5
A6
A6
T7
T7
T8
C9
C11
C11

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

Chain B: 25% 75%

C13 G16 A17 A18 T19 T20 C21 C21 C23 G22



#### 4.2.5 Score per residue for model 5

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

Chain A: 25% 75%

C1
G4
A5
A6
T7
T7
C9
C9
C11
G12

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

Chain B: 25% 75%

C13 G16 A17 A18 T19 C21 G22 C23 G22

#### 4.2.6 Score per residue for model 6

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

Chain A: 17% 83%

G1 644 A6 A6 A6 C9 C9 C11 C11

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

Chain B: 17% 83%

C13 A17 A17 T19 C21 C23 C23

#### 4.2.7 Score per residue for model 7

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

Chain A: 25% 75%

C1 A5 A6 A6 A6 C9 C9 C11 C11

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

Chain B: 33% 67%

C13
A17
A18
T19
T20
C21
G22
C23
G24



#### 4.2.8 Score per residue for model 8

• Molecule 1: DNA (5'-D(\*CP\*GP\*(5CM)P\*GP\*AP\*AP\*TP\*TP\*CP\*GP\*CP\*G)-3')
Chain A: 25% 75%

C1 G4 A5 A6 T7 T7 T8 C9 C9 C11 G12

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

Chain B: 33% 67%

C13 A17 A18 T20 C21 C21 C23 G24

### 4.2.9 Score per residue for model 9

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

Chain A: 33% 67%

C1 A5 A6 A6 T7 T7 C9 C9 C11 C11

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

Chain B: 33% 67%

C13 A17 A18 T19 T20 C21 C23 C23



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



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

Of the 18 calculated structures, 9 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	refinement	12
Amber	structure calculation	12

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	$input\_cs.cif$
Number of chemical shift lists	2
Total number of shifts	192
Number of shifts mapped to atoms	192
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%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

#### 5.1Too-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.

$\mathbf{Mol}$	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes
All	All	4392	2484	2484	ı

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.



## 5.2 Torsion angles (i)

### 5.2.1 Protein backbone (i)

There are no protein molecules in this entry.

### 5.2.2 Protein sidechains (i)

There are no protein molecules in this entry.

### 5.2.3 RNA (i)

There are no RNA molecules in this entry.

## 5.3 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	Tuno	Chain	Pog	Bond lengths			$ ag{ths}$
WIOI	туре	Chain	nes	Link	Counts	RMSZ	#Z>2
1	5CM	В	15	1	15,21,22	$1.08 \pm 0.01$	0±0 (0±0%)
1	5CM	A	3	1	15,21,22	$1.07 \pm 0.01$	0±0 (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	Т	Chain	Dag	T in le	Bond angles		
MIOI	Type	Chain	nes	Link	Counts	RMSZ	#Z>2
1	5CM	В	15	1	19,30,33	$1.08 \pm 0.01$	0±0 (0±0%)
1	5CM	A	3	1	19,30,33	$1.07 \pm 0.01$	0±0 (0±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
1	5CM	A	3	1	-	$0\pm0,4,21,22$	$0 \pm 0,2,2,2$
1	5CM	В	15	1	-	$0\pm0,4,21,22$	$0\pm0,2,2,2$

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.4 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.5 Ligand geometry (i)

There are no ligands in this entry.

## 5.6 Other polymers (i)

There are no such molecules in this entry.

## 5.7 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Chemical shift validation (i)

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

#### 6.1 Chemical shift list 1

File name: input cs.cif

Chemical shift list name: DD04\_D2O.str

### 6.1.1 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	166
Number of shifts mapped to atoms	166
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

## 6.1.2 Chemical shift referencing (i)

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

## 6.1.3 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 31%, i.e. 136 atoms were assigned a chemical shift out of a possible 440. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Sidechain	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Aromatic	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Overall	136/440 (31%)	136/264~(52%)	0/146~(0%)	0/30 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 31%, i.e. 136 atoms were assigned a chemical shift out of a possible 440. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.



	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	0/0 (%)	0/0 (—%)	0/0 (%)	0/0 (%)
Sidechain	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Aromatic	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Overall	$136/440 \ (31\%)$	136/264~(52%)	0/146 (0%)	0/30 (0%)

### 6.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

### 6.1.5 Random Coil Index (RCI) plots (i)

No random coil index (RCI) plot could be generated from the current chemical shift list (DD04\_D2O.str). RCI is only applicable to proteins.

#### 6.2 Chemical shift list 2

File name: input\_cs.cif

Chemical shift list name: DD04 H2O.str

## 6.2.1 Bookkeeping (1)

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	26
Number of shifts mapped to atoms	26
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

## 6.2.2 Chemical shift referencing (i)

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

## 6.2.3 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 5%, i.e. 22 atoms were assigned a chemical



shift out of a possible 440. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}{ m H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Sidechain	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (%)	0/0 (%)
Overall	22/440 (5%)	22/264~(8%)	0/146~(0%)	0/30 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 5%, i.e. 22 atoms were assigned a chemical shift out of a possible 440. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (%)	0/0 (%)
Aromatic	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Overall	22/440 (5%)	22/264~(8%)	0/146 (0%)	0/30 (0%)

### 6.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

## 6.2.5 Random Coil Index (RCI) plots (i)

No random coil index (RCI) plot could be generated from the current chemical shift list (DD04\_H2O.str). RCI is only applicable to proteins.

