

# Full wwPDB NMR Structure Validation Report (i)

#### Feb 13, 2022 - 08:37 PM EST

PDB ID	:	1IEY
Title	:	SOLUTION STRUCTURE OF THE DNA DUPLEX D(CCACCGGAAC).
		(GTTCCGGTGG) WITH A CHIRAL ALKYL-PHOSPHONATE MOIETY
		(DIAESTEREOISOMER R)
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Deposited on	:	2001-04-11

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:

Percentile statistics RCI	: : :	$\begin{array}{l} 1.8.5 \ (274361), \ \mathrm{CSD} \ \mathrm{as541be} \ (2020) \\ 20191225.v01 \ (\mathrm{using \ entries \ in \ the \ PDB \ archive \ December \ 25th \ 2019)} \\ \mathrm{v\_1n\_11\_5\_13\_A} \ (\mathrm{Berjanski \ et \ al., \ 2005)} \end{array}$
PANAV	:	Wang et al. $(2010)$
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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
Cl	ashscore		0
		Worse	Better
		Percentile relative to all structures	
		Percentile relative to all NMR structures	
	Metrie	Whole archive NMR 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 seg-
ment 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	10	60'	%	20%	20%
2	В	10	30%	40%		30%



## 2 Ensemble composition and analysis (i)

This entry contains 10 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. 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 3 unique types of molecules in this entry. The entry contains 656 atoms, of which 244 are hydrogens and 0 are deuteriums.

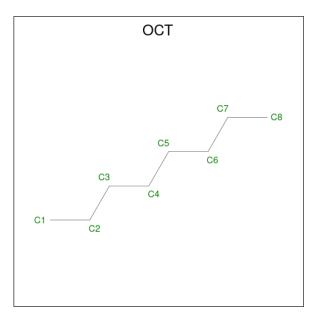
• Molecule 1 is a DNA chain called 5'-D(P\*CP\*CP\*AP\*CP\*CP\*(OCT)GP\*GP\*AP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms				Trace		
1	٨	10	Total	С	Н	Ν	0	Р	0
	A	10	311	95	112	40	54	10	0

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

Mol	Chain	Residues	Atoms				Trace		
2	D	10	Total	С	Н	Ν	0	Р	0
	D	10	320	98	115	37	61	9	0

• Molecule 3 is N-OCTANE (three-letter code: OCT) (formula:  $C_8H_{18}$ ).



N	lol	Chain	Residues	Atoms		
	2	٨	1	Total	С	Н
	3	А	1	25	8	17



# 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(P\*CP\*CP\*AP\*CP\*CP\*(OCT)GP\*GP\*AP\*AP\*C)-3'

Chain A:	60%		20%	20%		
C1 C5 C10 C10						
• Molecule 2: 5'-D(*GP*TP*TP*CP*CP*GP*GP*GP*GP*G)-3'						
Chain B:	30%	40%		30%		
G11 112 C14 C15 C15 C15 C15 C15 C19 C19 C19 C19 C20						

### 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

Chain A:	60%	20%	20%
C1 C4 C4 C10 C10			
• Molecule 2:	5'-D(*GP*TP*TP*CP*CP*	GP*GP*TP*GP*G	)-3'
Chain B:	30%	50%	20%



### 4.2.2 Score per residue for model 2

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

Chain A:	50%	30%	20%			
C1 A3 C4 C5 C5 C5 C5 C5 C5 C5 C10						
• Molecule 2: 5'-D(*GP*TP*TP*CP*CP*GP*GP*TP*GP*G)-3'						
Chain B: 30%		40%	30%			
611 112 113 113 014 015 016 017 017 019 019 019 020						

#### 4.2.3 Score per residue for model 3

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

Chain A:	50%	30%	20%
C1 C2 A3 G6 C10 C10			

• Molecule 2: 5'-D(\*GP\*TP\*TP\*CP\*CP\*GP\*GP\*TP\*GP\*G)-3'

Chain B:	30%	40%	30%
611 112 113 113 114 118 118 118 118 118 118 118 118 118			

#### 4.2.4 Score per residue for model 4

Chain A:	50%	30%	20%
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0			
• Molecule 2: 3	5'-D(*GP*TP*TP*CP*CP*	GP*GP*TP*GP*G	-3'





## 4.2.5 Score per residue for model 5

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

Chain A:	60%	20%	20%
C1 C4 C5 C5 C10 C10			
• Molecule 2:	5'-D(*GP*TP*TP*CP*CP*GP*G	P*TP*GP*G)	-3'
Chain B:	20% 60%		20%
611 112 113 113 113 113 616 116 118 118 118 619 619			

#### 4.2.6 Score per residue for model 6

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

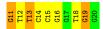
Chain A:	40%	50%	10%
C1 C2 C4 C5 C5 C5 C10 C10			

• Molecule 2: 5'-D(\*GP\*TP\*TP\*CP\*CP\*GP\*GP\*TP\*GP\*G)-3'

Chain B:	20%	70%	10%
611 112 112 113 113 113 113 115 115 116 118 118 118 118 118 118 118 118 118			

#### 4.2.7 Score per residue for model 7

Chain A:	40%	40%	20%		
C1 C5 C5 G6 G6 C10 C10					
• Molecule 2: 5'-D(*GP*TP*TP*CP*CP*GP*GP*GP*TP*GP*G)-3'					
Chain B:	20%	50%	30%		





## 4.2.8 Score per residue for model 8

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

Chain A:	50%	20%	30%
C1 C2 C5 C5 C5 C10			
• Molecule 2: 5'-I	D(*GP*TP*TP*CP*CF	P*GP*GP*TP*(	GP*G)-3'
Chain B: 10%	60%		30%
611 112 113 113 113 615 615 617 619 619 619			

#### 4.2.9 Score per residue for model 9

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

Chain A:	50%	30%	20%
C1 C5 G6 A8 A9 C10			

• Molecule 2: 5'-D(\*GP\*TP\*TP\*CP\*CP\*GP\*GP\*TP\*GP\*G)-3'

Chain B:	20%	60%	20%
611 112 113 113 113 113 114 118 116 117 118 118 118 118 118 118 118 118 118			

#### 4.2.10 Score per residue for model 10

Chain A:	20%	60%	20%
C1 C2 C2 C4 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5	010		
• Molecule 2	: 5'-D(*GI	P*TP*TP*CP*CP*GP*GP*TP*GP*	*G)-3'
Chain B:	20%	50%	30%
611 112 113 113 113 113 113 113 118 118 118 118			



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

The models were refined using the following method: *simulated, annealing molecular dynamics, matrix relaxation.* 

Of the 10 calculated structures, 10 were deposited, based on the following criterion:  $all \ calculated \ structures \ submitted.$ 

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

Software name	Classification	Version
Amber	refinement	5.0

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: OCT

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	
	Chain	RMSZ	#Z > 5	RMSZ	#Z>5
1	А	$8.25 \pm 21.08$	$0{\pm}0/223$ ( $0.0{\pm}$ $0.1\%)$	$1.96 {\pm} 0.18$	$7{\pm}1/339~(~1.9{\pm}~0.4\%)$
2	В	$1.36 {\pm} 0.03$	$0{\pm}0/229$ ( $0.0{\pm}$ $0.0\%)$	$1.99 {\pm} 0.03$	$8{\pm}2/353~(~2.2{\pm}~0.5\%)$
All	All	15.94	1/4511 ( $0.0%$ )	1.98	143/6911 ( $2.1%$ )

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	А	$0.0{\pm}0.0$	$1.9{\pm}0.3$
2	В	$0.0{\pm}0.0$	$4.1 \pm 0.8$
All	All	0	60

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$	Moo Worst	<b>lels</b> Total
1	А	1	DC	P-O5'	1067.34	12.27	1.59	1	1

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	Turne	Atoms	Z	Observed(°)	$Ideal(^{o})$	Mod	lels
	Unam	nes	Type	Atoms		Observed(*)	Ideal(*)	Worst	Total
1	А	1	DC	P-O5'-C5'	-30.33	72.37	120.90	1	1
1	А	6	DG	O4'-C1'-N9	9.09	114.36	108.00	3	5
2	В	18	DT	C6-C5-C7	-8.05	118.07	122.90	8	10
2	В	12	DT	C6-C5-C7	-7.92	118.14	122.90	9	10
2	В	13	DT	C6-C5-C7	-7.87	118.18	122.90	7	10
2	В	18	DT	O4'-C1'-N1	7.29	113.11	108.00	8	3

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Mol	Chain	Res	Turne	Atoms	Z	Observed(°)	$Ideal(^{o})$	Mod	lels
IVIOI	Unain	nes	Type	Atoms	L	Observed(*)	Ideal(*)	Worst	Total
2	В	11	DG	O4'-C1'-N9	7.05	112.94	108.00	6	9
1	А	5	DC	O4'-C1'-N1	6.83	112.78	108.00	10	5
1	А	6	DG	O4'-C4'-C3'	6.77	110.06	106.00	8	5
2	В	18	DT	P-O3'-C3'	6.73	127.77	119.70	4	1
2	В	13	DT	P-O3'-C3'	6.66	127.69	119.70	5	1
1	А	1	DC	O4'-C1'-N1	6.61	112.63	108.00	1	9
1	А	10	DC	O4'-C1'-N1	6.51	112.56	108.00	3	10
1	А	5	DC	O4'-C4'-C3'	6.32	109.79	106.00	10	6
1	А	8	DA	P-O3'-C3'	6.20	127.14	119.70	9	3
2	В	14	DC	P-O3'-C3'	6.17	127.11	119.70	7	1
1	А	4	DC	O4'-C1'-N1	5.97	112.18	108.00	1	5
1	А	1	DC	P-O3'-C3'	5.97	126.86	119.70	5	2
1	А	3	DA	P-O3'-C3'	5.92	126.80	119.70	6	3
2	В	11	DG	P-O3'-C3'	5.90	126.78	119.70	10	1
2	В	15	DC	O4'-C4'-C3'	5.85	109.51	106.00	8	8
2	В	16	DG	O4'-C1'-N9	5.72	112.01	108.00	9	6
1	А	2	DC	O4'-C4'-C3'	5.49	109.30	106.00	3	1
1	А	10	DC	N1-C2-O2	5.38	122.13	118.90	7	9
2	В	13	DT	O4'-C1'-N1	5.36	111.75	108.00	4	2
2	В	19	DG	O4'-C1'-N9	5.25	111.67	108.00	8	3
1	А	6	DG	P-O3'-C3'	5.24	125.99	119.70	7	1
2	В	16	DG	P-O3'-C3'	5.13	125.86	119.70	4	4
2	В	14	DC	O4'-C4'-C3'	5.13	109.08	106.00	8	3
1	А	9	DA	O4'-C4'-C3'	5.12	109.07	106.00	10	1
2	В	12	DT	C4-C5-C7	5.05	122.03	119.00	9	4
2	В	11	DG	N7-C8-N9	5.02	115.61	113.10	8	1

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There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	А	10	DC	Sidechain	10
2	В	13	DT	Sidechain	10
2	В	16	DG	Sidechain	10
2	В	19	DG	Sidechain	9
1	А	6	DG	Sidechain	8
2	В	11	DG	Sidechain	6
2	В	17	DG	Sidechain	5
1	А	9	DA	Sidechain	1
2	В	14	DC	Sidechain	1



### 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	198	112	112	$0\pm 0$
All	All	4111	2440	2439	3

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

Atom-1	Atom-2	$Clash(\lambda)$	Distance(Å)	Moo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:1:DC:H2"	1:A:2:DC:C6	0.40	2.51	10	3

### 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)

1 ligand 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.

Mol	Turne	Chain	Dec	Tiple		Bond leng	gths
	туре	Chain	nes	Link	Counts	RMSZ	#Z>2
3	OCT	А	11	1	7,7,7	$0.41 {\pm} 0.02$	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.

Mol	Type	Chain	Dog	Link		Bond ang	gles
	туре	Ullalli	nes	Link	Counts	RMSZ	#Z>2
3	OCT	А	11	1	6,6,6	$0.44{\pm}0.08$	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
3	OCT	А	11	1	-	$0\pm 0, 5, 5, 5$	-

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.



## 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

