

# Full wwPDB NMR Structure Validation Report (i)

### Feb 12, 2022 - 07:07 PM EST

PDB ID	:	1FV8
Title	:	NMR STUDY OF AN HETEROCHIRAL HAIRPIN
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Deposited on	:	2000-09-19

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:

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)	:	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	Percer	tile Ranks	Value		
C	Clashscore			8		
	Worse	2		Better		
	Perc	centile relative to all structures				
	Pero	centile relative to all NMR structures				
Γ	ъл . •	Whole archive	NMR archive	]		
	Metric	(# Entries)	(#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%

12864

Mol	Chain	Length	Quality of chain					
1	А	11	82%	9%	9%			



## 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 is only 1 type of molecule in this entry. The entry contains 348 atoms, of which 127 are hydrogens and 0 are deuteriums.

• Molecule 1 is a DNA chain called 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A) -3'.

Mol	Chain	Residues	Atoms						Trace
1	٨	11	Total	С	Η	Ν	Ο	Р	0
	A	11	348	108	127	39	64	10	0

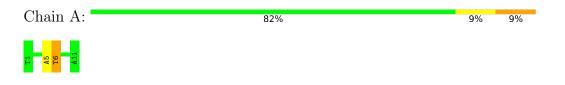


## 4 Residue-property plots (i)

## 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(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'

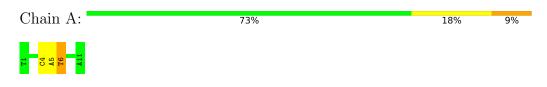


## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

### • Molecule 1: 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'



### 4.2.2 Score per residue for model 2

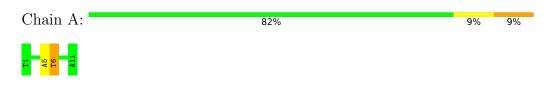
• Molecule 1: 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'





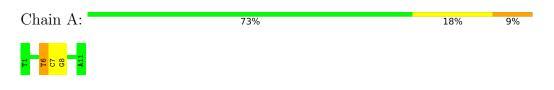
#### 4.2.3 Score per residue for model 3

• Molecule 1: 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'



#### 4.2.4 Score per residue for model 4

• Molecule 1: 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'

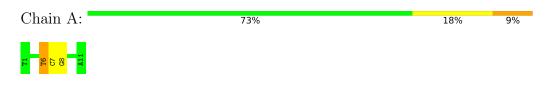


#### 4.2.5 Score per residue for model 5

• Molecule 1: 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'

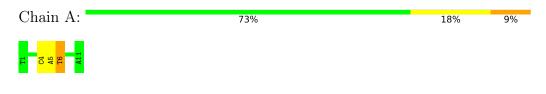
Chain A:	64%	27%	9%
T1 A2 A5 T6 A11			

- 4.2.6 Score per residue for model 6
- Molecule 1: 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'



#### 4.2.7 Score per residue for model 7

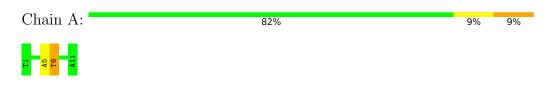
• Molecule 1: 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'





#### 4.2.8 Score per residue for model 8

• Molecule 1: 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'



#### 4.2.9 Score per residue for model 9

• Molecule 1: 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'

Chain A:	82%	9%	9%
ALL ALL			

#### 4.2.10 Score per residue for model 10

• Molecule 1: 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'

Chain A:	82%	9%	9%
AS A			

- 4.2.11 Score per residue for model 11
- Molecule 1: 5'-D(\*TP\*AP\*TP\*CP\*AP\*(0DT)P\*CP\*GP\*AP\*TP\*A)-3'





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

The models were refined using the following method: *simulated annealing, torsion angle dynamics.* 

Of the 50 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
CNS	structure solution	XPLOR 3.8
CNS	refinement	XPLOR 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:  $0\mathrm{DT}$ 

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	Sond lengths	Bond angles		
Moi Chain		RMSZ	$\#Z{>}5$	RMSZ	$\#Z{>}5$	
1	А	$0.55 {\pm} 0.95$	$2{\pm}5/224$ ( $0.8{\pm}$ $2.4\%$ )	$0.69 {\pm} 0.13$	$0{\pm}1/341~(~0.1{\pm}~0.2\%)$	
All	All	1.10	19/2464~(~0.8%)	0.71	2/3751~(~0.1%)	

All unique bond 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(Å)	Ideal(Å)	Mod	dels
	Ullalli	nes	Type	Atoms		Observeu(A)	Iueai(A)	Worst	Total
1	А	1	DT	O5'-C5'	-31.18	0.64	1.42	11	1
1	А	8	DG	P-O5'	-22.03	1.37	1.59	11	1
1	А	8	DG	P-OP2	-12.54	1.27	1.49	11	1
1	А	4	DC	P-O5'	-9.14	1.50	1.59	11	1
1	А	8	DG	O5'-C5'	-9.05	1.19	1.42	11	1
1	А	8	DG	P-OP1	-7.72	1.35	1.49	11	1
1	А	7	DC	C4-C5	-7.71	1.36	1.43	11	1
1	А	11	DA	O5'-C5'	-7.08	1.24	1.42	11	1
1	А	4	DC	C5'-C4'	-5.96	1.44	1.51	11	1
1	А	5	DA	P-O5'	-5.85	1.53	1.59	11	1
1	А	7	DC	N1-C2	-5.65	1.34	1.40	11	1
1	А	7	DC	C4'-C3'	-5.36	1.47	1.52	11	1
1	А	2	DA	P-O5'	-5.34	1.54	1.59	11	1
1	А	4	DC	P-OP2	-5.33	1.39	1.49	11	1
1	А	7	DC	C2'-C1'	-5.26	1.47	1.52	11	1
1	А	4	DC	C4'-C3'	-5.26	1.47	1.52	11	1
1	А	5	DA	P-OP1	-5.21	1.40	1.49	11	1
1	А	11	DA	P-O5'	-5.08	1.54	1.59	11	1
1	А	8	DG	C5'-C4'	-5.04	1.45	1.51	11	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	Dec	Trune	Atoma	ms	Z	7	7	7	Obconvod(0)	Ideal(°)	Models	
	Chain	$\operatorname{Res}$	Type	Atoms			Worst	Total					
1	А	1	DT	O5'-C5'-C4'	11.14	138.86	111.00	11	1				
1	А	8	DG	O5'-C5'-C4'	5.67	125.17	111.00	11	1				

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.

$\mathbf{M}$	ol	Chain	Non-H	H(model)	H(added)	Clashes
1	-	А	221	127	127	$3\pm 2$
A	11	All	2431	1397	1397	32

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Moo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:1:DT:O5'	1:A:1:DT:C4'	1.06	2.02	11	1
1:A:1:DT:O5'	1:A:1:DT:H5"	1.03	1.27	11	1
1:A:1:DT:O5'	1:A:1:DT:H5'	1.03	1.27	11	1
1:A:1:DT:O5'	1:A:1:DT:C5'	0.93	0.64	11	1
1:A:6:0DT:O5'	1:A:6:0DT:H6	0.72	1.84	1	5
1:A:5:DA:H2"	1:A:6:0DT:H71	0.63	1.71	8	7
1:A:4:DC:H2'	1:A:5:DA:C8	0.57	2.35	2	1
1:A:1:DT:C5'	1:A:1:DT:HO5'	0.51	1.21	11	1
1:A:7:DC:H2"	1:A:8:DG:O4'	0.51	2.06	4	2
1:A:6:0DT:H6	1:A:6:0DT:C5'	0.48	2.39	4	5
1:A:6:0DT:H6	1:A:6:0DT:O5'	0.45	2.11	10	1
1:A:5:DA:C2'	1:A:6:0DT:H71	0.44	2.41	3	1
1:A:2:DA:C2	1:A:11:DA:C2	0.43	3.07	5	1
1:A:7:DC:H2"	1:A:8:DG:O5'	0.43	2.14	2	1
1:A:4:DC:H2"	1:A:5:DA:C8	0.41	2.51	11	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)

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.

Mol	Type	Chain	Res	Link	Bond lengths			
					Counts	RMSZ	#Z>2	
1	0DT	А	6	1	15,21,22	$1.08 {\pm} 0.04$	$2\pm0$ (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	Type	Chain	Dog	Link		Bond ang	les
IVIOI	Type	Ullaill	nes		Counts	RMSZ	#Z>2
1	0DT	А	6	1	16,30,33	$3.68 \pm 0.04$	$1\pm0~(6\pm1\%)$

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	0DT	А	6	1	-	$0\pm0,4,21,22$	$0\pm 0,2,2,2$

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

Mol	Chain	Dog	Dec	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dog	Dec	Dec	Turna Atom	Atoms	7	Observed(Å)	Ideal(Å)	Models	
	Ullalli	nes	Type	Atoms		Observed(A)	Ideal(A)	Worst	Total																						
1	А	6	0DT	C4-N3	3.01	1.38	1.33	6	11																						
1	А	6	0DT	C6-C5	2.37	1.33	1.40	11	9																						

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

Mol	Chain	n Res Type	Tuna		7	$Observed(^{o})$		Models	
IVIOI			Type	Atoms	L	Observed(*)	$\mathrm{Ideal}(^{o})$	Worst	Total
1	А	6	0DT	C2-N3-C4	14.85	127.68	115.14	11	11
1	А	6	0DT	C5M-C5-C6	2.10	123.10	118.68	11	1

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

