



# wwPDB NMR Structure Validation Summary Report ⓘ

May 28, 2020 – 08:27 pm BST

PDB ID : 1SJL  
Title : A DUPLEX DNA WITH AN ABASIC SITE IN A DNA TRACT, BETA FORM,  
NMR, MINIMIZED AVERAGE STRUCTURE  
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Deposited on : 1997-07-22

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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



## 2 Ensemble composition and analysis

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 748 atoms, of which 270 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	12	380	117	135	51	66	11	0

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	12	368	112	135	37	73	11	0

## 4 Residue-property plots [i](#)


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.

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

Chain A: 

C1	C2	C3	A4	A5	A6	A7	A8	T9	G10	C11	G12
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- Molecule 2: DNA (5'-D(\*CP\*GP\*CP\*AP\*TP\*TP\*(AAB)P\*TP\*TP\*GP\*CP\*G)-3')

Chain B: 

C13	G14	C15	A16	T17	T18	T19	T20	T21	G22	C23	G24
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## 5 Refinement protocol and experimental data overview [i](#)

Of the 6 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	refinement	3.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 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	A	245	135	135	16
2	B	233	135	133	18
All	All	478	270	268	30

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 40.

5 of 30 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:22:DG:OP2	2:B:22:DG:P	1.49	1.09
2:B:22:DG:OP1	2:B:22:DG:P	1.46	1.08
1:A:1:DC:O5'	1:A:1:DC:C4'	1.21	1.86
1:A:1:DC:O5'	1:A:1:DC:H5'	0.96	1.19
1:A:1:DC:H5''	1:A:1:DC:O5'	0.95	1.19

### 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](#)

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
2	AAB	B	19	2	9,12,13	1.06	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	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	AAB	B	19	2	8,16,19	1.54	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
2	AAB	B	19	2	-	0,3,17,18	0,1,1,1

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

No chemical shift data were provided