



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:29 pm BST

PDB ID : 2KTT  
Title : Solution Structure of a Covalently Bound Pyrrolo[2,1-c][1,4]benzodiazepine-B  
enzimidazole Hybrid to a 10mer DNA Duplex  
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Deposited on : 2010-02-08

This is a Full wwPDB NMR Structure Validation 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)  
buster-report : 1.1.7 (2018)  
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 4 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.

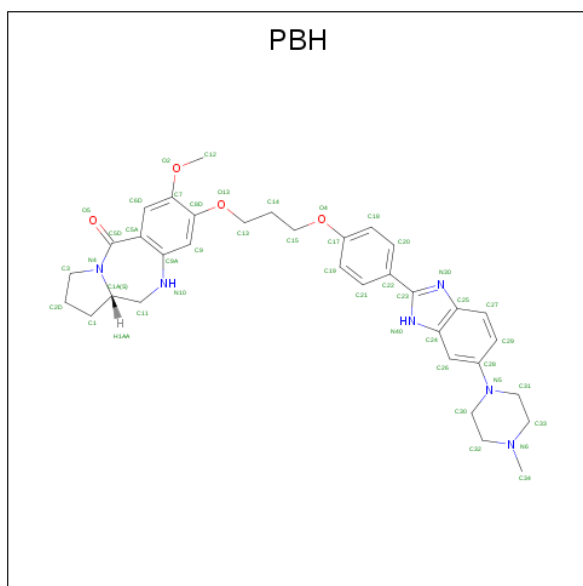
### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 718 atoms, of which 270 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(\*AP\*AP\*CP\*AP\*AP\*TP\*TP\*GP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
1	A	10	317	99	115	36	58	9	0
1	B	10	318	99	116	36	58	9	0

- Molecule 2 is (11aS)-7-methoxy-8-(3-{4-[6-(4-methylpiperazin-1-yl)-1H-benzimidazol-2-yl]phenoxy}propoxy)-1,2,3,10,11,11a-hexahydro-5H-pyrrolo[2,1-c][1,4]benzodiazepin-5-one (three-letter code: PBH) (formula: C<sub>34</sub>H<sub>40</sub>N<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	A	1	83	34	39	6	4

## 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.

- Molecule 1: 5'-D(\*AP\*AP\*CP\*AP\*AP\*TP\*TP\*GP\*TP\*T)-3'



- Molecule 1: 5'-D(\*AP\*AP\*CP\*AP\*AP\*TP\*TP\*GP\*TP\*T)-3'

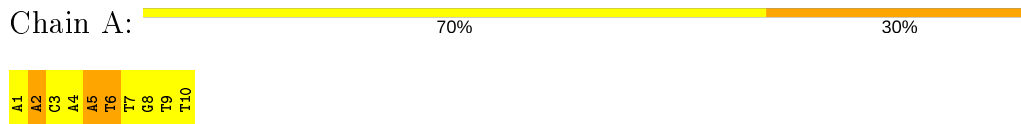


### 4.2 Scores per residue for each member of the ensemble

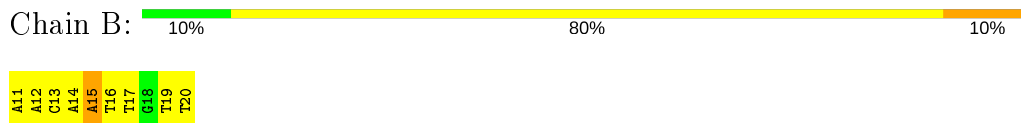
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: 5'-D(\*AP\*AP\*CP\*AP\*AP\*TP\*TP\*GP\*TP\*T)-3'



- Molecule 1: 5'-D(\*AP\*AP\*CP\*AP\*AP\*TP\*TP\*GP\*TP\*T)-3'



### 4.2.2 Score per residue for model 2

- Molecule 1: 5'-D(\*AP\*AP\*CP\*AP\*AP\*TP\*TP\*GP\*TP\*T)-3'



- Molecule 1: 5'-D(\*AP\*AP\*CP\*AP\*AP\*TP\*TP\*GP\*TP\*T)-3'



### 4.2.3 Score per residue for model 3

- Molecule 1: 5'-D(\*AP\*AP\*CP\*AP\*AP\*TP\*TP\*GP\*TP\*T)-3'

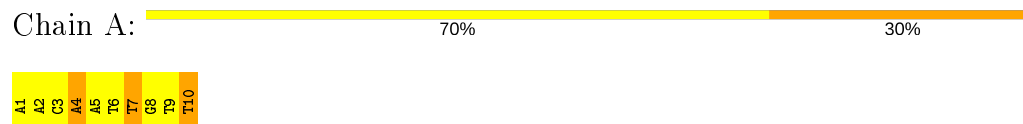


- Molecule 1: 5'-D(\*AP\*AP\*CP\*AP\*AP\*TP\*TP\*GP\*TP\*T)-3'

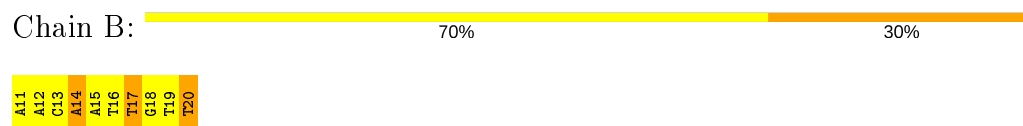


### 4.2.4 Score per residue for model 4

- Molecule 1: 5'-D(\*AP\*AP\*CP\*AP\*AP\*TP\*TP\*GP\*TP\*T)-3'



- Molecule 1: 5'-D(\*AP\*AP\*CP\*AP\*AP\*TP\*TP\*GP\*TP\*T)-3'



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

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

Of the 15000 calculated structures, 4 were deposited, based on the following criterion: *representative conformers of clusters*.

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

Software name	Classification	Version
AMBER	refinement	9

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

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### 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	B	202	116	114	0±1
2	A	44	39	39	0±1
All	All	1792	1080	1064	2

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:22:PBH:H34B	1:B:19:DT:H4'	0.45	1.87	3	1
2:A:22:PBH:H34B	1:B:19:DT:C4'	0.41	2.46	3	1

### 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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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### 5.5 Other polymers [i](#)

There are no such molecules in this entry.

### 5.6 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Chemical shift validation

No chemical shift data were provided