



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1PYJ
Title : Solution Structure of an O6-[4-oxo-4-(3-pyridyl)butyl]guanine adduct in an 11mer DNA duplex
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Deposited on : 2003-07-09

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 ⓘ symbol.

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

There are 2 unique types of molecules in this entry. The entry contains 715 atoms, of which 259 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
1	A	11	363	114	134	40	65	10	0

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

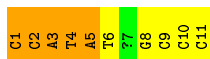
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
2	B	11	352	108	125	45	64	10	0

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.

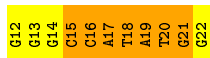
- Molecule 1: 5'-D(*CP*CP*AP*TP*AP*TP*GP*GP*CP*CP*C)-3'

Chain A: 



- Molecule 2: 5'-D*GP*GP*GP*CP*CP*AP*TP*AP*TP*GP*G)-3'

Chain B: 



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular mechanics in torsion angle space*.

Of the ? 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
DUPLEX	structure solution	
DUPLEX	refinement	

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	A	229	134	135	4
2	B	227	125	125	5
All	All	456	259	260	7

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:3:DA:C2	2:B:21:DG:C2	0.53	2.96
1:A:5:DA:C2	2:B:19:DA:C2	0.52	2.97
1:A:1:DC:C2	1:A:2:DC:C5	0.50	2.99
1:A:3:DA:C2	1:A:4:DT:C2	0.48	3.01
2:B:17:DA:C2	2:B:18:DT:C2	0.45	3.04
2:B:15:DC:C2	2:B:16:DC:C4	0.42	3.07
2:B:19:DA:C2	2:B:20:DT:C2	0.42	3.08

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.

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5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 Ligand geometry [i](#)

There are no ligands in this entry.

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