

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1GIP
Title	:	THE NMR STRUCTURE OF DNA DODECAMER DETERMINED IN
		AQUEOUS DILUTE LIQUID CRYSTALLINE PHASE
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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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
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	:	2.29
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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.

There are no overall percentile quality scores available for this entry.

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%

Mol	Chain	Length	Quality of chain
1	А	12	100%
1	В	12	100%



2 Ensemble composition and analysis (i)

This entry contains 2 models. Identification of well-defined residues and clustering analysis are not possible.



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 758 atoms, of which 272 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms				Trace		
1	Δ	12	Total	С	Η	Ν	Ο	Р	0
	12	379	116	136	46	70	11	0	
1	р	12	Total	С	Η	Ν	Ο	Р	0
	12	379	116	136	46	70	11	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(*CP*GP*CP*GP*AP*AP*TP*TP*CP*GP*CP*G)-3'

Chain A:	100%
C1 C2 C3 C3 C3 C3 C3 C3 C1 C11 C11 C11 C11 C1	
• Molecule 1: 5'-	D(*CP*GP*CP*GP*AP*AP*TP*TP*CP*GP*CP*G)-3'
Chain B:	100%
113 114 115 115 119 119 122 122 122 122 122	

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(*CP*GP*CP*GP*AP*AP*TP*TP*CP*GP*CP*G)-3'

 Chain A:
 100%

 58555555
 •

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

 Chain B:
 100%

 5555555555



4.2.2 Score per residue for model 2

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

Chain A:

100%

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

Chain B:

100%

C13 C15 C15 C15 C15 A17 A17 A18 T19 C21 C21 C21 C21 C23 C23 C23



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: SIMULATED ANNEALING IN TORSION ANGLE SPACE USING A SIXTH ORDER PREDICTOR-CORRECTOR METHOD WITH AU-TOMATIC TIME STEP SELECTION (C. SCHWIETERS AND G.M. CLORE).

Of the 40 calculated structures, 2 were deposited, based on the following criterion: *THE RE-STRAINED REGULARIZED MEAN STRUCTURES*.

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

Software name	
NIH VERSION OF XPLOR (AVAILABLE TO ACADEMIC USERS BY ANONYMOUS FTP	AT PORTA
NMRPIPE 1.7	
XwinNMR	
PIPP/CAPP	

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	0	0	0	-

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is -.

There are no clashes.

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)

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

