

wwPDB NMR Structure Validation Summary Report (i)

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PDB ID : 1EMQ

Title : NMR OBSERVATION OF T-TETRADS IN A PARALLEL STRANDED

DNA QUADRUPLEX FORMED BY SACCHAROMYCES CEREVISIAE

TELOMERE REPEATS

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This is a wwPDB NMR Structure Validation Summary 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 (i)) 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	A	7	100%		
1	В	7	100%		
1	С	7	100%		
1	D	7	100%		



2 Ensemble composition and analysis (i)

This entry contains 1 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 900 atoms, of which 324 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms				Trace		
1	A	7	Total	С	Н	N	О	Р	0
			225	69	81	27	42	6	
1	В	7	Total	С	Н	N	О	Р	0
			225	69	81	27	42	6	0
1	С	7	Total	С	Н	N	О	Р	0
			225	69	81	27	42	6	
1	D	D 7	Total	С	Н	N	О	Р	0
			225	69	81	27	42	6	



4 Residue-property plots (i)

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: DNA (5'-D(*TP*GP*C	GP*TP*GP*GP*C)-3')
Chain A:	100%
1101 6103 6103 6105 6106 6106	
• Molecule 1: DNA (5'-D(*TP*GP*C	GP*TP*GP*GP*C)-3')
Chain B:	100%
1201 6202 6203 1204 6205 6206 6206	
• Molecule 1: DNA (5'-D(*TP*GP*C	GP*TP*GP*GP*C)-3')
Chain C:	100%
7401 6403 6403 7405 6405 6406 6406	
• Molecule 1: DNA (5'-D(*TP*GP*C	GP*TP*GP*GP*C)-3')
Chain D:	100%
1301 63302 7303 63305 63305 63306 63307	



5 Refinement protocol and experimental data overview (i)



The models were refined using the following method: An initial model of quadruplex was generated on a IRIS workastation. Energy minimization by steepest descent followed by conjugate gradients methods was done using AMBER force field. Conformational search for the equadruplex was performed by simulated annealing-reastarined molecular dynamics using AMBER forcefield. Relaxation matrix refinement was performed...

Of the 8 calculated structures, 1 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	
Discover	structure solution	3.1	
IRMA	refinement	2.3	

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 clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore 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

