



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1EMQ
Title : NMR OBSERVATION OF T-TETRADES IN A PARALLEL STRANDED
DNA QUADRUPLEX FORMED BY SACCHAROMYCES CEREVISIAE
TELOMERE REPEATS
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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
<http://wwpdb.org/validation/2016/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 : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

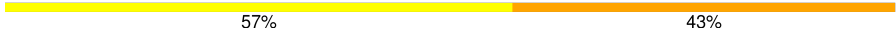
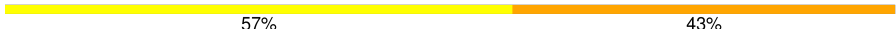
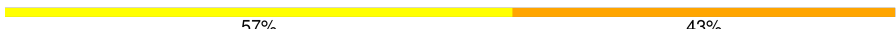

The overall completeness of chemical shifts assignment is 38%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain	
1	A	7		
1	B	7		
1	C	7		
1	D	7		

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 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	C	H	N	O	P	0
			225	69	81	27	42	6	
1	B	7	Total	C	H	N	O	P	0
			225	69	81	27	42	6	
1	C	7	Total	C	H	N	O	P	0
			225	69	81	27	42	6	
1	D	7	Total	C	H	N	O	P	0
			225	69	81	27	42	6	

4 Residue-property plots

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(*TP*GP*GP*TP*GP*GP*C)-3')

Chain A: 



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

Chain B: 




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

Chain C: 



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

Chain D: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *An initial model of quadruplex was generated on a IRIS workstation. Energy minimization by steepest descent followed by conjugate gradients methods was done using AMBER force field. Conformational search for the quadruplex was performed by simulated annealing-restrained 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

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 4609
Number of chemical shift lists	1
Total number of shifts	236
Number of shifts mapped to atoms	236
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.59	0/161 (0.0%)	2.55	16/248 (6.5%)
1	B	1.59	0/161 (0.0%)	2.45	13/248 (5.2%)
1	C	1.58	0/161 (0.0%)	2.53	15/248 (6.0%)
1	D	1.54	0/161 (0.0%)	2.47	11/248 (4.4%)
All	All	1.58	0/644 (0.0%)	2.50	55/992 (5.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	2
All	All	0	11

There are no bond-length outliers.

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	404	DT	C6-C5-C7	-8.64	117.72	122.90
1	D	304	DT	C6-C5-C7	-8.29	117.93	122.90
1	A	104	DT	C6-C5-C7	-8.23	117.96	122.90
1	D	301	DT	C6-C5-C7	-8.23	117.96	122.90
1	A	101	DT	C6-C5-C7	-7.79	118.23	122.90
1	C	401	DT	C6-C5-C7	-7.73	118.26	122.90
1	B	204	DT	C6-C5-C7	-7.72	118.27	122.90
1	B	201	DT	C6-C5-C7	-7.71	118.28	122.90
1	A	107	DC	N3-C4-N4	-7.69	112.62	118.00
1	B	207	DC	N3-C4-N4	-7.08	113.05	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	304	DT	O4'-C1'-C2'	-7.07	100.24	105.90
1	A	106	DG	N3-C2-N2	-7.03	114.98	119.90
1	C	404	DT	O4'-C1'-C2'	-7.02	100.28	105.90
1	A	104	DT	O4'-C1'-C2'	-6.78	100.47	105.90
1	B	204	DT	O4'-C1'-C2'	-6.61	100.61	105.90
1	C	407	DC	N3-C4-N4	-6.42	113.51	118.00
1	C	401	DT	N3-C2-O2	-6.07	118.66	122.30
1	C	404	DT	N1-C2-N3	6.01	118.21	114.60
1	D	304	DT	N1-C2-N3	5.98	118.19	114.60
1	B	204	DT	N1-C2-N3	5.96	118.17	114.60
1	A	106	DG	C5-C6-N1	5.90	114.45	111.50
1	A	104	DT	N1-C2-N3	5.87	118.12	114.60
1	C	406	DG	N3-C2-N2	-5.86	115.80	119.90
1	D	302	DG	C5-C6-N1	5.83	114.41	111.50
1	B	201	DT	O4'-C1'-N1	5.82	112.08	108.00
1	C	403	DG	C5-C6-N1	5.78	114.39	111.50
1	D	303	DG	C5-C6-N1	5.75	114.37	111.50
1	B	204	DT	N3-C2-O2	-5.74	118.86	122.30
1	A	102	DG	C5-C6-N1	5.73	114.36	111.50
1	C	404	DT	N3-C2-O2	-5.73	118.86	122.30
1	B	203	DG	C5-C6-N1	5.73	114.36	111.50
1	D	304	DT	N3-C2-O2	-5.72	118.86	122.30
1	B	202	DG	C5-C6-N1	5.69	114.35	111.50
1	B	205	DG	C5-C6-N1	5.67	114.33	111.50
1	B	201	DT	N3-C2-O2	-5.67	118.90	122.30
1	A	103	DG	C5-C6-N1	5.65	114.33	111.50
1	A	104	DT	N3-C2-O2	-5.65	118.91	122.30
1	A	105	DG	C5-C6-N1	5.65	114.33	111.50
1	C	401	DT	O4'-C4'-C3'	-5.62	102.25	104.50
1	C	402	DG	C5-C6-N1	5.61	114.30	111.50
1	D	305	DG	C5-C6-N1	5.56	114.28	111.50
1	B	205	DG	C8-N9-C4	-5.46	104.22	106.40
1	B	206	DG	C5-C6-N1	5.45	114.22	111.50
1	D	305	DG	C8-N9-C4	-5.44	104.22	106.40
1	A	105	DG	C8-N9-C4	-5.42	104.23	106.40
1	A	101	DT	N3-C2-O2	-5.38	119.07	122.30
1	A	101	DT	O4'-C1'-N1	5.37	111.76	108.00
1	C	406	DG	C5-C6-N1	5.37	114.18	111.50
1	C	405	DG	C8-N9-C4	-5.34	104.27	106.40
1	C	405	DG	C5-C6-N1	5.33	114.17	111.50
1	C	401	DT	N1-C2-N3	5.29	117.78	114.60
1	A	107	DC	N3-C4-C5	5.20	123.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	105	DG	N7-C8-N9	5.18	115.69	113.10
1	D	306	DG	C5-C6-N1	5.12	114.06	111.50
1	D	301	DT	N3-C2-O2	-5.11	119.23	122.30

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	C	406	DG	Sidechain
1	A	107	DC	Sidechain
1	D	302	DG	Sidechain
1	B	207	DC	Sidechain
1	A	102	DG	Sidechain
1	A	104	DT	Sidechain
1	B	202	DG	Sidechain
1	C	407	DC	Sidechain
1	B	204	DT	Sidechain
1	C	402	DG	Sidechain
1	D	304	DT	Sidechain

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	576	324	324	-

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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 38% for the well-defined parts and 38% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4609

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	236
Number of shifts mapped to atoms	236
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 38%, i.e. 212 atoms were assigned a chemical shift out of a possible 560. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	212/560 (38%)	212/336 (63%)	0/180 (0%)	0/44 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 38%, i.e. 212 atoms were assigned a chemical shift out of a possible 560. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	212/560 (38%)	212/336 (63%)	0/180 (0%)	0/44 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.