

Full wwPDB NMR Structure Validation Report (i)

May 29, 2020 - 07:33 am BST

PDB ID	:	5LQG
Title	:	A two-quartet G-quadruplex formed by human telomere in KCl solution at
		neutral pH
Authors	:	Galer, P.; Wang, B.; Sket, P.; Plavec, J.
Deposited on	:	2016-08-17

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

Cyrange	:	Kirchner and Güntert (2011)
$\operatorname{NmrClust}$:	Kelley et al. (1996)
$\operatorname{MolProbity}$:	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)
${ m ShiftChecker}$:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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	Perce	ntile Ranks	Value
Clashscore			0
	Worse		Better
	Percentile relative to all structu	res	
	Percentile relative to all NMR st	ructures	
			7
Ъ <i>Т</i> - 4 ² -	Whole archive	NMR archive	

Metric	$egin{array}{c} Whole \ { m archive} \ (\#{ m Entries}) \end{array}$	${f NMR} ext{ archive} \ (\# ext{Entries})$
Clashscore	158937	12864

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	22	9%	73%	18%



2 Ensemble composition and analysis (i)

This entry contains 10 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 is only 1 type of molecule in this entry. The entry contains 714 atoms, of which 251 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms				Trace		
1	Λ	22	Total	С	Η	Ν	Ο	Р	0
	A	22	714	220	251	89	133	21	0



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: DNA (5'-D(*TP*AP*GP*GP*GP*TP*TP*AP*GP*GP*GP*TP*TP*AP*GP*GP *GP*TP*TP*AP*GP*G)-3')

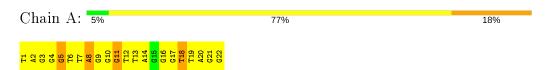
Chain A:	9%	73%	18%
11 42 63 17 17 69 69	C10 112 113 113 113 113 113 113 113 113 113		

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

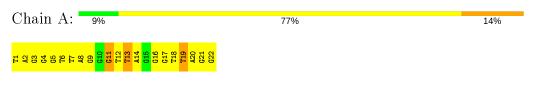
4.2.1 Score per residue for model 1

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



4.2.2 Score per residue for model 2

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





4.2.3 Score per residue for model 3

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

Chain A:	14%	73%	14%
11 A2 63 65 17 A8 A8	611 112 113 113 114 113 615 616 616 616 621 621 621		

4.2.4 Score per residue for model 4

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

Chain A:	9%	64%	27%
T1 A2 G3 G5 G5 T7	A8 60 61 712 712 713 713 713 713 713 713 713 713 713 713		

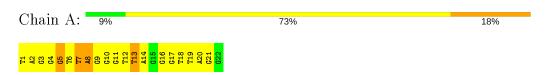
4.2.5 Score per residue for model 5

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

Chain A:	14%	77%	9%
11 63 17 17 65 71 75 71 75 71 75 75 75 75 75 75 75 75 75 75 75 75 75	A8 69 610 112 113 113 114	0115 0116 1118 1119 1119 021 022	

4.2.6 Score per residue for model 6

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



4.2.7 Score per residue for model 7

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



86%

5%

Chain A: 9%

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4.2.8 Score per residue for model 8

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

Chain A:	14%	55%	32%
<mark>년 1</mark> 2 2 2 2 2 2 1 1	A8 69 610 712 713 713 713 615 615	017 119 1138 120 021 022 022	

4.2.9 Score per residue for model 9

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

Chain A:	14%	64%	23%
11 63 17 17 17 17 17 17 17 17 17 17 17 17 17	A8 610 712 712 713 714 715 715 715 715 715 715 715 720 720 720 720		

4.2.10 Score per residue for model 10

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

Chain A:	9%	68%	23%
48 12 13 13 13 13 13 13 13 13 13 13 13 13 13	69 611 611 112 112 113 113 113 616 616 616 621 622 622		



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: simulated annealing.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
Amber	structure calculation	
Amber	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	182
Number of shifts mapped to atoms	182
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.

COVALENT-GEOMETRY INFOmissingINFO

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
All	All	4630	2510	2510	-

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.



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.

5.5 Ligand geometry (i)

There are no ligands in this entry.

5.6 Other polymers (i)

There are no such molecules in this entry.

5.7 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Chemical shift validation (i)

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

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: TD_chemical_shift_php.txt

6.1.1 Bookkeeping (i)

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	182
Number of shifts mapped to atoms	182
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

6.1.2 Chemical shift referencing (i)

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

6.1.3 Completeness of resonance assignments (i)

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. 165 atoms were assigned a chemical shift out of a possible 437. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
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	165/437~(38%)	165/261~(63%)	0/143~(0%)	0/33~(0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 38%, i.e. 165 atoms were assigned a chemical shift out of a possible 437. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.



	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
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	165/437~(38%)	165/261~(63%)	0/143~(0%)	0/33~(0%)

6.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

6.1.5 Random Coil Index (RCI) plots (1)

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

