wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2KKA
Title	:	Human telomere DNA two-tetrad quadruplex structure in K+ solution
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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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

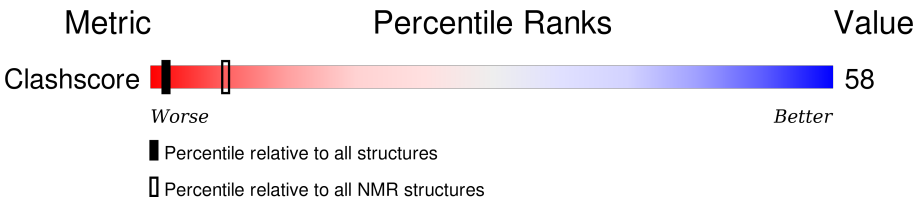
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 41%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	23	. 96%

2 Ensemble composition and analysis (i)

This entry contains 8 models. This entry does not contain protein, 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 745 atoms, of which 261 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(*AP*GP*GP*GP*TP*TP*AP*GP*GP*GP*TP*TP*AP*IP*GP*GP*TP*TP*AP*GP*GP*GP*T)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	23	745	230	261	93	139	22	0

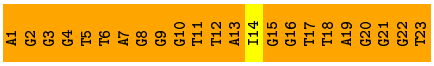
4 Residue-property plots (i)

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: 5'-D(*AP*GP*GP*GP*TP*TP*AP*GP*GP*GP*TP*TP*AP*IP*GP*GP*TP*TP*AP*GP*GP*GP*T)-3'

Chain A:

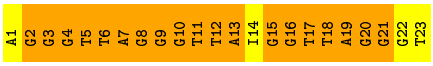


4.2 Residue scores for the representative (author defined) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

• Molecule 1: 5'-D(*AP*GP*GP*GP*TP*TP*AP*GP*GP*GP*TP*TP*AP*IP*GP*GP*TP*TP*AP*GP*GP*GP*T)-3'

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DGSA-distance geometry simulated annealing.*

Of the 100 calculated structures, 8 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
X-PLOR NIH	refinement	

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 16356
Number of chemical shift lists	1
Total number of shifts	210
Number of shifts mapped to atoms	201
Number of unparsed shifts	0
Number of shifts with mapping errors	9
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

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	1.28±0.01	3±1/520 (0.6±0.2%)	2.41±0.01	53±1/803 (6.6±0.2%)
All	All	1.28	26/4160 (0.6%)	2.41	421/6424 (6.6%)

5 of 8 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	6	DT	C5-C7	5.97	1.53	1.50	2	8
1	A	5	DT	C5-C7	5.37	1.53	1.50	5	2
1	A	18	DT	C5-C7	5.18	1.53	1.50	6	3
1	A	17	DT	C5-C7	5.16	1.53	1.50	6	3
1	A	11	DT	C5-C7	5.12	1.53	1.50	7	4

5 of 59 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	10	DG	N7-C8-N9	9.70	117.95	113.10	3	8
1	A	4	DG	N7-C8-N9	9.57	117.88	113.10	3	8
1	A	8	DG	N7-C8-N9	9.51	117.85	113.10	4	8
1	A	16	DG	N7-C8-N9	9.40	117.80	113.10	3	8
1	A	15	DG	N7-C8-N9	9.30	117.75	113.10	6	8

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
1	A	484	261	261	43±4
All	All	3872	2088	2088	344

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 58.

5 of 182 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:DI:H2"	1:A:14:DI:N3	0.86	1.83	6	3
1:A:20:DG:N3	1:A:20:DG:H5'	0.84	1.87	4	2
1:A:14:DI:H3'	1:A:14:DI:N3	0.80	1.92	8	2
1:A:14:DI:N3	1:A:14:DI:H2"	0.79	1.91	4	3
1:A:10:DG:H2"	1:A:11:DT:O5'	0.76	1.80	3	5

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 (i)

The completeness of assignment taking into account all chemical shift lists is 41% for the well-defined parts and 41% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16356

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 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	210
Number of shifts mapped to atoms	201
Number of unparsed shifts	0
Number of shifts with mapping errors	9
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. First 5 (of 9) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	14	INO	H2"	2.766	-1.0	1
A	14	INO	H5"	3.888	-1.0	1
A	14	INO	H2'	2.811	-1.0	1
A	14	INO	H1'	6.358	-1.0	1
A	14	INO	H4'	4.234	-1.0	1

7.1.2 Chemical shift referencing (i)

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

7.1.3 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 41%, i.e. 180 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}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	180/437 (41%)	180/261 (69%)	0/143 (0%)	0/33 (0%)

7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	12	DT	H2'	0.91	3.17 – 1.07	-5.8
1	A	8	DG	H8	6.59	8.85 – 6.75	-5.8
1	A	6	DT	H5"	2.97	5.01 – 3.01	-5.2
1	A	5	DT	H2"	1.41	3.34 – 1.44	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

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.