Full wwPDB NMR Structure Validation Report (i)

Aug 20, 2022 – 08:21 AM EDT

PDB ID	:	1D6D
Title	:	SOLUTION DNA STRUCTURE CONTAINING (A-A)-T TRIADS INTERDIGITATED BETWEEN A-T BASE PAIRS AND GGGG TETRADS; NMR, 8 STRUCT.
Authors	:	Kuryavyi, V.V.; Kettani, A.; Wang, W.; Jones, R.; Patel, D.J.
Deposited on	:	1999-10-13

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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Percentile statistics	:	FAILED
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	12	8% 92%
1	B	12	17% 83%

2 Ensemble composition and analysis (i)

This entry contains 8 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 774 atoms, of which 276 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	12	387	120	138	48	70	11	0
1	B	12	387	120	138	48	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(*AP*AP*GP*GP*TP*TP*TP*TP*AP*AP*GP*G)-3'

Chain A: 8% 92%

A1 A2 G3 G4 T5 T6 T7 T8 A9 A10 G11 G12

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

Chain B: 17% 83%

A1 A2 G3 G4 T5 T6 T7 T8 A9 A10 G11 G12

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

Chain A: 17% 83%

A1 A2 G3 G4 T5 T6 T7 T8 A9 A10 G11 G12

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

Chain B: 17% 83%

A1 A2 G3 G4 T5 T6 T7 T8 A9 A10 G11 G12

4.2.2 Score per residue for model 2

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

Chain A: 33% 67%

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

Chain B: 33% 67%

4.2.3 Score per residue for model 3

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

Chain A: 33% 67%

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

Chain B: 33% 67%

4.2.4 Score per residue for model 4

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

Chain A: 17% 83%

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

Chain B: 25% 75%

4.2.5 Score per residue for model 5

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

Chain A: 42% 58%

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

Chain B: 42% 58%

4.2.6 Score per residue for model 6

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

Chain A: 25% 75%

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

Chain B: 25% 75%

4.2.7 Score per residue for model 7

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

Chain A: 33% 67%

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

Chain B: 33% 67%

4.2.8 Score per residue for model 8

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

Chain A:

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

Chain B:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DISTANCE GEOMETRY AND SIMULATED ANNEALING, DISTANCE RESTRAINED MOLECULAR DYNAMICS REFINEMENT AND RELAXATION MATRIX INTENSITY REFINEMENT.*

Of the 100 calculated structures, 8 were deposited, based on the following criterion: *BACK CALCULATED DATA AGREE WITH EXPERIMENTAL NOESY SPECTRUM,STRUCTURES WITH ACCEPTABLE COVALENT GEOMETRY,STRUCTURES WITH FAVORABLE NON-BOND ENERGY, STRUCTURES WITH THE LEAST RESTRAINT VIOLATIONS,STRUCTURES WITH THE LOWEST ENERGY.*

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	3.1

No chemical shift data was provided.

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	1.39±0.02	3±1/280 (1.2± 0.4%)	2.40±0.01	30±3/432 (6.9± 0.6%)
1	B	1.40±0.02	3±1/280 (1.2± 0.4%)	2.40±0.01	30±2/432 (6.9± 0.4%)
All	All	1.39	53/4480 (1.2%)	2.40	479/6912 (6.9%)

All 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	B	7	DT	C5-C7	5.76	1.53	1.50	4	8
1	A	7	DT	C5-C7	5.71	1.53	1.50	3	8
1	B	11	DG	N9-C8	-5.48	1.34	1.37	7	2
1	B	5	DT	C5-C7	5.47	1.53	1.50	2	6
1	A	5	DT	C5-C7	5.42	1.53	1.50	2	7
1	B	8	DT	C5-C7	5.28	1.53	1.50	3	6
1	A	11	DG	N9-C8	-5.27	1.34	1.37	7	2
1	B	6	DT	C5-C7	5.26	1.53	1.50	4	4
1	A	6	DT	C5-C7	5.24	1.53	1.50	4	5
1	B	10	DA	C5'-C4'	5.20	1.57	1.51	8	1
1	A	8	DT	C5-C7	5.18	1.53	1.50	7	3
1	A	10	DA	C5'-C4'	5.16	1.57	1.51	8	1

All 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	B	11	DG	N7-C8-N9	10.51	118.36	113.10	7	8
1	A	11	DG	N7-C8-N9	10.46	118.33	113.10	7	8
1	A	4	DG	N7-C8-N9	9.71	117.96	113.10	8	8
1	B	4	DG	N7-C8-N9	9.69	117.94	113.10	1	8
1	B	3	DG	N7-C8-N9	9.54	117.87	113.10	7	8
1	A	3	DG	N7-C8-N9	9.51	117.86	113.10	7	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	12[*]	DG	N7-C8-N9	9.44	117.82	113.10	8	8
1	B	12[*]	DG	N7-C8-N9	9.35	117.78	113.10	8	8
1	B	5	DT	O4'-C1'-N1	8.81	114.17	108.00	2	6
1	A	5	DT	O4'-C1'-N1	8.80	114.16	108.00	2	6
1	A	10	DA	N7-C8-N9	8.62	118.11	113.80	6	8
1	B	10	DA	N7-C8-N9	8.57	118.09	113.80	6	8
1	B	9	DA	N7-C8-N9	8.54	118.07	113.80	6	8
1	A	9	DA	N7-C8-N9	8.47	118.04	113.80	6	8
1	B	1	DA	N7-C8-N9	8.39	117.99	113.80	1	8
1	A	1	DA	N7-C8-N9	8.31	117.95	113.80	1	8
1	B	12[*]	DG	C8-N9-C4	-7.78	103.29	106.40	5	8
1	A	12[*]	DG	C8-N9-C4	-7.57	103.37	106.40	5	8
1	A	2	DA	N7-C8-N9	7.52	117.56	113.80	8	8
1	A	11	DG	O4'-C1'-N9	7.52	113.26	108.00	5	4
1	B	11	DG	O4'-C1'-N9	7.49	113.24	108.00	5	4
1	B	2	DA	N7-C8-N9	7.48	117.54	113.80	6	8
1	A	11	DG	C8-N9-C4	-6.72	103.71	106.40	3	8
1	A	3	DG	C8-N9-C4	-6.71	103.72	106.40	2	8
1	B	3	DG	C8-N9-C4	-6.70	103.72	106.40	2	8
1	B	4	DG	C8-N9-C4	-6.65	103.74	106.40	1	8
1	A	4	DG	C8-N9-C4	-6.59	103.76	106.40	8	8
1	B	11	DG	C8-N9-C4	-6.46	103.81	106.40	3	8
1	B	8	DT	C6-C5-C7	-6.14	119.22	122.90	6	8
1	A	8	DT	C6-C5-C7	-6.08	119.25	122.90	6	8
1	B	2	DA	C8-N9-C4	-6.01	103.39	105.80	4	8
1	A	2	DA	C8-N9-C4	-5.98	103.41	105.80	4	8
1	B	4	DG	O4'-C1'-N9	5.97	112.18	108.00	1	3
1	B	10	DA	C5-N7-C8	-5.91	100.95	103.90	7	6
1	A	11	DG	C5-N7-C8	-5.90	101.35	104.30	4	8
1	A	4	DG	O4'-C1'-N9	5.87	112.11	108.00	1	3
1	B	4	DG	C5-N7-C8	-5.86	101.37	104.30	3	8
1	B	5	DT	C6-C5-C7	-5.86	119.39	122.90	1	8
1	A	2	DA	O4'-C1'-N9	5.83	112.08	108.00	7	2
1	B	2	DA	O4'-C1'-N9	5.83	112.08	108.00	7	2
1	A	10	DA	C5-N7-C8	-5.83	100.99	103.90	7	7
1	B	11	DG	C5-N7-C8	-5.83	101.39	104.30	2	8
1	B	6	DT	C6-C5-C7	-5.80	119.42	122.90	1	8
1	A	5	DT	C6-C5-C7	-5.80	119.42	122.90	1	8
1	A	7	DT	O4'-C1'-N1	5.78	112.05	108.00	7	5
1	A	6	DT	C6-C5-C7	-5.78	119.43	122.90	3	8
1	A	3	DG	C5-N7-C8	-5.74	101.43	104.30	7	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	4	DG	C5-N7-C8	-5.72	101.44	104.30	3	8
1	B	7	DT	O4'-C1'-N1	5.72	112.00	108.00	7	5
1	B	3	DG	C5-N7-C8	-5.66	101.47	104.30	7	6
1	B	6	DT	O4'-C1'-N1	5.63	111.94	108.00	8	2
1	A	6	DT	O4'-C1'-N1	5.60	111.92	108.00	8	2
1	A	8	DT	O4'-C1'-N1	5.55	111.89	108.00	7	5
1	B	8	DT	O4'-C1'-N1	5.53	111.87	108.00	7	5
1	A	1	DA	O4'-C1'-N9	5.51	111.86	108.00	3	5
1	B	9	DA	C5-N7-C8	-5.50	101.15	103.90	3	5
1	B	1	DA	O4'-C1'-N9	5.50	111.85	108.00	7	5
1	A	9	DA	C5-N7-C8	-5.49	101.15	103.90	3	4
1	B	12[*]	DG	C5-N7-C8	-5.45	101.57	104.30	2	8
1	A	7	DT	C6-C5-C7	-5.43	119.64	122.90	6	5
1	B	7	DT	C6-C5-C7	-5.42	119.65	122.90	8	5
1	A	12[*]	DG	C5-N7-C8	-5.39	101.61	104.30	8	7
1	B	8	DT	C4-C5-C6	5.36	121.22	118.00	6	8
1	B	10	DA	C8-N9-C4	-5.36	103.66	105.80	2	4
1	A	6	DT	C4-C5-C6	5.33	121.20	118.00	3	5
1	B	6	DT	C4-C5-C6	5.31	121.18	118.00	3	6
1	B	9	DA	C8-N9-C4	-5.29	103.69	105.80	6	2
1	A	10	DA	C8-N9-C4	-5.29	103.69	105.80	8	3
1	A	9	DA	C8-N9-C4	-5.28	103.69	105.80	6	2
1	A	1	DA	C8-N9-C4	-5.28	103.69	105.80	2	5
1	A	8	DT	C4-C5-C6	5.27	121.16	118.00	7	8
1	B	1	DA	C8-N9-C4	-5.25	103.70	105.80	2	4
1	A	3	DG	O4'-C1'-N9	5.21	111.65	108.00	1	2
1	B	3	DG	O4'-C1'-N9	5.18	111.63	108.00	1	2
1	A	5	DT	C4-C5-C6	5.18	121.11	118.00	6	4
1	A	9	DA	O4'-C1'-N9	5.16	111.61	108.00	7	2
1	B	5	DT	C4-C5-C6	5.16	121.09	118.00	3	3
1	B	9	DA	O4'-C1'-N9	5.14	111.60	108.00	7	2
1	B	2	DA	C5-N7-C8	-5.13	101.34	103.90	2	1
1	B	1	DA	C5-N7-C8	-5.13	101.34	103.90	6	2
1	A	1	DA	C5-N7-C8	-5.08	101.36	103.90	6	2
1	A	9	DA	N1-C2-N3	-5.06	126.77	129.30	1	1

There are no chirality outliers.

There are no planarity outliers.

CLOSE-CONTACTS INFOmissingINFO

6.2 Torsion angles (i)

6.2.1 Protein backbone (i)

There are no protein molecules in this entry.

6.2.2 Protein sidechains (i)

There are no protein molecules in this entry.

6.2.3 RNA (i)

There are no RNA molecules in this entry.

6.3 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.4 Carbohydrates (i)

There are no monosaccharides in this entry.

6.5 Ligand geometry (i)

There are no ligands in this entry.

6.6 Other polymers (i)

There are no such molecules in this entry.

6.7 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided