wwPDB NMR Structure Validation Summary Report (i)

Apr 26, 2016 – 03:57 PM BST

PDB ID	:	1N14
Title	:	Structure and Dynamics of Thioguanine-modified Duplex DNA in Comparison with Unmodified DNA; Structure of Unmodified Duplex DNA
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Deposited on	:	2002-10-16

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:

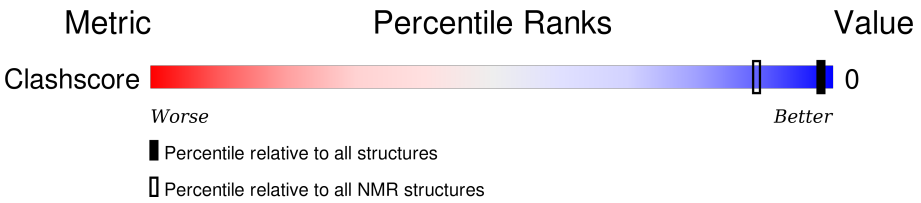
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 was not calculated.

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	13	38% 62%
2	B	13	15% 85%

2 Ensemble composition and analysis (i)

This entry contains 20 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 are 2 unique types of molecules in this entry. The entry contains 823 atoms, of which 296 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	13	413	127	146	56	72	12	0

- Molecule 2 is a DNA chain called 5'-D(*GP*GP*CP*TP*TP*TP*CP*CP*TP*TP*AP*GP*C)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	13	410	126	150	42	80	12	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(*GP*CP*TP*AP*AP*GP*GP*AP*AP*AP*GP*CP*C)-3'

Chain A:

- Molecule 2: 5'-D(*GP*GP*CP*TP*TP*TP*CP*CP*TP*TP*AP*GP*C)-3'

Chain B:

4.2 Residue scores for the first model from the NMR ensemble

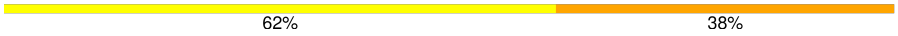
No representative models were identified. Colouring as in section 4.1 above.

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

Chain A:

- Molecule 2: 5'-D(*GP*GP*CP*TP*TP*TP*CP*CP*TP*TP*AP*GP*C)-3'

Chain B:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *restrained molecular dynamics, relaxation matrix analysis.*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *back calculated data agree with experimental NOESY spectrum.*

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

Software name	Classification	Version
X-PLOR	refinement	3.1

No chemical shift data was provided. 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	3.18±0.14	35±6/301 (11.7±1.9%)	4.25±0.20	93±7/463 (20.0±1.4%)
2	B	3.41±0.17	39±5/289 (13.6±1.6%)	4.07±0.18	86±8/444 (19.3±1.7%)
All	All	3.30	1493/11800 (12.7%)	4.17	3567/18140 (19.7%)

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	0.0±0.0	7.4±2.0
2	B	0.0±0.0	8.0±2.2
All	All	0	308

5 of 426 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
2	B	23	DT	P-O5'	16.85	1.76	1.59	14	6
2	B	19	DT	C5-C7	16.19	1.59	1.50	9	11
2	B	18	DT	C5-C7	15.81	1.59	1.50	5	9
1	A	4	DA	N7-C5	15.47	1.48	1.39	16	8
2	B	23	DT	C4'-O4'	-15.24	1.29	1.45	1	8

5 of 572 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	11	DG	O4'-C1'-N9	22.63	123.84	108.00	13	16
2	B	24	DA	N1-C6-N6	-22.61	105.04	118.60	19	19
1	A	4	DA	C4-C5-C6	-21.96	106.02	117.00	6	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	4	DA	C5-C6-N1	21.01	128.21	117.70	6	14
1	A	1	DG	O4'-C1'-N9	20.90	122.63	108.00	8	16

There are no chirality outliers.

5 of 26 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	11	DG	Sidechain	18
2	B	26	DC	Sidechain	17
2	B	25	DG	Sidechain	17
1	A	1	DG	Sidechain	16
1	A	13	DC	Sidechain	16

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	267	146	134	0±1
2	B	260	150	148	0±0
All	All	10540	5920	5660	8

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 0.

5 of 8 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:DG:N2	2:B:22:DT:C2	0.52	2.78	10	1
1:A:11:DG:C6	1:A:12:DC:C5	0.45	3.05	8	1
1:A:11:DG:C5	1:A:12:DC:C5	0.43	3.05	8	1
1:A:4:DA:C2	2:B:24:DA:C2	0.43	3.06	14	1
1:A:8:DA:C2	1:A:9:DA:C5	0.43	3.07	9	1

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)

No chemical shift data were provided