wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1JU0
Title	:	NMR solution structure of a DNA kissing complex
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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:

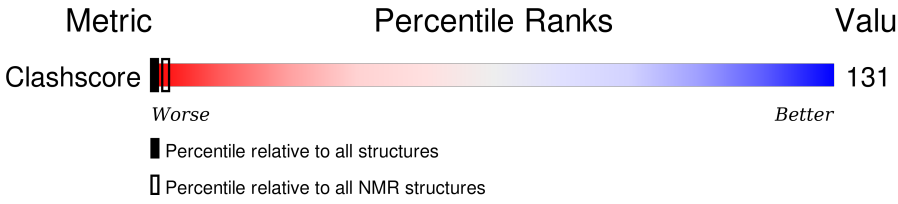
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal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

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	23	43% 35% 22%
1	B	23	39% 30% 30%

2 Ensemble composition and analysis (i)

This entry contains 16 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 1366 atoms, of which 424 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	23	Total	C	H	N	O	P	0
			683	223	212	92	134	22	
1	B	23	Total	C	H	N	O	P	0
			683	223	212	92	134	22	

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

Chain A:

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

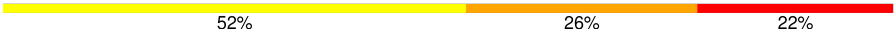
Chain B:

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

The representative model is number 5. Colouring as in section 4.1 above.

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

Chain A:



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

Chain B:


C1
T2
T3
G4
C5
T6
G7
A8
A9
G10
C11
G12
C13
G14
C15
A16
C17
G18
G19
C20
A21
A22
G23

5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing matrix relaxation chemical shift back calculation.*

Of the 16 calculated structures, 16 were deposited, based on the following criterion: *back calculated data agree with experimental NOESY spectrum, structures with acceptable covalent geometry, 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
CNS	structure solution	1.0
CNS	refinement	1.0

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

6.1 Standard geometry

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	1.34±0.02	6±1/529 (1.1±0.2%)	1.81±0.03	23±2/815 (2.9±0.2%)
1	B	1.32±0.01	5±1/529 (1.0±0.1%)	1.81±0.02	23±1/815 (2.9±0.2%)
All	All	1.33	175/16928 (1.0%)	1.81	748/26080 (2.9%)

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	6.1±0.9
1	B	0.0±0.0	6.9±0.9
All	All	0	209

5 of 15 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	12	DG	C2'-C1'	-6.71	1.45	1.52	14	16
1	A	12	DG	C2'-C1'	-6.71	1.45	1.52	14	16
1	A	12	DG	C2-N2	6.33	1.40	1.34	7	4
1	A	20	DC	C2'-C1'	-6.29	1.46	1.52	9	16
1	B	20	DC	C2'-C1'	-6.28	1.46	1.52	15	16

5 of 63 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	14	DG	O4'-C1'-N9	-11.50	99.95	108.00	1	16
1	A	14	DG	O4'-C1'-N9	-11.32	100.08	108.00	4	16
1	A	12	DG	N3-C2-N2	10.80	127.46	119.90	2	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	7	DG	O4'-C1'-N9	10.75	115.52	108.00	9	16
1	B	7	DG	O4'-C1'-N9	10.38	115.27	108.00	3	16

There are no chirality outliers.

5 of 18 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	B	13	DC	Sidechain	16
1	A	13	DC	Sidechain	16
1	A	12	DG	Sidechain	16
1	B	14	DG	Sidechain	16
1	B	12	DG	Sidechain	16

6.2 Too-close contacts

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	471	212	258	106±6
1	B	471	212	258	104±9
All	All	15072	6784	8256	3061

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 131.

5 of 367 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:DA:H1'	1:A:9:DA:N7	1.07	1.65	1	16
1:B:8:DA:H1'	1:B:9:DA:N7	1.04	1.68	3	16
1:B:10:DG:H2"	1:B:11:DC:C5	0.90	2.01	2	16
1:B:15:DC:H4'	1:B:16:DA:C5	0.90	2.01	13	8
1:A:15:DC:OP1	1:A:16:DA:C2	0.90	2.25	14	9

6.3 Torsion angles

6.3.1 Protein backbone

There are no protein molecules in this entry.

6.3.2 Protein sidechains

There are no protein molecules in this entry.

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided