

Full wwPDB NMR Structure Validation Report (i)

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PDB ID : 1EFS

Title : CONFORMATION OF A DNA-RNA HYBRID

Authors : Larue, V.; Hantz, E.

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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 : 20191225.v01 (using entries in the PDB archive December 25th 2019)

wwPDB-RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

wwPDB-ShiftChecker : v1.2

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

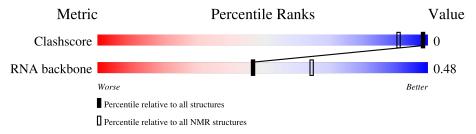
 $Validation\ Pipeline\ (wwPDB-VP) \quad : \quad 2.36.2$

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 $(\# \mathrm{Entries})$	$rac{ m NMR~archive}{ m (\#Entries)}$		
Clashscore	158937	12864		
RNA backbone	4643	676		

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	В	13		100%				



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 are 2 unique types of molecules in this entry. The entry contains 812 atoms, of which 281 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms					Trace	
1	Λ	19	Total	С	Н	N	О	Р	0
1	A	13	419	130	144	65	68	12	U

• Molecule 2 is a RNA chain called RNA (5'-R(*UP*UP*CP*UP*UP*CP*UP*CP*UP*UP*CP*UP*UP*UP*CP*UP*UP*CP*UP*UP*CP*UP*UP*UP*CP*UP*UP*UP*CP*UP*UP*CP*UP*UP*UP*UP*CP*UP*UP*UP*CP*UP*UP*UP*U

Mol	Chain	Residues	Atoms					Trace	
9	D	19	Total	С	Н	N	О	Р	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	15	393	117	137	32	95	12	U	



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.



Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2

4.2.1 Score per residue for model 1

There are no outlier residues in this chain.

 $\bullet \ \, \text{Molecule 1: DNA (5'-D(*GP*AP*GP*AP*GP*AP*GP*AP*AP*GP*AP*A)-3')}$



 $\bullet \ \, \text{Molecule 2: RNA (5'-R(*UP*UP*CP*UP*CP*UP*CP*UP*CP*UP*CP*UP*CP*UP*C)-3')}$

Chain B:

There are no outlier residues in this chain.



4.2.2	Score per	residue for model	1 2		
• Molec	cule 1: DNA	A (5'-D(*GP*AP*GP	*AP*GP*GP*AP	*AP*GP*AP*(GP*AP*A)-3')

Chain A: 46% 46% 8%



• Molecule 2: RNA (5'-R(*UP*UP*CP*UP*CP*UP*CP*UP*CP*UP*CP*UP*C)-3')

Chain B: 100%

There are no outlier residues in this chain.

4.2.3 Score per residue for model 3

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

Chain A: 38% 62%



 $\bullet \ \mathrm{Molecule} \ 2: \ \mathrm{RNA} \ (5'-\mathrm{R}(^*\mathrm{UP}^*\mathrm{UP}^*\mathrm{CP}^*\mathrm{UP}^*\mathrm{CP}^*\mathrm{UP}^*\mathrm{CP}^*\mathrm{UP}^*\mathrm{CP}^*\mathrm{UP}^*\mathrm{CP}^*\mathrm{UP}^*\mathrm{C})-3')$

Chain B:

There are no outlier residues in this chain.

4.2.4 Score per residue for model 4

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

Chain A: 54% 46%



 $\bullet \ \mathrm{Molecule} \ 2: \ \mathrm{RNA} \ (5'-\mathrm{R}(^*\mathrm{UP}^*\mathrm{UP}^*\mathrm{CP}^*\mathrm{UP}^*\mathrm{CP}^*\mathrm{UP}^*\mathrm{CP}^*\mathrm{UP}^*\mathrm{CP}^*\mathrm{UP}^*\mathrm{CP}^*\mathrm{UP}^*\mathrm{C})-3')$

Chain B:

There are no outlier residues in this chain.



4.2.5 Score per residue for r	model 5
• Molecule 1: DNA (5'-D(*GP*A	.P*GP*AP*GP*GP*AP*AP*GP*AP*A)-3
Chain A: 31%	69%
61 63 63 66 66 66 67 69 60 611 612 613 613 614 614 615 616 617 617 618 618 619 619 619 619 619 619 619 619	
• Molecule 2: RNA (5'-R(*UP*U	P*CP*UP*CP*UP*CP*CP*UP*CP*UP*C)-3')
Chain B:	100%
There are no outlier residues in the	his chain.
4.2.6 Score per residue for n	model 6
• Molecule 1: DNA (5'-D(*GP*A	.P*GP*AP*GP*AP*AP*AP*GP*AP*A)-3
Chain A: 31%	69%
01 A2 A2 A3 A6 A1 A12 A13	
• Molecule 2: RNA (5'-R(*UP*U	P*CP*UP*CP*UP*CP*CP*UP*CP*UP*C)-3')
Chain B:	100%
There are no outlier residues in the	his chain.
4.2.7 Score per residue for n	model 7
• Molecule 1: DNA (5'-D(*GP*A	.P*GP*AP*GP*GP*AP*AP*GP*AP*A)-3
Chain A: 54%	46%
63 63 64 65 65 69 69 A13	
• Molecule 2: RNA (5'-R(*UP*U	P*CP*UP*CP*UP*CP*CP*UP*CP*UP*C)-3')

There are no outlier residues in this chain.

Chain B:



100%

Chain B:

4.2.8 Score per residue for model 8
\bullet Molecule 1: DNA (5'-D(*GP*AP*GP*AP*GP*AP*GP*AP*AP*GP*AP*AP*A)-3
Chain A: 31% 69%
1
$ \bullet \ \text{Molecule 2: RNA (5'-R(*UP*UP*CP*UP*CP*UP*CP*UP*CP*UP*CP*UP*CP*UP*C})-3') }$
Chain B: 100%
There are no outlier residues in this chain.
4.2.9 Score per residue for model 9
Chain A: 54% 46%
A2 A4
Chain B: 100%
There are no outlier residues in this chain.
4.2.10 Score per residue for model 10
\bullet Molecule 1: DNA (5'-D(*GP*AP*GP*AP*GP*AP*GP*AP*AP*GP*AP*A)-3
Chain A: 69% 31%
A 2 A 2 A 3 A 4 1 2 A 4 1 3 A
$ \bullet \ \text{Molecule 2: RNA (5'-R(*UP*UP*CP*UP*CP*UP*CP*UP*CP*UP*CP*UP*CP*UP*C)-3')} $

92%

8%



5 Refinement protocol and experimental data overview (i)



The models were refined using the following method: molecular mechanics distance geometry matrix relaxation.

Of the 10 calculated structures, 10 were deposited, based on the following criterion: back calculated data agree with experimental NOESY spectrum, 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
JUMNA	structure solution	10
IRMA	refinement	95

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		В	Sond lengths	Bond angles		
		RMSZ	#Z>5	RMSZ	#Z>5	
1	A	1.01 ± 0.02	$0\pm0/313~(~0.0\pm~0.0\%)$	1.45 ± 0.02	$8\pm2/484~(~1.5\pm~0.4\%)$	
2	В	0.76 ± 0.02	$0\pm0/281~(~0.0\pm~0.0\%)$	1.32 ± 0.01	$0\pm0/433~(~0.0\pm~0.1\%)$	
All	All	0.90	0/5940 (0.0%)	1.39	76/9170 (0.8%)	

There are no bond-length outliers.

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

Mal	Mol Chain		Trino	Atoma	\mathbf{z}	Observed(0)	$\operatorname{Ideal}({}^{o})$	Models	
IVIOI	Chain	Res	Type	Atoms		$\mathrm{Observed}(^{o})$	ideai(*)	Worst	Total
1	A	10	DA	O4'-C1'-N9	6.45	112.52	108.00	2	7
1	A	12	DA	O4'-C1'-N9	6.19	112.33	108.00	5	10
1	A	10	DA	O4'-C1'-C2'	-6.08	101.03	105.90	2	1
1	A	4	DA	O4'-C1'-N9	5.79	112.05	108.00	7	9
1	A	3	DG	O4'-C1'-N9	5.77	112.04	108.00	10	8
1	A	5	DG	O4'-C1'-N9	5.74	112.02	108.00	5	10
1	A	2	DA	O4'-C1'-N9	5.65	111.96	108.00	7	9
1	A	8	DA	O4'-C1'-N9	5.50	111.85	108.00	8	6
1	A	11	DG	O4'-C1'-N9	5.38	111.77	108.00	5	2
1	A	9	DG	O4'-C1'-N9	5.30	111.71	108.00	1	6
1	A	12	DA	O4'-C1'-C2'	-5.21	101.73	105.90	2	2
1	A	4	DA	O4'-C4'-C3'	5.20	109.12	106.00	2	1
1	A	7	DA	O4'-C1'-N9	5.20	111.64	108.00	5	3
2	В	22	С	C3'-C2'-C1'	5.14	105.61	101.50	10	1
1	A	7	DA	C1'-O4'-C4'	-5.12	104.98	110.10	5	1

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	275	144	142	0±0
All	All	5310	2810	2770	1

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.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2 Clash(Å) Distance(Å)		Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:9:DG:H2"	1:A:10:DA:C8	0.43	2.48	2	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)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	В	12/13 (92%)	0±0 (0±0%)	0±0 (0±0%)	0.48 ± 0.11
All	All	120/130 (92%)	0 (0%)	0 (0%)	0.48

The overall RNA backbone suiteness is 0.48.

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.



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 monosaccharides 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

