



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1R3X
Title : INTRAMOLECULAR DNA TRIPLEX WITH RNA THIRD STRAND,
NMR, 10 STRUCTURES
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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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk30686
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

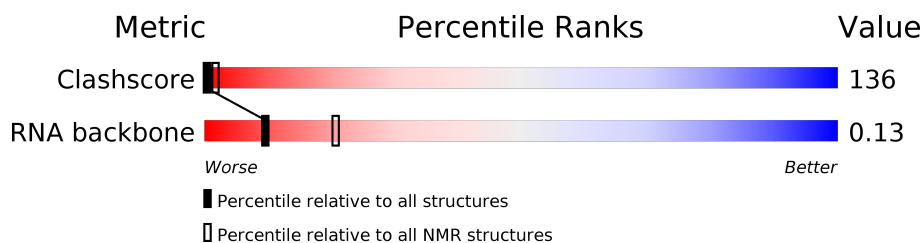
1 Overall quality at a glance

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	136279	12091
RNA backbone	3744	647

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	8	
2	B	8	
3	C	8	

2 Ensemble composition and analysis ⓘ

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 3 unique types of molecules in this entry. The entry contains 752 atoms, of which 273 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	8	Total	C	H	N	O	P	0
			258	80	90	40	41	7	

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*CP*TP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms						Trace
2	B	8	Total	C	H	N	O	P	0
			249	77	95	19	51	7	

- Molecule 3 is a RNA chain called RNA (5'-R(*UP*CP*UP*CP*UP*CP*UP*U)-3').

Mol	Chain	Residues	Atoms						Trace
3	C	8	Total	C	H	N	O	P	0
			245	72	88	19	59	7	

4 Residue-property plots

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

Chain A: 

A1 G2 A3 G4 A5 G6 A7 A8

- Molecule 2: DNA (5'-D(*TP*TP*CP*TP*CP*TP*CP*T)-3')

Chain B: 

T9 T10 C11 T12 C13 T14 C15 T16

- Molecule 3: RNA (5'-R(*UP*CP*UP*CP*UP*CP*UP*U)-3')

Chain C: 

U17 C18 U19 C20 U21 C22 U23 U24

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

Chain A: 

A1 G2 A3 G4 A5 G6 A7 A8

- Molecule 2: DNA (5'-D(*TP*TP*CP*TP*CP*TP*CP*T)-3')

Chain B: 

T9	T10	C11	T12	C13	T14	C15	T16
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- Molecule 3: RNA (5'-R(*UP*CP*UP*CP*UP*CP*UP*U)-3')



U17	C18	U19	C20	U21	C22	U23	U24
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY/ SIMULATED ANNEALING*.

Of the 20 calculated structures, 10 were deposited, based on the following criterion: *LOWEST OVERALL 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. 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	2.25±0.04	8±1/191 (4.2±0.4%)	3.93±0.15	39±6/294 (13.3±2.0%)
2	B	2.65±0.08	13±2/169 (7.4±1.1%)	4.43±0.18	45±4/258 (17.4±1.7%)
3	C	1.48±0.06	1±1/172 (0.6±0.3%)	2.81±0.05	24±2/264 (9.2±0.9%)
All	All	2.18	216/5320 (4.1%)	3.79	1083/8160 (13.3%)

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
2	B	0.1±0.3	0.3±0.5
All	All	1	3

5 of 40 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	14	DT	C5-C7	-11.76	1.43	1.50	8	10
2	B	14	DT	N1-C6	-11.37	1.30	1.38	4	10
2	B	12	DT	C5-C7	-10.42	1.43	1.50	3	10
1	A	8	DA	N9-C4	-10.24	1.31	1.37	2	10
2	B	9	DT	N1-C6	-9.37	1.31	1.38	1	10

5 of 208 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(°)	Ideal(°)	Models	
								Worst	Total
1	A	3	DA	O4'-C1'-N9	37.78	134.44	108.00	8	9
1	A	6	DG	O4'-C1'-N9	26.07	126.25	108.00	4	10
1	A	4	DG	O4'-C1'-N9	19.86	121.90	108.00	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	10	DT	C6-C5-C7	-19.70	111.08	122.90	9	10
2	B	9	DT	C6-C5-C7	-19.28	111.33	122.90	5	10

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	16	DT	C4'	1

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	13	DC	Sidechain	3

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	168	90	90	60±8
2	B	154	95	95	23±4
3	C	157	88	85	41±7
All	All	4790	2730	2700	1015

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 136.

5 of 263 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:DG:C4	1:A:3:DA:C8	1.11	2.39	6	10
1:A:4:DG:C4	1:A:5:DA:C8	0.94	2.56	6	10
1:A:1:DA:C8	3:C:18:C:O2	0.88	2.27	1	10
3:C:18:C:O2'	3:C:19:U:O4'	0.87	1.93	3	10
1:A:2:DG:C2	1:A:3:DA:C4	0.86	2.64	3	10

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
3	C	8/8 (100%)	5±1 (68±11%)	4±1 (44±17%)	0.14±0.09
All	All	79/80 (99%)	54 (68%)	35 (44%)	0.15

The overall RNA backbone suiteness is 0.13.

5 of 7 unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
3	C	24	U	10
3	C	18	C	10
3	C	19	U	10
3	C	20	C	8
3	C	23	U	8

5 of 6 unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
3	C	18	C	10
3	C	17	U	9
3	C	19	U	5
3	C	22	C	4
3	C	23	U	4

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

No chemical shift data were provided