



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:24 pm BST

PDB ID : 1W86
Title : Solution structure of an dsDNA:LNA triplex
Authors : Sorensen, J.J.; Nielsen, J.T.; Petersen, M.
Deposited on : 2004-09-16

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 ⓘ 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

2 Ensemble composition and analysis

This entry contains 20 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

There are 3 unique types of molecules in this entry. The entry contains 771 atoms, of which 286 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called INTRAMOLECULAR DSDNA-LNA TRIPLEX.

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

- Molecule 2 is a DNA chain called INTRAMOLECULAR DSDNA-LNA TRIPLEX.

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

- Molecule 3 is a DNA chain called INTRAMOLECULAR DSDNA-LNA TRIPLEX.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
3	C	8	264	83	101	19	54	7	0

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: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



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: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain B:  25% 75%

T9
T10
C11
T12
C13
T14
C15
T16

- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain C:  25% 63% 13%

T17
M18
T19
N20
T21
N22
T23
T24

4.2.2 Score per residue for model 2

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain A:  25% 75%

A1
G2
A3
G4
A5
G6
A7
A8

- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain B:  25% 75%

T9
T10
C11
T12
C13
T14
C15
T16

- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain C:  25% 63% 13%

T17
M18
T19
N20
T21
N22
T23
T24

4.2.3 Score per residue for model 3

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain A:  50% 50%

A1
G2
A3
G4
A5
A8

- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain B:  13% 88%

T9
T10
C11
T12
C13
T14
C15
T16

- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain C: 



4.2.4 Score per residue for model 4

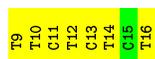
- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain A: 



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain B: 



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain C: 



4.2.5 Score per residue for model 5

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain A: 

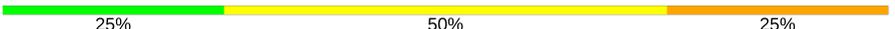


- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain B: 



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain C: 



4.2.6 Score per residue for model 6

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.7 Score per residue for model 7

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.8 Score per residue for model 8

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.9 Score per residue for model 9

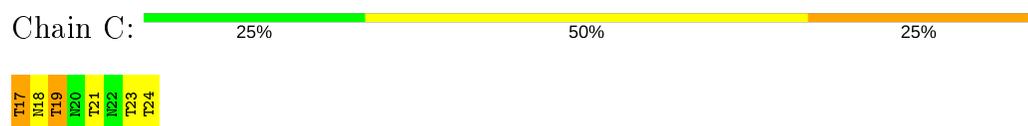
- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.10 Score per residue for model 10

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX





- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.11 Score per residue for model 11

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.12 Score per residue for model 12

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX

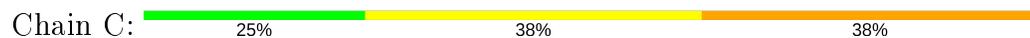


- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX





- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.13 Score per residue for model 13

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX

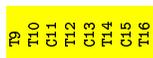


4.2.14 Score per residue for model 14

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX

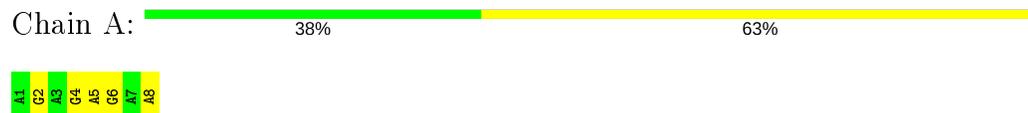


- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.15 Score per residue for model 15

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.16 Score per residue for model 16

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.17 Score per residue for model 17

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.18 Score per residue for model 18

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX



4.2.19 Score per residue for model 19

- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain A:  50% 38% 13%

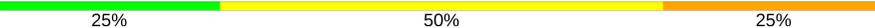


- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain B:  25% 75%



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain C:  25% 50% 25%



4.2.20 Score per residue for model 20

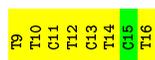
- Molecule 1: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain A:  50% 50%



- Molecule 2: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain B:  13% 88%



- Molecule 3: INTRAMOLECULAR DSDNA-LNA TRIPLEX

Chain C:  25% 63% 13%



5 Refinement protocol and experimental data overview [i](#)

The models were refined using the following method: *simulated annealing*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
AMBER	refinement	
AMBER	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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
3	C	163	101	101	1±0
All	All	9700	5720	5720	20

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:18:LCC:H2'1	3:C:19:DT:C6	0.57	2.34	3	20

5.2 Torsion angles [i](#)

5.2.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.2.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

MODRES-GEOMETRY INFOmissingINFO

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 Ligand geometry [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such molecules in this entry.

5.6 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

No chemical shift data were provided