

Full wwPDB NMR Structure Validation Report (i)

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PDB ID : 7W0V BMRB ID : 36455

Title : C4'-SCF3-DT modifeid DNA-DNA duplex

Authors: Li, Q.; Trajkovski, M.; Fan, C.; Chen, J.; Zhou, Y.; Lu, K.; Li, H.; Su, X.; Xi,

Z.; Plavec, J.; Zhou, C.

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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 (1)) were used in the production of this report:

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 : 2.31.2

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

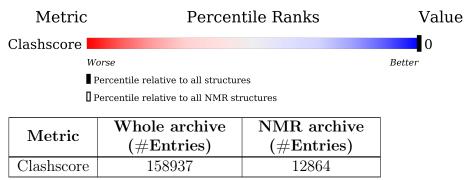
Validation Pipeline (wwPDB-VP) : 2.31.2

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 is 43%.

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.



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	10	100%					
2	В	10	30%	70%				



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 638 atoms, of which 229 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues		${f Atoms}$					Trace		
1	Λ	10	Total	С	F	Н	N	О	Р	S	0
1	A	10	318	98	3	114	35	58	9	1	U

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

Mol	Chain	Residues		Atoms					
9	D	10	Total	С	Н	N	О	Р	0
	Б	10	320	99	115	39	58	9	0



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.

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

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: DNA (5'-D(*CP*CP*AP*TP*(DSW)P*AP*TP*AP*GP*C)-3')





4.2.2	Score per residue for model 2
• Molecu	ıle 1: DNA (5'-D(*CP*CP*AP*TP*(DSW)P*AP*TP*AP*GP*C)-3'
Chain A	: 100%
C1 C2 A3 T4 84E5 A6	177 60 010 010
• Molecu	ale 2: DNA (5'-D(*GP*CP*TP*AP*TP*AP*AP*TP*GP*G)-3')
Chain B	: 30% 70%
G11 C12 T13 A14 T15 A16	A17
4.2.3	Score per residue for model 3
• Molecu	ıle 1: DNA (5'-D(*CP*CP*AP*TP*(DSW)P*AP*TP*AP*GP*C)-3'
Chain A	: 100%
C1 C2 A3 T4 84E5 A6	174 010 010
• Molecu	ule 2: DNA (5'-D(*GP*CP*TP*AP*TP*AP*AP*TP*GP*G)-3')
Chain B	: 30% 70%
G11 C12 T13 A14 T15 A16	11
4.2.4	Score per residue for model 4
• Molecu	ıle 1: DNA (5'-D(*CP*CP*AP*TP*(DSW)P*AP*TP*AP*GP*C)-3'
Chain A	: 100%
C1 C2 A3 T4 84E5 A6	17 69 69 610
• Molecu	ale 2: DNA (5'-D(*GP*CP*TP*AP*TP*AP*AP*TP*GP*G)-3')
Chain B	: 30% 70%



4.2.5	Score per r	esidue for model 5
• Mole	cule 1: DNA (5'-D(*CP*CP*AP*TP*(DSW)P*AP*TP*AP*GP*C)-
Chain	A:	100%
C1 C2 A3 T4 84E5	A6 T7 A8 G9 C10	
• Mole	cule 2: DNA (5'-D(*GP*CP*TP*AP*TP*AP*AP*TP*GP*G)-3')
Chain	В: 30%	70%
G11 C12 T13 A14 T15	A16 A17 T18 G20	
4.2.6	Score per r	esidue for model 6
• Mole	cule 1: DNA (5'-D(*CP*CP*AP*TP*(DSW)P*AP*TP*AP*GP*C)-
Chain	A:	100%
C1 C2 A3 T4 84E5	A6 T7 A8 G9 C10	
• Mole	cule 2: DNA (5'-D(*GP*CP*TP*AP*TP*AP*AP*TP*GP*G)-3')
Chain	В: 30%	70%
G11 C12 T13 A14 T15	A16 A17 T18 G20 G20	
4.2.7	Score per r	esidue for model 7
• Mole	cule 1: DNA (5'-D(*CP*CP*AP*TP*(DSW)P*AP*TP*AP*GP*C)-
Chain	A:	100%
C1 C2 A3 T4 84E5	A6 T7 A8 G9 C10	
• Mole	cule 2: DNA (5'-D(*GP*CP*TP*AP*TP*AP*AP*TP*GP*G)-3')
Chain	B: 20%	80%



4.2.8 Score	e per residue for model 8
• Molecule 1:	DNA (5'-D(*CP*CP*AP*TP*(DSW)P*AP*TP*AP*GP*C)-3
Chain A:	100%
C1 C2 A3 T4 T4 T7 A6 G9 C10	
• Molecule 2:	DNA (5'-D(*GP*CP*TP*AP*TP*AP*AP*TP*GP*G)-3')
Chain B:	30% 70%
611 C12 T13 A14 T15 A16 A17 T18 G19 G20	
4.2.9 Score	e per residue for model 9
• Molecule 1:	DNA (5'-D(*CP*CP*AP*TP*(DSW)P*AP*TP*AP*GP*C)-3
Chain A:	100%
C1 C2 A3 T4 84E5 A6 T7 A8 G9	
• Molecule 2:	DNA (5'-D(*GP*CP*TP*AP*TP*AP*AP*TP*GP*G)-3')
Chain B:	30% 70%
G11 C12 A14 A14 A16 A17 T18 G19 G20	
4.2.10 Sco	re per residue for model 10
• Molecule 1:	DNA (5'-D(*CP*CP*AP*TP*(DSW)P*AP*TP*AP*GP*C)-3
Chain A:	100%
C1 C2 A3 T4 84E5 A6 T7 A8 G9	
• Molecule 2:	DNA (5'-D(*GP*CP*TP*AP*TP*AP*AP*TP*GP*G)-3')
Chain B:	20% 80%



5 Refinement protocol and experimental data overview (i)



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

Of the 50 calculated structures, 10 were deposited, based on the following criterion: structures with the lowest energy.

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

Software name	Classification	Version
Amber	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	187
Number of shifts mapped to atoms	187
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	43%



6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 84E

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	Е	ond lengths	Bond angles		
MIOI	Chain	RMSZ	#Z>5	RMSZ	#Z>5	
1	A	1.53 ± 0.00	$0\pm0/199$ ($0.0\pm$ 0.0%)	2.46 ± 0.01	$20\pm0/302$ ($6.7\pm$ 0.2%)	
2	В	1.57 ± 0.00	$0\pm0/230~(~0.0\pm~0.0\%)$	2.34 ± 0.01	$17\pm0/354$ ($4.9\pm$ 0.1%)	
All	All	1.55	0/4290 (0.0%)	2.39	375/6560 (5.7%)	

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.

Mol	Chain	Dag	Trmo	Atoma	\mathbf{z}	Observed(0)	Ideal(0)	Mod	dels
MIOI	Chain	Res	Type	Atoms	L	$Observed(^o)$	$\operatorname{Ideal}(^{o})$	Worst	Total
2	В	17	DA	N1-C6-N6	-8.57	113.46	118.60	3	10
2	В	16	DA	N1-C6-N6	-8.27	113.64	118.60	7	10
1	A	3	DA	N1-C6-N6	-8.08	113.75	118.60	3	10
2	В	14	DA	N1-C6-N6	-7.98	113.81	118.60	4	10
1	A	8	DA	N1-C6-N6	-7.90	113.86	118.60	4	10
1	A	10	DC	N3-C2-O2	-7.50	116.65	121.90	3	10
1	A	2	DC	N3-C2-O2	-7.43	116.70	121.90	2	10
1	A	6	DA	C5-C6-N1	7.42	121.41	117.70	6	10
1	A	3	DA	C5-C6-N1	7.37	121.38	117.70	5	10
1	A	1	DC	N3-C2-O2	-7.34	116.76	121.90	1	10
1	A	8	DA	C5-C6-N1	7.32	121.36	117.70	5	10
1	A	6	DA	N1-C6-N6	-7.10	114.34	118.60	10	10
2	В	16	DA	C5-C6-N1	7.06	121.23	117.70	3	10
2	В	17	DA	C5-C6-N1	6.86	121.13	117.70	2	10
2	В	14	DA	C5-C6-N1	6.82	121.11	117.70	4	10
2	В	16	DA	C4-C5-C6	-6.82	113.59	117.00	3	10
2	В	17	DA	C4-C5-C6	-6.77	113.61	117.00	7	10
2	В	12	DC	N3-C2-O2	-6.74	117.18	121.90	2	10
2	В	14	DA	C4-C5-C6	-6.71	113.64	117.00	2	10
1	A	3	DA	C4-C5-C6	-6.70	113.65	117.00	2	10

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Mol	Chain	Res	Type	Atoma	\mathbf{Z}	Observed (0)	Ideal(0)	Mod	dels
MIOI	Chain	nes	Type	Atoms	L	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$	Worst	Total
1	A	8	DA	C4-C5-C6	-6.53	113.74	117.00	2	10
2	В	13	DT	C6-C5-C7	-6.36	119.09	122.90	1	10
1	A	7	DT	C6-C5-C7	-6.21	119.17	122.90	3	10
1	A	4	DT	C6-C5-C7	-6.04	119.28	122.90	10	10
1	A	10	DC	N1-C2-O2	6.02	122.51	118.90	3	10
1	A	6	DA	C4-C5-C6	-5.98	114.01	117.00	5	10
2	В	15	DT	N3-C2-O2	-5.93	118.74	122.30	2	10
2	В	18	DT	C6-C5-C7	-5.88	119.37	122.90	2	10
2	В	18	DT	N3-C2-O2	-5.87	118.78	122.30	2	10
2	В	15	DT	C6-C5-C7	-5.81	119.41	122.90	1	10
1	A	1	DC	N1-C2-O2	5.80	122.38	118.90	7	10
1	A	2	DC	N1-C2-O2	5.70	122.32	118.90	9	10
1	A	7	DT	N3-C2-O2	-5.61	118.94	122.30	6	10
2	В	12	DC	N1-C2-O2	5.54	122.23	118.90	8	10
2	В	13	DT	N3-C2-O2	-5.45	119.03	122.30	4	10
1	A	4	DT	N3-C2-O2	-5.29	119.13	122.30	6	10
1	A	9	DG	O4'-C1'-N9	5.26	111.68	108.00	2	10
1	A	4	DT	C5-C6-N1	-5.13	120.62	123.70	6	3
2	В	20	DG	O4'-C1'-N9	5.12	111.58	108.00	7	2

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.

\mathbf{Mol}	Chain	Non-H	H(model)	H(added)	Clashes
All	All	4090	2290	2180	-

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 -.

There are no clashes.



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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Pos	Bond lengths			ths
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	#Z>2
1	84E	A	5	1,2	21,26,27	0.97 ± 0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Pos	Link	Bond ang		gles	
IVIOI			nes	LIIIK	Counts	RMSZ	#Z>2	
1	84E	A	5	1,2	29,40,43	1.65 ± 0.05	5±0 (17±1%)	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical



component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	84E	A	5	1,2	-	$0\pm0,9,31,32$	$0 \pm 0,2,2,2$

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.

Mol	Chain	Res	Type	Atoms	\mathbf{z}	Observed(°)	$Ideal(^{o})$	Models	
MIOI	Chain	nes	Type	Atoms	Z Observed()		ideai()	Worst	Total
1	A	5	84E	O5'-C5'-C4'	5.06	115.42	108.56	3	10
1	A	5	84E	C6'-S4'-C4'	3.58	106.86	102.14	2	10
1	A	5	84E	C7-C5-C6	3.14	118.65	122.85	7	10
1	A	5	84E	C6-C5-C4	2.98	120.52	118.03	6	10
1	A	5	84E	C5-C6-N1	2.58	120.68	123.34	6	10
1	A	5	84E	O4'-C1'-N1	2.01	110.13	107.91	6	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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)

The completeness of assignment taking into account all chemical shift lists is 43% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: working cs.cif

Chemical shift list name: chem_shift_T5STF_DSW.str

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	187
Number of shifts mapped to atoms	187
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 43%, i.e. 162 atoms were assigned a chemical shift out of a possible 374. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Sidechain	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Aromatic	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Overall	162/374~(43%)	$162/222 \ (73\%)$	0/129 (0%)	0/23~(0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 162 atoms were assigned a chemical shift out of a possible 374. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.



	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}\mathbf{N}$
Backbone	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Sidechain	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Aromatic	0/0 (%)	0/0 (%)	0/0 (%)	0/0 (%)
Overall	162/374 (43%)	$162/222 \ (73\%)$	0/129 (0%)	$0/23 \ (0\%)$

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

No random coil index (RCI) plot could be generated from the current chemical shift list (chem_shift_T5STF_RCI is only applicable to proteins.

