Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 12:40 AM BST

PDB ID	:	2L8I
Title	:	A biocompatible backbone modification? - Structure and dynamics of a triazole-linked DNA duplex
Authors	:	El-Sagheer, A.; Brown, T.; Ernsting, N.; Dehmel, L.; Griesinger, C.; Mugge, C.
Deposited on	:	2011-01-13

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
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:

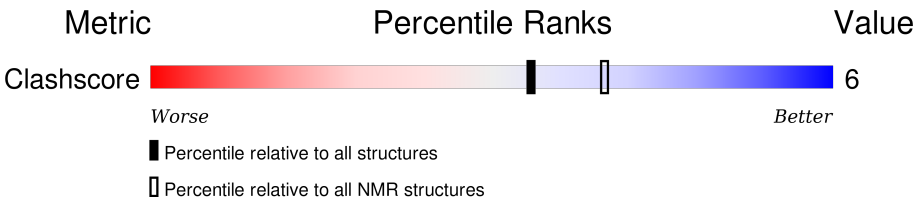
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 55%.

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	13	85% 15%
2	B	12	42% 58%

2 Ensemble composition and analysis (i)

This entry contains 11 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 are 2 unique types of molecules in this entry. The entry contains 827 atoms, of which 298 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	13	411	126	147	51	75	12	0

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	12	416	129	151	51	74	11	0

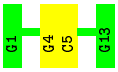
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

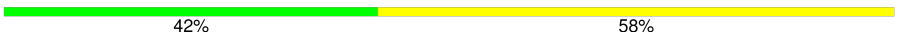
These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain 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: DNA (5'-D(*GP*CP*TP*GP*CP*AP*AP*AP*CP*GP*TP*CP*G)-3')

Chain A:



• Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

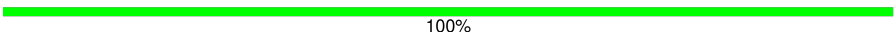
Chain B: 

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

Chain A: 

There are no outlier residues in this chain.

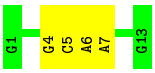
• Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

Chain B:

4.2.2 Score per residue for model 2

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

Chain A: 69% 31%



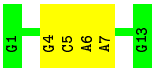
- Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

Chain B: 25% 75%

4.2.3 Score per residue for model 3

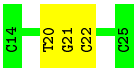
- Molecule 1: DNA (5'-D(*GP*CP*TP*GP*CP*AP*AP*AP*CP*GP*TP*CP*G)-3')

Chain A: 69% 31%



- Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

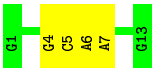
Chain B: 75% 25%



4.2.4 Score per residue for model 4

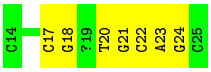
- Molecule 1: DNA (5'-D(*GP*CP*TP*GP*CP*AP*AP*AP*CP*GP*TP*CP*G)-3')

Chain A: 69% 31%



- Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

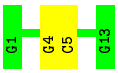
Chain B: 42% 58%



4.2.5 Score per residue for model 5

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

Chain A: 85% 15%



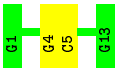
- Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

Chain B: 25% 75%

4.2.6 Score per residue for model 6

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

Chain A: 85% 15%



- Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

Chain B: 25% 75%

4.2.7 Score per residue for model 7

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

Chain A: 69% 31%

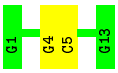
- Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

Chain B: 42% 58%

4.2.8 Score per residue for model 8

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

Chain A: 85% 15%



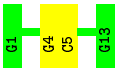
- Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

Chain B: 42% 58%

4.2.9 Score per residue for model 9

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

Chain A: 85% 15%



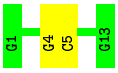
- Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

Chain B: 42% 58%

4.2.10 Score per residue for model 10

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

Chain A: 85% 15%



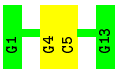
- Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

Chain B: 25% 75%

4.2.11 Score per residue for model 11

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

Chain A: 85% 15%



- Molecule 2: DNA (5'-D(*CP*GP*AP*CP*G*(2L8)P*TP*GP*CP*AP*GP*C)-3')

Chain B: 42% 58%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 11 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
X-PLOR NIH	refinement	2.20
X-PLOR NIH	structure solution	2.20

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)	2l8i_cs.str
Number of chemical shift lists	1
Total number of shifts	306
Number of shifts mapped to atoms	283
Number of unparsed shifts	18
Number of shifts with mapping errors	5
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	55%

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)

Bond lengths and bond angles in the following residue types are not validated in this section: 2L8

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	264	147	147	1±1
2	B	265	151	151	4±1
All	All	5819	3278	3278	58

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:DG:C2	1:A:5:DC:C2	0.52	2.98	8	10
2:B:20:DT:C2	2:B:21:DG:N7	0.49	2.81	8	10
2:B:17:DC:C2	2:B:18:DG:C8	0.47	3.02	9	9
2:B:21:DG:C4	2:B:22:DC:C5	0.47	3.03	9	11
2:B:15:DG:C6	2:B:16:DA:N6	0.45	2.84	8	8
2:B:23:DA:C2	2:B:24:DG:C4	0.41	3.08	10	5
1:A:6:DA:C2	1:A:7:DA:C4	0.41	3.08	3	4
1:A:6:DA:C4	1:A:7:DA:C8	0.40	3.09	3	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)

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	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	2L8	B	19	2	28,46,47	0.98±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	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	2L8	B	19	2	35,67,70	1.08±0.01	0±0 (0±0%)

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
2	2L8	B	19	2	-	0±0,8,46,47	0±0,5,5,5

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 (i)

The completeness of assignment taking into account all chemical shift lists is 55% for the well-defined parts and 55% for the entire structure.

7.1 Chemical shift list 1

File name: 2l8i_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

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	306
Number of shifts mapped to atoms	283
Number of unparsed shifts	18
Number of shifts with mapping errors	5
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	40

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 18 occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
30	A	3	THY	H7	1.67	.	1
31	A	3	THY	H7	1.67	.	1
122	A	11	THY	H7	1.40	.	1
123	A	11	THY	H7	1.40	.	1
210	B	19	THY	H7	1.37	.	1
211	B	19	THY	H7	1.37	.	1
220	B	19	2L8	C1'1	86.1	.	1
222	B	19	2L8	C3'1	74.8	.	1
224	B	19	2L8	C61	134.9	.	1
226	B	19	2L8	H11'	5.76	.	1
228	B	19	2L8	H12'	2.77	.	1
229	B	19	2L8	H13'	4.79	.	1
230	B	19	2L8	H14'	4.17	.	1
233	B	19	2L8	H1C6	7.00	.	1
236	B	19	2L8	H1N3	13.95	.	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
238	B	19	2L8	HC2'	1.94	.	1
246	B	21	THY	H7	1.75	.	1
247	B	21	THY	H7	1.75	.	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 5 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	11	THY	H7	1.4	-1.0	1
B	21	THY	H7	1.75	-1.0	1
A	3	THY	H7	1.67	-1.0	1
B	20	TAL	H7	1.63	-1.0	1
B	19	THY	H7	1.37	-1.0	1

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 55%, i.e. 265 atoms were assigned a chemical shift out of a possible 482. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}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	265/482 (55%)	180/290 (62%)	85/160 (53%)	0/32 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 55%, i.e. 265 atoms were assigned a chemical shift out of a possible 482. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	265/482 (55%)	180/290 (62%)	85/160 (53%)	0/32 (0%)

7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
2	B	25	DC	C5	95.00	100.78 – 96.68	-9.1
1	A	9	DC	C5	95.20	100.78 – 96.68	-8.6
2	B	17	DC	C5	95.40	100.78 – 96.68	-8.1
1	A	5	DC	C5	95.50	100.78 – 96.68	-7.9
2	B	22	DC	C5	95.50	100.78 – 96.68	-7.9
1	A	2	DC	C5	95.70	100.78 – 96.68	-7.4
1	A	11	DT	C6	135.80	141.81 – 136.91	-7.3
1	A	9	DC	C6	139.00	146.45 – 140.25	-7.0
1	A	7	DA	C1'	81.50	88.48 – 82.48	-6.6
2	B	17	DC	C6	139.30	146.45 – 140.25	-6.5
1	A	8	DA	C8	138.00	144.55 – 138.85	-6.5
1	A	12	DC	C5	96.10	100.78 – 96.68	-6.4
1	A	7	DA	C8	138.10	144.55 – 138.85	-6.3
1	A	6	DA	C1'	81.70	88.48 – 82.48	-6.3
1	A	11	DT	C1'	82.70	90.81 – 83.51	-6.1
1	A	7	DA	C2	151.00	158.48 – 151.68	-6.0
1	A	8	DA	C1'	81.90	88.48 – 82.48	-6.0
2	B	16	DA	C8	138.30	144.55 – 138.85	-6.0
1	A	5	DC	C6	139.70	146.45 – 140.25	-5.9
1	A	3	DT	C1'	82.90	90.81 – 83.51	-5.8
2	B	20	DT	C1'	82.90	90.81 – 83.51	-5.8
2	B	16	DA	C1'	82.10	88.48 – 82.48	-5.6
2	B	23	DA	C1'	82.10	88.48 – 82.48	-5.6
1	A	3	DT	C6	136.60	141.81 – 136.91	-5.6
2	B	22	DC	C6	139.90	146.45 – 140.25	-5.6
1	A	6	DA	C2	151.30	158.48 – 151.68	-5.6
2	B	24	DG	C1'	81.20	89.32 – 81.62	-5.5
2	B	15	DG	C1'	81.30	89.32 – 81.62	-5.4
2	B	21	DG	C1'	81.30	89.32 – 81.62	-5.4
1	A	4	DG	C1'	81.40	89.32 – 81.62	-5.3
2	B	23	DA	C2	151.50	158.48 – 151.68	-5.3
1	A	2	DC	C6	140.10	146.45 – 140.25	-5.2

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
2	B	14	DC	C5	96.60	100.78 – 96.68	-5.2
1	A	9	DC	C1'	83.10	92.11 – 83.21	-5.1
1	A	6	DA	C8	138.80	144.55 – 138.85	-5.1
2	B	23	DA	C8	138.80	144.55 – 138.85	-5.1
2	B	25	DC	C6	140.20	146.45 – 140.25	-5.1
2	B	25	DC	C3'	68.80	85.86 – 68.86	-5.0
2	B	24	DG	C8	134.50	143.32 – 134.52	-5.0
2	B	17	DC	C1'	83.20	92.11 – 83.21	-5.0

7.1.5 Random Coil Index (RCI) plots (i)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.