



wwPDB NMR Structure Validation Summary Report ⓘ

Jun 22, 2024 – 06:00 PM EDT

PDB ID : 6KFI
BMRB ID : 36267
Title : NMR solution structure of the 1:1 complex of Tel26 G-quadruplex and a tripodal cationic fluorescent probe NBTE
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Deposited on : 2019-07-07

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
buster-report : 1.1.7 (2018)
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) : 2.37.1

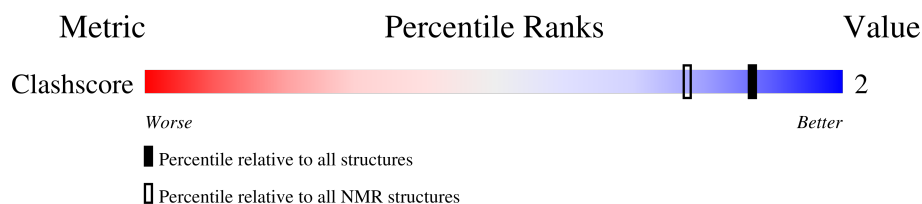
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

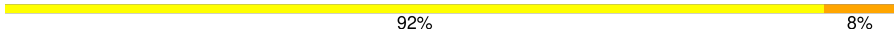
The overall completeness of chemical shifts assignment is 44%.

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	158937	12864

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	26	 92% 8%

2 Ensemble composition and analysis ⓘ

This entry contains 15 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.

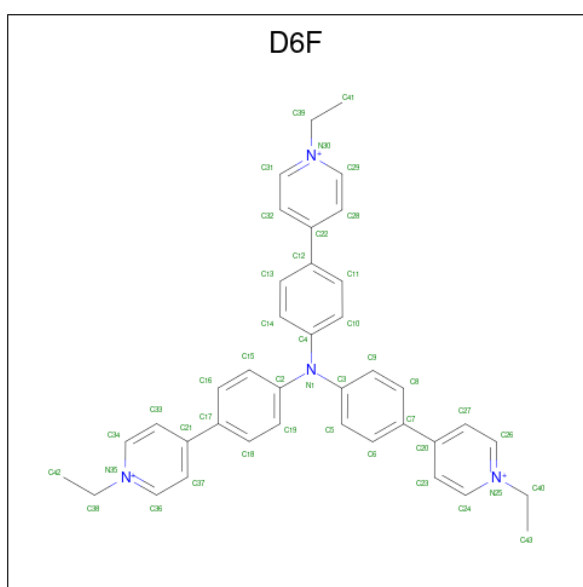
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 925 atoms, of which 333 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called G-quadruplex DNA (26-MER).

Mol	Chain	Residues	Atoms						Trace
1	A	26	Total	C	H	N	O	P	0
			843	260	294	112	152	25	

- Molecule 2 is 4,4',4''-(nitrilotris(benzene-4,1-diyl))tris(1-ethylpyridin-1-ium) iodide (three-letter code: D6F) (formula: C₃₉H₃₉N₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	N
			82	39	39	4

4 Residue-property plots

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: G-quadruplex DNA (26-MER)

Chain A: 

A1	A2	A3	G4	G5	G6	T7	T8	A9	G10	G11	G12	T13	T14	A15	G16	G17	G18	T19	T20	A21	G22	G23	G24	A25	A26
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4.2 Residue scores for the representative (author defined) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: G-quadruplex DNA (26-MER)

Chain A: 

A1	A2	A3	G4	G5	G6	T7	T8	A9	G10	G11	G12	T13	T14	A15	G16	G17	G18	T19	T20	A21	G22	G23	G24	A25	A26
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing, molecular dynamics*.

Of the 100 calculated structures, 15 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	
X-PLOR NIH	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	285
Number of shifts mapped to atoms	246
Number of unparsed shifts	0
Number of shifts with mapping errors	39
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	44%

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: D6F

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	2.85±0.36	51±19/620 (8.2± 3.1%)	3.86±0.39	165±29/960 (17.2± 3.1%)
All	All	2.87	759/9300 (8.2%)	3.88	2475/14400 (17.2%)

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
1	A	0.0±0.0	0.7±1.1
All	All	0	10

5 of 194 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
1	A	13	DT	N1-C6	16.71	1.50	1.38	7	7
1	A	14	DT	N1-C6	14.92	1.48	1.38	7	6
1	A	20	DT	N1-C6	13.70	1.47	1.38	7	7
1	A	8	DT	N1-C6	13.69	1.47	1.38	7	7
1	A	19	DT	N1-C6	13.56	1.47	1.38	7	7

5 of 531 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	15	DA	O4'-C1'-N9	-28.90	87.77	108.00	14	7
1	A	23	DG	C2-N3-C4	24.10	123.95	111.90	10	9
1	A	16	DG	C2-N3-C4	20.36	122.08	111.90	7	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	17	DG	C2-N3-C4	20.28	122.04	111.90	7	7
1	A	11	DG	C2-N3-C4	19.17	121.49	111.90	7	8

There are no chirality outliers.

5 of 6 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	19	DT	Sidechain	3
1	A	21	DA	Sidechain	3
1	A	7	DT	Sidechain	1
1	A	10	DG	Sidechain	1
1	A	6	DG	Sidechain	1

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	549	294	294	2±1
All	All	8880	4995	4408	26

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 2.

5 of 18 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:N3	1:A:4:DG:H2'	0.50	2.21	9	1
1:A:22:DG:H1'	1:A:23:DG:OP1	0.49	2.07	13	1
1:A:16:DG:N3	1:A:16:DG:H2'	0.49	2.23	15	1
1:A:4:DG:H1'	1:A:5:DG:O4'	0.47	2.09	14	7
1:A:4:DG:H4'	1:A:5:DG:OP1	0.47	2.10	10	2

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](#)

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](#)

1 ligand 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	D6F	A	101	-	48,48,48	1.75±0.26	11±3 (23±5%)

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	D6F	A	101	-	66,66,66	0.68±0.07	0±1 (0±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
2	D6F	A	101	-	-	0±0,30,30,30	0±0,6,6,6

5 of 12 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	A	101	D6F	C3-N1	4.67	1.33	1.42	10	15
2	A	101	D6F	C4-N1	4.65	1.33	1.42	9	14
2	A	101	D6F	C2-N1	4.64	1.33	1.42	2	14
2	A	101	D6F	C21-C17	4.06	1.39	1.49	9	14
2	A	101	D6F	C12-C22	4.05	1.39	1.49	3	14

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	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	101	D6F	C10-C4-N1	2.82	124.37	120.45	12	1
2	A	101	D6F	C3-N1-C4	2.61	114.23	119.70	7	1
2	A	101	D6F	C5-C3-N1	2.35	123.72	120.45	12	1
2	A	101	D6F	C15-C2-N1	2.26	123.59	120.45	12	1

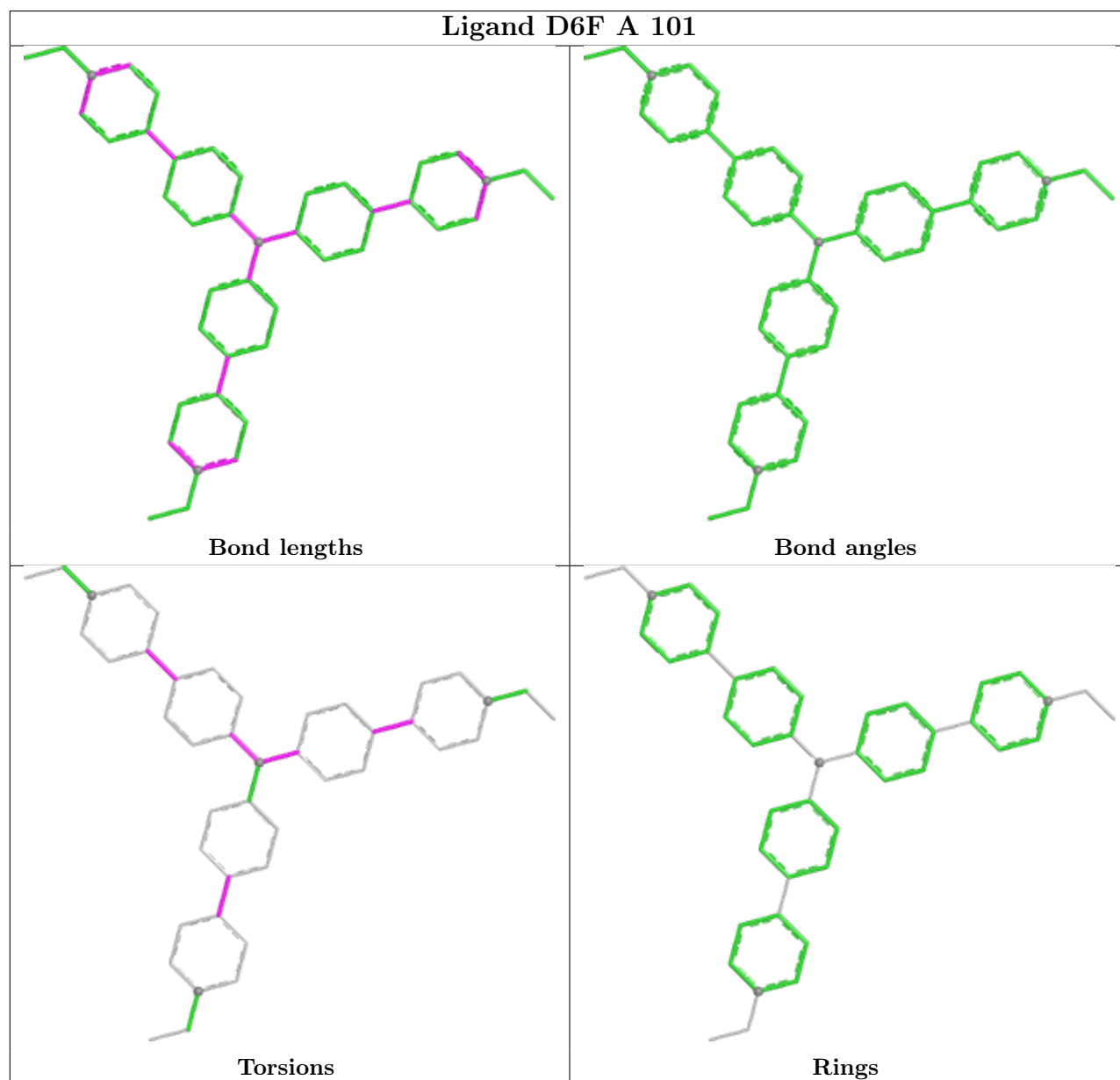
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 44% for the well-defined parts and 44% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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	285
Number of shifts mapped to atoms	246
Number of unparsed shifts	0
Number of shifts with mapping errors	39
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- No matching atom found in the structure. First 5 (of 39) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	D6F	H10	6.682	.	.
1	A	27	D6F	H14	6.682	.	.
1	A	27	D6F	H11	7.423	.	.
1	A	27	D6F	H13	7.423	.	.
1	A	27	D6F	H28	7.831	.	.
1	A	27	D6F	H32	7.839	.	.
1	A	27	D6F	H29	8.549	.	.
1	A	27	D6F	H31	8.549	.	.
1	A	27	D6F	H39	4.441	.	.
1	A	27	D6F	H9M	4.441	.	.
1	A	27	D6F	H41	1.573	.	.
1	A	27	D6F	H9O	1.573	.	.
1	A	27	D6F	H9P	1.573	.	.
1	A	27	D6F	H15	6.934	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	D6F	H19	6.934	.	.
1	A	27	D6F	H16	7.722	.	.
1	A	27	D6F	H18	7.722	.	.
1	A	27	D6F	H33	8.122	.	.
1	A	27	D6F	H37	8.122	.	.
1	A	27	D6F	H34	8.78	.	.
1	A	27	D6F	H36	8.78	.	.
1	A	27	D6F	H38	4.441	.	.
1	A	27	D6F	H9L	4.441	.	.
1	A	27	D6F	H42	1.573	.	.
1	A	27	D6F	H9Q	1.573	.	.
1	A	27	D6F	H9R	1.573	.	.
1	A	27	D6F	H5	6.141	.	.
1	A	27	D6F	H9	6.141	.	.
1	A	27	D6F	H6	7.122	.	.
1	A	27	D6F	H8	7.122	.	.
1	A	27	D6F	H23	7.348	.	.
1	A	27	D6F	H27	7.348	.	.
1	A	27	D6F	H24	8.024	.	.
1	A	27	D6F	H26	8.024	.	.
1	A	27	D6F	H40	4.441	.	.
1	A	27	D6F	H9N	4.441	.	.
1	A	27	D6F	H43	1.573	.	.
1	A	27	D6F	H9S	1.573	.	.
1	A	27	D6F	H9T	1.573	.	.

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 44%, i.e. 228 atoms were assigned a chemical shift out of a possible 520. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	182/312 (58%)	182/182 (100%)	0/130 (0%)	0/0 (—%)
Base	46/208 (22%)	46/130 (35%)	0/40 (0%)	0/38 (0%)
Overall	228/520 (44%)	228/312 (73%)	0/170 (0%)	0/38 (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.

List Id	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
1	A	15	DA	H5'	2.74	2.78 – 5.31	-5.2
1	A	20	DT	H2'	0.76	0.76 – 3.44	-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. RCI is only applicable to proteins