

# Full wwPDB NMR Structure Validation Report (i)

### Oct 28, 2022 – 01:14 am BST

PDB ID	:	8ABD
BMRB ID	:	34740
Title	:	Solution structure of Phen-DC3 intercalating into a quadruplex-duplex hybrid
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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	:	1.8.4, CSD as $541$ be (2020)
buster-report	:	1.1.7(2018)
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

Clashscore

# 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 36%.

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 Percentile F		ntile Ranks	Value
C	lashscore			0
	I.	Vorse		Better
		Percentile relative to all structures		
	[	Percentile relative to all NMR structures		
	<b>Ъ</b> <i>Т</i> а́а́а:-	Whole archive	NMR archive	
	Metric	(#Entries)	(#Entries)	

158937

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%

12864

Mol	Chain	Length	Quality of chain		
1	А	36	28%	72%	



# 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.



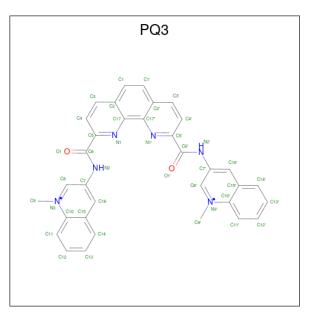
# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1228 atoms, of which 436 are hydrogens and 0 are deuteriums.

• Molecule 1 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues		Atoms			Trace		
1	٨	36	Total	С	Н	Ν	0	Р	0
1	A	- 50	1160	357	410	138	220	35	0

• Molecule 2 is N2,N9-bis (1-methylquinolin-3-yl)-1,10-phenanthroline-2,9-dicarboxa mide (three-letter code: PQ3) (formula:  $\rm C_{34}H_{26}N_6O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ate	oms		
9	۸	1	Total	С	Η	Ν	0
	A	1	68	34	26	6	2



# 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 (36-MER)

Chain A:	28%	72%
THM1 T2 A3 G5 G5 G7 G7	T10 A11 715 715 712 723 723 723 724 724 724 724 724	125 127 127 128 123 133 133 133 133 133 133 133 133 133

### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

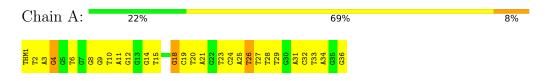
• Molecule 1: DNA (36-MER)

### 4.2.1 Score per residue for model 1

Chain A: 19% 75% 6%

## 4.2.2 Score per residue for model 2

• Molecule 1: DNA (36-MER)





#### 4.2.3 Score per residue for model 3

• Molecule 1: DNA (36-MER)



### 4.2.4 Score per residue for model 4

• Molecule 1: DNA (36-MER)



### 4.2.5 Score per residue for model 5

• Molecule 1: DNA (36-MER)

Chain A:	25%	64%	11%
THM1 T2 A3 G4 G5 G5 G7	110 411 612 615 616 617 617 720 720 721	123 724 724 725 726 727 727 728 733 733 733 733 733 733 733 733 733 73	

### 4.2.6 Score per residue for model 6

• Molecule 1: DNA (36-MER)



### 4.2.7 Score per residue for model 7

• Molecule 1: DNA (36-MER)





6%

### 4.2.8 Score per residue for model 8

• Molecule 1: DNA (36-MER)



### 4.2.9 Score per residue for model 9

### 4.2.10 Score per residue for model 10

• Molecule 1: DNA (36-MER)

Chain A:	: 14%	83%
T2 A3 G5 16 57 77	67 68 69 613 612 613	115 616 616 618 7120 7120 7120 7120 7128 7129 7129 7128 7129 7129 7128 7129 7128 7128 7128 7128 7128 7128 7128 7128



# 5 Refinement protocol and experimental data overview (i)

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

Of the 10 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	refinement	18
X-PLOR NIH	structure calculation	3.0.3

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	290
Number of shifts mapped to atoms	281
Number of unparsed shifts	0
Number of shifts with mapping errors	9
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	36%



# 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: PQ3, THM  $\,$ 

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	B	Sond lengths	Bond angles		
	Unam	RMSZ	$\#Z{>}5$	RMSZ	$\#Z{>}5$	
1	А	$1.56 {\pm} 0.01$	$0{\pm}0/823~(~0.0{\pm}~0.0\%)$	$2.34{\pm}0.02$	$57{\pm}4/1273~(~4.5{\pm}~0.3\%)$	
All	All	1.56	1/8230 ( $0.0%$ )	2.34	574/12730~(~4.5%)	

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	А	$0.0{\pm}0.0$	$3.2{\pm}1.2$
All	All	0	32

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)	Moo Worst	<b>dels</b> Total
1	А	28	DT	C5-C7	5.16	1.53	1.50	8	1

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	Turne	Atoma	Z	$Observed(^{o})$	$Ideal(^{o})$	Moo	dels
	Ullalli	nes	Type	Atoms		Observed()	Ideal()	Worst	Total
1	А	3	DA	N1-C6-N6	-11.54	111.67	118.60	2	10
1	А	2	DT	O4'-C1'-N1	10.41	115.28	108.00	6	4
1	А	27	DT	O4'-C1'-N1	9.96	114.97	108.00	3	5
1	А	11	DA	N1-C6-N6	-9.70	112.78	118.60	3	10
1	А	34	DA	N1-C6-N6	-9.12	113.13	118.60	3	10
1	А	25	DA	N1-C6-N6	-9.01	113.19	118.60	10	10
1	А	6	DT	O4'-C1'-N1	8.82	114.17	108.00	5	2
1	А	36	DG	O4'-C1'-N9	8.73	114.11	108.00	1	4



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	$Ideal(^{o})$	Mo	dels
WIOI	Ullalli	nes	туре	Atoms		Observed()	Iueai()	Worst	Total
1	А	21	DA	N1-C6-N6	-8.71	113.38	118.60	6	10
1	А	31	DA	N1-C6-N6	-8.66	113.40	118.60	8	10
1	А	26	DT	O4'-C1'-N1	8.26	113.78	108.00	4	7
1	А	20	DT	O4'-C1'-N1	8.20	113.74	108.00	8	7
1	А	3	DA	O4'-C1'-N9	8.13	113.69	108.00	5	2
1	А	19	DC	N3-C2-O2	-7.99	116.31	121.90	5	10
1	А	3	DA	C5-C6-N1	7.95	121.67	117.70	10	10
1	А	2	DT	C6-C5-C7	-7.89	118.16	122.90	5	10
1	А	26	DT	C6-C5-C7	-7.89	118.17	122.90	3	10
1	А	24	DC	N3-C2-O2	-7.87	116.39	121.90	6	10
1	А	20	DT	C6-C5-C7	-7.84	118.20	122.90	2	10
1	А	11	DA	C5-C6-N1	7.77	121.58	117.70	6	10
1	А	25	DA	C5-C6-N1	7.70	121.55	117.70	4	10
1	А	32	DC	N3-C2-O2	-7.67	116.53	121.90	2	10
1	А	10	DT	C6-C5-C7	-7.45	118.43	122.90	10	10
1	А	31	DA	C5-C6-N1	7.37	121.38	117.70	5	10
1	А	30	DG	O4'-C1'-N9	7.24	113.07	108.00	8	9
1	А	27	DT	C6-C5-C7	-7.24	118.56	122.90	6	10
1	А	9	DG	O4'-C1'-N9	7.22	113.06	108.00	10	4
1	А	21	DA	C5-C6-N1	7.21	121.30	117.70	4	10
1	А	11	DA	C4-C5-C6	-7.21	113.40	117.00	3	10
1	А	12	DG	P-O3'-C3'	7.05	128.16	119.70	8	2
1	А	34	DA	C5-C6-N1	7.00	121.20	117.70	5	10
1	А	18	DG	O4'-C1'-N9	7.00	112.90	108.00	2	2
1	А	3	DA	C4-C5-C6	-6.95	113.52	117.00	10	10
1	А	6	DT	C6-C5-C7	-6.94	118.74	122.90	3	10
1	А	28	DT	C6-C5-C7	-6.84	118.80	122.90	2	10
1	А	31	DA	C4-C5-C6	-6.75	113.63	117.00	2	10
1	А	25	DA	C4-C5-C6	-6.73	113.64	117.00	9	10
1	А	7	DG	P-O3'-C3'	6.68	127.72	119.70	5	2
1	А	15	DT	C6-C5-C7	-6.63	118.92	122.90	6	10
1	А	34	DA	C4-C5-C6	-6.62	113.69	117.00	6	10
1	А	4	DG	P-O3'-C3'	6.45	127.44	119.70	3	2
1	А	23	DT	C6-C5-C7	-6.39	119.07	122.90	8	10
1	А	21	DA	C4-C5-C6	-6.38	113.81	117.00	4	10
1	А	29	DT	O4'-C1'-N1	6.36	112.45	108.00	2	1
1	А	2	DT	N3-C2-O2	-6.28	118.53	122.30	7	9
1	А	29	DT	C6-C5-C7	-6.25	119.15	122.90	10	10
1	A	24	DC	N1-C2-O2	6.24	122.65	118.90	4	10
1	A	12	DG	O4'-C1'-N9	6.19	112.33	108.00	10	3
1	A	32	DC	N1-C2-O2	6.17	122.60	118.90	2	10

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Mol	Chain	Res	Turne	Atoma	Z	Observed(0)	Ideal(0)	Mo	dels
IVIOI	Unain	nes	Type	Atoms	L	$\mathbf{Observed}(^{o})$	$\mathrm{Ideal}(^{o})$	Worst	Total
1	А	27	DT	P-O3'-C3'	6.16	127.10	119.70	4	2
1	А	20	DT	N3-C2-O2	-6.09	118.65	122.30	8	10
1	А	4	DG	O4'-C1'-N9	6.08	112.25	108.00	2	2
1	А	15	DT	N3-C2-O2	-6.05	118.67	122.30	8	10
1	А	5	DG	P-O3'-C3'	6.03	126.93	119.70	1	1
1	А	33	DT	C6-C5-C7	-6.00	119.30	122.90	8	10
1	А	28	DT	N3-C2-O2	-5.97	118.72	122.30	8	9
1	А	19	DC	N1-C2-O2	5.95	122.47	118.90	5	10
1	А	35	DG	O4'-C1'-N9	5.92	112.14	108.00	3	1
1	А	6	DT	N3-C2-O2	-5.88	118.77	122.30	5	10
1	А	26	DT	N3-C2-O2	-5.88	118.77	122.30	8	8
1	А	10	DT	N3-C2-O2	-5.85	118.79	122.30	8	10
1	А	36	DG	N3-C4-C5	-5.84	125.68	128.60	2	8
1	А	23	DT	N3-C2-O2	-5.82	118.81	122.30	8	10
1	А	29	DT	N3-C2-O2	-5.80	118.82	122.30	3	10
1	А	5	DG	O4'-C1'-N9	5.72	112.00	108.00	5	2
1	А	27	DT	N3-C2-O2	-5.66	118.90	122.30	8	9
1	А	35	DG	P-O3'-C3'	5.62	126.45	119.70	8	1
1	А	25	DA	O4'-C4'-C3'	5.53	109.32	106.00	3	1
1	А	33	DT	N3-C2-O2	-5.49	119.01	122.30	7	10
1	А	9	DG	N3-C2-N2	-5.40	116.12	119.90	6	1
1	А	14	DG	N3-C2-N2	-5.39	116.13	119.90	10	3
1	А	15	DT	O4'-C1'-C2'	-5.37	101.61	105.90	8	1
1	А	12	DG	N3-C2-N2	-5.35	116.16	119.90	2	5
1	А	8	DG	P-O3'-C3'	5.35	126.12	119.70	6	1
1	А	15	DT	P-O3'-C3'	5.34	126.11	119.70	10	1
1	А	10	DT	P-O3'-C3'	5.31	126.08	119.70	8	1
1	А	11	DA	O4'-C1'-N9	5.27	111.69	108.00	7	2
1	А	27	DT	C5-C6-N1	-5.25	120.55	123.70	3	1
1	А	4	DG	N3-C2-N2	-5.19	116.27	119.90	10	5
1	А	17	DG	N3-C2-N2	-5.18	116.28	119.90	4	4
1	А	36	DG	C1'-O4'-C4'	-5.17	104.93	110.10	2	3
1	А	7	DG	O4'-C1'-N9	5.16	111.61	108.00	1	1
1	А	16	DG	O4'-C1'-N9	5.12	111.59	108.00	10	1
1	А	18	DG	O4'-C4'-C3'	5.10	109.06	106.00	8	1
1	А	8	DG	N3-C2-N2	-5.10	116.33	119.90	2	1
1	А	19	DC			109.05	106.00	10	1
1	А	35	DG	N1-C6-O6	-5.08	116.85	119.90	3	2
1	А	36	DG	C5-C6-N1	5.07	114.03	111.50	6	1
1	А	16	DG	N3-C2-N2	-5.07	116.35	119.90	10	3
1	А	7	DG	N3-C2-N2	-5.06	116.36	119.90	1	1

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Mol	Chain	Dec	Trune	Atoma	7	Observed <sup>(0)</sup>	$Ideal(^{o})$	Mod	dels
	Chain	$\operatorname{Res}$	Type	Atoms		$\mathbf{Observed}(^{o})$	Ideal(*)	Worst	Total
1	А	2	DT	C5-C6-N1	-5.06	120.67	123.70	9	1
1	А	22	DG	N1-C6-O6	-5.04	116.87	119.90	6	1
1	А	13	DG	N3-C2-N2	-5.03	116.38	119.90	3	1
1	А	4	DG	C5-C6-N1	5.02	114.01	111.50	2	1
1	А	5	DG	N3-C2-N2	-5.01	116.39	119.90	8	1

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There are no chirality outliers.

All 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	А	23	DT	Sidechain	4
1	А	25	DA	Sidechain	4
1	А	4	DG	Sidechain	4
1	А	2	DT	Sidechain	4
1	А	33	DT	Sidechain	4
1	А	36	DG	Sidechain	4
1	А	7	DG	Sidechain	3
1	А	26	DT	Sidechain	2
1	А	18	DG	Sidechain	1
1	А	29	DT	Sidechain	1
1	А	15	DT	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
All	All	7920	4360	4360	-

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.

Mal	Tuno	Chain	Dog	Link		Bond leng	ths
	Type	Ullalli	nes	Link	Counts	RMSZ	#Z>2
1	THM	А	1	1	$18,\!18,\!18$	$0.67 {\pm} 0.02$	$0\pm0~(0\pm0\%)$

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	Turne	Chain	Dec	Tink		Bond an	gles
10101	Type	Chain	nes	LIIIK	Counts	RMSZ	#Z>2
1	THM	А	1	1	26,26,26	$1.31 \pm 0.08$	3±0 (13±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	THM	А	1	1	-	$0\pm 0,\!6,\!18,\!18$	$0\pm0,2,2,2$

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	Dec	Trune	Atoma	Z	Observed <sup>(0)</sup>	Ideal(°)	Moo	lels
	Chain	$\operatorname{Res}$	Type	Atoms	L	$\mathbf{Observed}(^{o})$	Ideal(*)	Worst	Total
1	А	1	THM	C6-C5-C4	3.23	120.73	118.03	5	10
1	А	1	THM	C5M-C5-C6	3.06	118.76	122.85	5	10
1	А	1	THM	O4'-C1'-N1	3.01	113.23	107.86	2	4
1	А	1	THM	O3'-C3'-C4'	2.54	119.81	110.10	9	1
1	А	1	THM	C5-C6-N1	2.53	120.73	123.34	9	9

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)

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.

Mal	Turne	Chain	Dec	Tink		Bond len	$\mathbf{gths}$
10101	туре	Unam	nes	Link	Counts	RMSZ	#Z>2
2	PQ3	А	101	-	48,48,48	$1.58 {\pm} 0.01$	8±1 (15±1%)



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.

Mal	Type	Chain	Dog	Link		Bond an	igles
WIOI	Type	Ullalli	nes	Link	Counts	RMSZ	#Z>2
2	PQ3	А	101	-	66,70,70	$1.67 {\pm} 0.04$	$16\pm0$ (23 $\pm0\%$ )

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	PQ3	А	101	-	-	$0\pm0,16,62,62$	$0\pm 0,7,7,7$

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Tuno	Atoms	ms Z $Observed(Å)$		Ideal(Å)	Moo	dels
	Ullalli	nes	Type	Atoms	L	Observeu(A)	Iueai(A)	Worst	Total
2	А	101	PQ3	C8'-N3'	4.32	1.38	1.33	10	10
2	А	101	PQ3	C8-N3	4.20	1.38	1.33	9	10
2	А	101	PQ3	C4-C5	3.06	1.44	1.39	3	10
2	А	101	PQ3	C4'-C5'	3.03	1.44	1.39	10	10
2	А	101	PQ3	C16'-C7'	2.72	1.43	1.37	10	10
2	А	101	PQ3	C16-C7	2.62	1.43	1.37	2	10
2	А	101	PQ3	C8-C7	2.15	1.35	1.39	1	8
2	А	101	PQ3	C8'-C7'	2.15	1.35	1.39	7	8

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mal	Mol Chain		Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$	Models	
	Ullaili	$\operatorname{Res}$	туре	Atoms		Observed()	Ideal()	Worst	Total
2	А	101	PQ3	C5'-N1'-C17'	3.65	121.70	117.50	6	10
2	А	101	PQ3	C9-N3-C8	3.59	115.02	118.81	7	10
2	А	101	PQ3	C5-N1-C17	3.51	121.54	117.50	8	10
2	А	101	PQ3	C11-C10-N3	3.38	129.01	120.84	7	10
2	А	101	PQ3	C9'-N3'-C8'	3.37	115.25	118.81	7	7
2	А	101	PQ3	C11'-C10'-N3'	3.36	128.97	120.84	7	10



N/ al	Mol Chain		<b>T</b> 0	<b>A t a m a</b>	7	$Oh$ a series $d(\theta)$		Mod	dels
IVIOI	Chain	$\operatorname{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathrm{Ideal}(^{o})$	Worst	Total
2	А	101	PQ3	C8'-N3'-C10'	3.13	124.33	121.59	3	10
2	А	101	PQ3	C4'-C5'-N1'	3.07	119.62	123.42	3	10
2	А	101	PQ3	C8-N3-C10	3.02	124.24	121.59	3	10
2	А	101	PQ3	C4-C5-N1	2.89	119.84	123.42	7	10
2	А	101	PQ3	C16'-C15'-C10'	2.81	123.12	118.92	7	10
2	А	101	PQ3	C16-C15-C10	2.73	123.01	118.92	3	10
2	А	101	PQ3	C15-C10-N3	2.64	111.97	118.13	7	10
2	А	101	PQ3	C15'-C10'-N3'	2.63	112.01	118.13	7	10
2	А	101	PQ3	C6'-C5'-N1'	2.55	123.59	116.94	8	10
2	А	101	PQ3	C6-C5-N1	2.46	123.35	116.94	7	10

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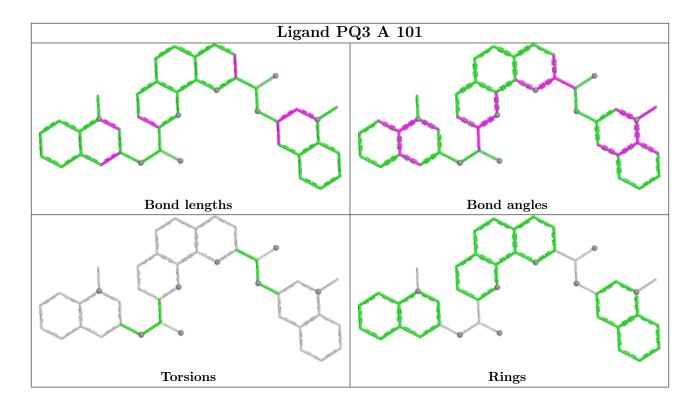
There are no chirality outliers.

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 then 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 sufficient 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 (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 36% for the well-defined parts and 36% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list* 

### 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	290
Number of shifts mapped to atoms	281
Number of unparsed shifts	0
Number of shifts with mapping errors	9
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

• Residue not found in structure. All 9 occurences are reported below.

Chain	Dec	Turne	Atom		Shift Data	1 I
Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
А	1	DT	C6	139.428	-1.0	1
А	1	DT	H3'	4.326	0.003	1
A	1	DT	H2'	1.954	0.002	1
А	1	DT	H2"	2.139	0.003	1
А	1	DT	H6	7.33	0.002	1
А	1	DT	H73	1.551	0.004	1
А	1	DT	H71	1.551	0.004	1
А	1	DT	H72	1.551	0.004	1
А	1	DT	H1'	5.623	0.004	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 36%, i.e. 248 atoms were assigned a chemical shift out of a possible 693. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}$ 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	248/693~(36%)	208/413~(50%)	40/230~(17%)	0/50~(0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 36%, i.e. 248 atoms were assigned a chemical shift out of a possible 693. 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	248/693~(36%)	208/413~(50%)	40/230~(17%)	0/50~(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 (assigned\_chem\_shift\_list). RCI is only applicable to proteins.

