



# Full wwPDB NMR Structure Validation Report ⓘ

Jan 4, 2021 – 08:30 PM JST

PDB ID : 6LNZ  
Title : NMR solution structure of VEGF G-quadruplex bound a non-planar cyclometalated-carbene platinum(II) complex  
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Deposited on : 2020-01-02

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (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 : 2.16  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.16



## 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.

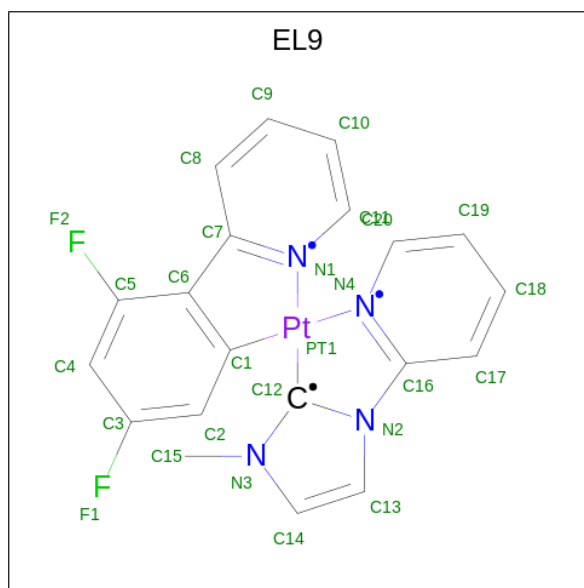
### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 749 atoms, of which 262 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	22	707	215	247	91	133	21	0

- Molecule 2 is cyclometalated-carbene platinum(II) complex (three-letter code: EL9) (formula: C<sub>20</sub>H<sub>15</sub>F<sub>2</sub>N<sub>4</sub>Pt) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					
			Total	C	F	H	N	Pt
2	A	1	42	20	2	15	4	1

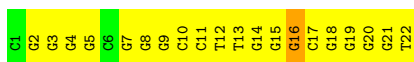
## 4 Residue-property plots

### 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: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

Chain A: 



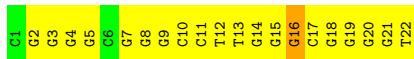
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

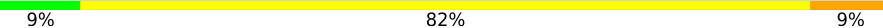
- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

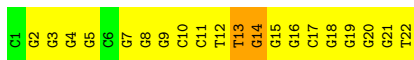
Chain A: 



#### 4.2.2 Score per residue for model 2

- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

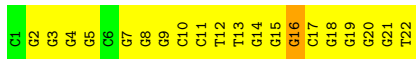
Chain A: 



### 4.2.3 Score per residue for model 3

- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

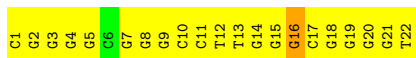
Chain A:  9% 86% 5%



### 4.2.4 Score per residue for model 4

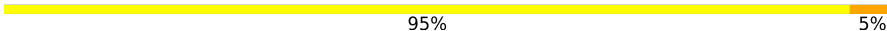
- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

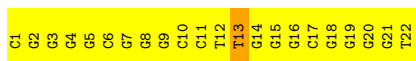
Chain A:  5% 91% 5%



### 4.2.5 Score per residue for model 5

- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

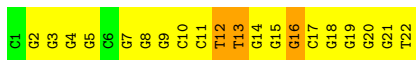
Chain A:  95% 5%



### 4.2.6 Score per residue for model 6

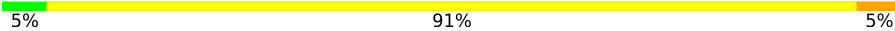
- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

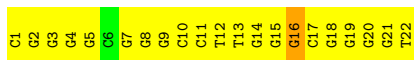
Chain A:  9% 77% 14%



### 4.2.7 Score per residue for model 7

- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

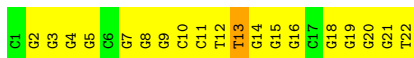
Chain A:  5% 91% 5%



#### 4.2.8 Score per residue for model 8

- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

Chain A:  14% 82% 5%



#### 4.2.9 Score per residue for model 9

- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

Chain A:  14% 73% 14%



#### 4.2.10 Score per residue for model 10

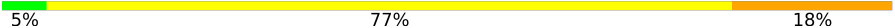
- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

Chain A:  9% 77% 14%



#### 4.2.11 Score per residue for model 11

- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

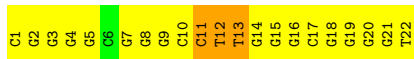
Chain A:  5% 77% 18%



#### 4.2.12 Score per residue for model 12

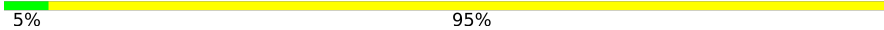
- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

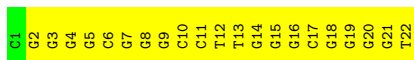
Chain A:  5% 82% 14%



#### 4.2.13 Score per residue for model 13


- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

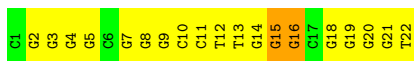
Chain A:  5% 95%



#### 4.2.14 Score per residue for model 14

- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

Chain A:  14% 77% 9%



#### 4.2.15 Score per residue for model 15

- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*TP\*TP\*GP\*GP\*GP\*CP\*GP\*GP\*GP\*GP\*T)-3')

Chain A:  9% 77% 14%





## 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	
Discovery Studio	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	230
Number of shifts mapped to atoms	230
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

## 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: EL9

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	2.09±0.16	19±6/517 ( 3.6± 1.2%)	3.17±0.18	76±15/800 ( 9.5± 1.8%)
All	All	2.10	279/7755 ( 3.6%)	3.17	1142/12000 ( 9.5%)

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	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	12	DT	C4'-C3'	12.64	1.66	1.53	1	6
1	A	14	DG	C5'-C4'	12.61	1.65	1.51	12	2
1	A	12	DT	C5'-C4'	11.86	1.64	1.51	1	11
1	A	11	DC	C4'-C3'	10.67	1.64	1.53	13	6
1	A	9	DG	C5'-C4'	10.62	1.63	1.51	8	3
1	A	9	DG	P-O5'	10.44	1.70	1.59	8	3
1	A	12	DT	O3'-P	-10.41	1.48	1.61	4	3
1	A	6	DC	O3'-P	10.12	1.73	1.61	5	2
1	A	11	DC	C5'-C4'	10.01	1.62	1.51	12	8
1	A	13	DT	C5'-C4'	9.66	1.61	1.51	8	4
1	A	14	DG	P-O5'	9.61	1.69	1.59	12	3
1	A	14	DG	O3'-P	-9.56	1.49	1.61	7	5
1	A	9	DG	O3'-P	-9.53	1.49	1.61	15	4
1	A	17	DC	O3'-P	-9.53	1.49	1.61	13	2
1	A	9	DG	C2'-C1'	9.14	1.61	1.52	7	4
1	A	8	DG	O3'-P	-8.88	1.50	1.61	11	4
1	A	22	DT	C5-C7	8.78	1.55	1.50	3	15
1	A	12	DT	C5-C7	8.78	1.55	1.50	10	15
1	A	13	DT	C5-C7	8.72	1.55	1.50	12	15
1	A	13	DT	C2'-C1'	8.60	1.60	1.52	12	3
1	A	12	DT	C2'-C1'	8.21	1.60	1.52	5	3
1	A	21	DG	C2'-C1'	8.20	1.60	1.52	14	1
1	A	13	DT	P-OP1	7.82	1.62	1.49	5	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	13	DT	P-OP2	7.61	1.61	1.49	5	7
1	A	12	DT	C3'-C2'	7.55	1.61	1.52	5	3
1	A	21	DG	C5'-C4'	7.46	1.59	1.51	5	7
1	A	17	DC	P-O5'	-7.40	1.52	1.59	12	1
1	A	21	DG	O3'-P	-7.34	1.52	1.61	7	2
1	A	12	DT	P-OP2	7.11	1.61	1.49	12	4
1	A	12	DT	P-O5'	7.03	1.66	1.59	13	2
1	A	11	DC	O3'-P	6.93	1.69	1.61	12	3
1	A	10	DC	C3'-C2'	6.92	1.60	1.52	14	7
1	A	15	DG	P-OP1	6.84	1.60	1.49	15	11
1	A	14	DG	P-OP2	6.84	1.60	1.49	10	5
1	A	2	DG	C5'-C4'	6.81	1.58	1.51	11	5
1	A	14	DG	P-OP1	6.62	1.60	1.49	12	6
1	A	9	DG	P-OP2	6.62	1.60	1.49	11	6
1	A	13	DT	O3'-P	-6.62	1.53	1.61	11	3
1	A	21	DG	C4'-C3'	6.54	1.59	1.53	13	1
1	A	10	DC	O3'-P	6.54	1.69	1.61	12	2
1	A	22	DT	P-O5'	-6.48	1.53	1.59	9	3
1	A	16	DG	C4'-O4'	-6.46	1.38	1.45	7	1
1	A	12	DT	C3'-O3'	6.44	1.52	1.44	5	2
1	A	9	DG	C3'-C2'	6.29	1.59	1.52	13	2
1	A	18	DG	C5'-C4'	6.24	1.58	1.51	5	1
1	A	22	DT	C4'-O4'	-6.22	1.38	1.45	11	1
1	A	15	DG	P-OP2	6.09	1.59	1.49	1	8
1	A	6	DC	P-O5'	-6.09	1.53	1.59	5	1
1	A	3	DG	P-O5'	-5.94	1.53	1.59	8	1
1	A	10	DC	P-OP2	5.92	1.59	1.49	1	2
1	A	6	DC	P-OP1	5.90	1.58	1.49	13	1
1	A	9	DG	C4'-O4'	-5.90	1.39	1.45	15	1
1	A	11	DC	P-OP2	5.85	1.58	1.49	13	3
1	A	11	DC	C2'-C1'	5.78	1.58	1.52	7	1
1	A	9	DG	P-OP1	5.75	1.58	1.49	6	4
1	A	12	DT	P-OP1	5.71	1.58	1.49	4	4
1	A	11	DC	C4'-O4'	-5.70	1.39	1.45	10	1
1	A	16	DG	P-OP1	5.70	1.58	1.49	14	10
1	A	13	DT	P-O5'	5.65	1.65	1.59	11	2
1	A	16	DG	P-OP2	5.61	1.58	1.49	5	6
1	A	7	DG	P-OP2	5.60	1.58	1.49	5	1
1	A	10	DC	P-OP1	5.56	1.58	1.49	9	6
1	A	7	DG	P-OP1	5.51	1.58	1.49	5	1
1	A	5	DG	C5'-C4'	5.44	1.57	1.51	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	13	DT	C4'-C3'	5.44	1.58	1.53	5	1
1	A	21	DG	C3'-C2'	5.38	1.58	1.52	14	1
1	A	15	DG	C5'-C4'	5.34	1.57	1.51	13	2
1	A	10	DC	C5'-C4'	5.30	1.57	1.51	4	1
1	A	9	DG	C4'-C3'	5.24	1.58	1.53	3	1
1	A	11	DC	P-OP1	5.18	1.57	1.49	9	1
1	A	18	DG	P-OP2	5.16	1.57	1.49	13	1
1	A	21	DG	P-OP1	5.13	1.57	1.49	4	1
1	A	13	DT	C4'-O4'	-5.10	1.40	1.45	9	1
1	A	17	DC	P-OP2	5.09	1.57	1.49	2	1
1	A	21	DG	C5-C4	5.09	1.42	1.38	8	1
1	A	16	DG	C5'-C4'	5.09	1.56	1.51	13	1
1	A	14	DG	C4'-O4'	-5.03	1.40	1.45	13	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	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	10	DC	O4'-C1'-N1	-34.97	83.52	108.00	4	12
1	A	14	DG	P-O3'-C3'	22.35	146.52	119.70	7	12
1	A	10	DC	N1-C1'-C2'	18.96	148.63	112.60	11	14
1	A	13	DT	O4'-C1'-N1	16.85	119.79	108.00	4	8
1	A	1	DC	P-O3'-C3'	15.92	138.80	119.70	11	5
1	A	12	DT	O3'-P-O5'	15.81	134.03	104.00	6	13
1	A	13	DT	O5'-P-OP2	-15.64	91.62	105.70	11	10
1	A	9	DG	O4'-C1'-C2'	-15.57	93.44	105.90	13	8
1	A	12	DT	O4'-C1'-C2'	-15.29	93.67	105.90	9	7
1	A	9	DG	OP1-P-OP2	-15.15	96.87	119.60	13	7
1	A	11	DC	O4'-C1'-N1	-15.04	97.47	108.00	2	8
1	A	22	DT	O4'-C4'-C3'	-14.95	97.03	106.00	11	2
1	A	14	DG	O4'-C4'-C3'	-14.93	97.04	106.00	13	2
1	A	9	DG	O4'-C4'-C3'	-14.65	97.21	106.00	3	6
1	A	13	DT	O4'-C4'-C3'	-14.37	97.38	106.00	8	8
1	A	12	DT	O5'-P-OP1	-14.06	93.05	105.70	12	5
1	A	13	DT	O4'-C1'-C2'	-13.98	94.71	105.90	12	8
1	A	11	DC	O3'-P-O5'	13.89	130.40	104.00	13	12
1	A	8	DG	O3'-P-O5'	13.69	130.01	104.00	13	6
1	A	16	DG	OP1-P-OP2	-13.56	99.27	119.60	3	14
1	A	14	DG	OP1-P-OP2	-13.39	99.51	119.60	2	7
1	A	12	DT	O4'-C4'-C3'	-13.23	98.06	106.00	4	5
1	A	11	DC	O4'-C1'-C2'	-13.17	95.36	105.90	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	10	DC	O5'-P-OP2	-13.01	93.99	105.70	9	7
1	A	13	DT	OP1-P-OP2	-12.92	100.22	119.60	8	10
1	A	12	DT	O5'-P-OP2	-12.85	94.14	105.70	8	7
1	A	11	DC	N1-C2-O2	12.82	126.59	118.90	13	1
1	A	12	DT	O4'-C1'-N1	12.77	116.94	108.00	1	5
1	A	14	DG	P-O5'-C5'	12.58	141.03	120.90	10	6
1	A	16	DG	O4'-C1'-N9	-12.52	99.24	108.00	7	5
1	A	9	DG	O5'-P-OP2	-12.35	94.59	105.70	14	4
1	A	13	DT	C4'-C3'-C2'	-12.17	92.14	103.10	5	2
1	A	14	DG	O5'-P-OP2	-12.13	94.78	105.70	8	3
1	A	10	DC	O4'-C1'-C2'	-12.12	96.20	105.90	4	10
1	A	15	DG	OP1-P-OP2	-11.96	101.66	119.60	12	13
1	A	20	DG	O3'-P-O5'	11.69	126.20	104.00	14	8
1	A	10	DC	OP1-P-OP2	-11.65	102.13	119.60	1	15
1	A	11	DC	P-O3'-C3'	11.64	133.66	119.70	7	11
1	A	16	DG	O4'-C4'-C3'	-11.60	99.04	106.00	13	3
1	A	20	DG	P-O3'-C3'	11.51	133.51	119.70	9	4
1	A	9	DG	O4'-C1'-N9	-11.51	99.95	108.00	14	6
1	A	15	DG	O4'-C1'-N9	-11.20	100.16	108.00	13	5
1	A	10	DC	O3'-P-O5'	10.98	124.86	104.00	4	14
1	A	13	DT	P-O3'-C3'	-10.84	106.69	119.70	11	4
1	A	13	DT	C3'-C2'-C1'	10.65	115.28	102.50	12	5
1	A	12	DT	C1'-O4'-C4'	10.53	120.63	110.10	5	8
1	A	13	DT	O3'-P-O5'	10.43	123.82	104.00	4	7
1	A	22	DT	O4'-C1'-N1	-10.32	100.77	108.00	11	1
1	A	2	DG	O4'-C1'-N9	-10.17	100.88	108.00	5	2
1	A	22	DT	O4'-C1'-C2'	-10.12	97.80	105.90	11	1
1	A	15	DG	P-O3'-C3'	10.08	131.80	119.70	13	11
1	A	11	DC	OP1-P-OP2	-9.95	104.67	119.60	2	15
1	A	11	DC	N3-C2-O2	-9.94	114.94	121.90	13	1
1	A	14	DG	O4'-C1'-C2'	-9.88	98.00	105.90	13	1
1	A	10	DC	O5'-P-OP1	-9.74	96.93	105.70	3	2
1	A	13	DT	O5'-P-OP1	-9.66	97.00	105.70	13	5
1	A	9	DG	P-O3'-C3'	9.64	131.27	119.70	7	6
1	A	16	DG	O4'-C1'-C2'	-9.64	98.19	105.90	11	5
1	A	10	DC	O4'-C4'-C3'	-9.61	100.23	106.00	13	5
1	A	11	DC	C4'-C3'-C2'	9.53	111.68	103.10	8	4
1	A	12	DT	P-O5'-C5'	-9.52	105.66	120.90	10	6
1	A	15	DG	N7-C8-N9	9.41	117.80	113.10	11	15
1	A	2	DG	N7-C8-N9	9.40	117.80	113.10	11	15
1	A	5	DG	N7-C8-N9	9.39	117.79	113.10	11	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	7	DG	N7-C8-N9	9.37	117.79	113.10	9	15
1	A	3	DG	N7-C8-N9	9.37	117.78	113.10	3	15
1	A	8	DG	N7-C8-N9	9.35	117.78	113.10	1	15
1	A	4	DG	N7-C8-N9	9.35	117.77	113.10	3	15
1	A	16	DG	N7-C8-N9	9.34	117.77	113.10	10	15
1	A	21	DG	O4'-C1'-N9	-9.32	101.47	108.00	11	6
1	A	14	DG	N7-C8-N9	9.31	117.75	113.10	9	15
1	A	19	DG	N7-C8-N9	9.30	117.75	113.10	4	15
1	A	21	DG	N7-C8-N9	9.29	117.74	113.10	4	15
1	A	20	DG	N7-C8-N9	9.28	117.74	113.10	3	15
1	A	9	DG	N7-C8-N9	9.27	117.73	113.10	3	15
1	A	18	DG	N7-C8-N9	9.26	117.73	113.10	2	15
1	A	12	DT	C4'-C3'-C2'	-9.23	94.79	103.10	11	4
1	A	10	DC	C1'-O4'-C4'	9.18	119.28	110.10	4	4
1	A	15	DG	O3'-P-O5'	9.05	121.20	104.00	13	9
1	A	12	DT	P-O3'-C3'	9.04	130.55	119.70	5	5
1	A	15	DG	N9-C1'-C2'	9.04	129.78	112.60	11	11
1	A	6	DC	OP1-P-OP2	-9.04	106.04	119.60	5	2
1	A	14	DG	OP1-P-O3'	9.03	125.06	105.20	12	4
1	A	11	DC	N1-C1'-C2'	-9.00	95.51	112.60	11	6
1	A	5	DG	P-O3'-C3'	8.93	130.42	119.70	13	2
1	A	14	DG	O4'-C1'-N9	-8.81	101.83	108.00	13	2
1	A	21	DG	OP1-P-OP2	-8.80	106.40	119.60	12	12
1	A	12	DT	C3'-C2'-C1'	8.79	113.05	102.50	6	10
1	A	14	DG	C5'-C4'-C3'	8.79	129.92	114.10	12	1
1	A	11	DC	O4'-C4'-C3'	-8.70	100.78	106.00	10	7
1	A	9	DG	C3'-C2'-C1'	8.65	112.88	102.50	13	4
1	A	17	DC	N1-C1'-C2'	-8.64	96.18	112.60	13	2
1	A	9	DG	OP2-P-O3'	8.62	124.16	105.20	15	2
1	A	9	DG	C4'-C3'-C2'	-8.59	95.37	103.10	7	3
1	A	12	DT	OP1-P-OP2	-8.39	107.02	119.60	9	9
1	A	17	DC	OP1-P-OP2	-8.37	107.05	119.60	2	4
1	A	2	DG	O3'-P-O5'	8.12	119.44	104.00	8	1
1	A	21	DG	C4'-C3'-C2'	-8.11	95.81	103.10	14	2
1	A	11	DC	OP2-P-O3'	-7.97	87.67	105.20	8	2
1	A	15	DG	C8-N9-C4	-7.91	103.23	106.40	13	15
1	A	3	DG	C8-N9-C4	-7.90	103.24	106.40	3	15
1	A	13	DT	C1'-O4'-C4'	7.89	118.00	110.10	7	6
1	A	3	DG	OP1-P-OP2	-7.89	107.77	119.60	8	1
1	A	15	DG	O5'-P-OP2	-7.88	98.61	105.70	1	2
1	A	4	DG	C8-N9-C4	-7.87	103.25	106.40	15	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	2	DG	C8-N9-C4	-7.86	103.25	106.40	11	15
1	A	20	DG	C8-N9-C4	-7.86	103.25	106.40	6	15
1	A	12	DT	OP2-P-O3'	7.85	122.47	105.20	9	2
1	A	6	DC	P-O3'-C3'	7.84	129.11	119.70	5	1
1	A	16	DG	C8-N9-C4	-7.78	103.29	106.40	12	15
1	A	21	DG	O4'-C1'-C2'	-7.77	99.68	105.90	14	2
1	A	21	DG	C8-N9-C4	-7.77	103.29	106.40	15	15
1	A	2	DG	N9-C1'-C2'	-7.75	97.87	112.60	12	1
1	A	5	DG	C8-N9-C4	-7.75	103.30	106.40	10	15
1	A	14	DG	OP2-P-O3'	7.75	122.24	105.20	9	4
1	A	3	DG	O5'-P-OP2	-7.72	98.76	105.70	8	1
1	A	14	DG	C8-N9-C4	-7.71	103.31	106.40	15	15
1	A	8	DG	C8-N9-C4	-7.71	103.32	106.40	8	15
1	A	9	DG	OP1-P-O3'	7.70	122.15	105.20	11	4
1	A	7	DG	C8-N9-C4	-7.70	103.32	106.40	15	15
1	A	9	DG	C8-N9-C4	-7.70	103.32	106.40	6	15
1	A	18	DG	C8-N9-C4	-7.69	103.32	106.40	14	15
1	A	19	DG	C8-N9-C4	-7.67	103.33	106.40	5	15
1	A	11	DC	C1'-O4'-C4'	-7.61	102.49	110.10	5	3
1	A	12	DT	C5'-C4'-O4'	7.60	123.74	109.30	4	1
1	A	2	DG	OP1-P-OP2	-7.59	108.22	119.60	4	7
1	A	18	DG	OP1-P-OP2	-7.54	108.28	119.60	13	2
1	A	9	DG	C5'-C4'-C3'	7.48	127.56	114.10	8	4
1	A	15	DG	O5'-P-OP1	-7.47	98.97	105.70	11	3
1	A	9	DG	O3'-P-O5'	7.44	118.13	104.00	8	11
1	A	13	DT	P-O5'-C5'	-7.42	109.02	120.90	10	2
1	A	15	DG	OP1-P-O3'	7.38	121.43	105.20	15	4
1	A	6	DC	O5'-P-OP1	7.32	119.48	110.70	13	1
1	A	21	DG	C3'-C2'-C1'	7.28	111.23	102.50	14	1
1	A	15	DG	O4'-C1'-C2'	-7.06	100.25	105.90	1	2
1	A	16	DG	O3'-P-O5'	7.02	117.35	104.00	2	3
1	A	12	DT	OP1-P-O3'	7.01	120.61	105.20	2	5
1	A	14	DG	O3'-P-O5'	6.99	117.28	104.00	1	8
1	A	9	DG	O5'-P-OP1	6.99	119.09	110.70	8	1
1	A	12	DT	N1-C1'-C2'	6.96	125.83	112.60	13	2
1	A	2	DG	C4'-C3'-C2'	6.93	109.34	103.10	8	1
1	A	13	DT	C5'-C4'-C3'	6.92	126.56	114.10	5	1
1	A	9	DG	C1'-O4'-C4'	6.88	116.98	110.10	7	5
1	A	22	DT	OP1-P-OP2	-6.88	109.29	119.60	11	3
1	A	2	DG	P-O3'-C3'	6.82	127.88	119.70	11	1
1	A	12	DT	C5'-C4'-C3'	6.81	126.36	114.10	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	DC	C5'-C4'-O4'	-6.77	96.43	109.30	11	2
1	A	14	DG	O5'-P-OP1	-6.74	99.64	105.70	2	1
1	A	13	DT	N1-C1'-C2'	6.70	125.32	112.60	9	1
1	A	21	DG	O3'-P-O5'	6.68	116.69	104.00	7	3
1	A	15	DG	O4'-C4'-C3'	-6.57	101.87	104.50	1	5
1	A	6	DC	N1-C1'-C2'	-6.55	100.15	112.60	13	1
1	A	21	DG	C1'-O4'-C4'	6.43	116.53	110.10	11	2
1	A	21	DG	P-O3'-C3'	6.43	127.42	119.70	14	4
1	A	11	DC	C4'-C3'-O3'	6.42	125.75	109.70	1	3
1	A	14	DG	N9-C1'-C2'	6.42	124.79	112.60	13	1
1	A	5	DG	O3'-P-O5'	6.35	116.07	104.00	5	2
1	A	21	DG	OP1-P-O3'	6.35	119.17	105.20	9	1
1	A	6	DC	O4'-C1'-N1	-6.31	103.59	108.00	13	1
1	A	2	DG	C1'-O4'-C4'	6.29	116.39	110.10	11	2
1	A	11	DC	O5'-P-OP2	-6.29	100.04	105.70	12	2
1	A	6	DC	O4'-C4'-C3'	-6.28	101.99	104.50	13	1
1	A	11	DC	O5'-P-OP1	6.21	118.16	110.70	15	1
1	A	5	DG	O4'-C1'-C2'	-6.16	100.97	105.90	5	1
1	A	8	DG	OP2-P-O3'	-6.13	91.72	105.20	14	1
1	A	6	DC	C4'-C3'-C2'	6.12	108.61	103.10	13	1
1	A	16	DG	N9-C1'-C2'	6.07	124.14	112.60	13	1
1	A	21	DG	OP2-P-O3'	6.05	118.52	105.20	11	1
1	A	22	DT	O5'-P-OP2	-6.05	100.26	105.70	9	1
1	A	12	DT	C4'-C3'-O3'	6.04	124.81	109.70	5	1
1	A	1	DC	OP2-P-O3'	6.01	118.42	105.20	11	1
1	A	18	DG	C5'-C4'-O4'	5.96	120.61	109.30	5	1
1	A	17	DC	C4'-C3'-C2'	5.88	108.39	103.10	13	1
1	A	8	DG	P-O3'-C3'	5.82	126.69	119.70	15	2
1	A	17	DC	O4'-C4'-C3'	-5.77	102.19	104.50	5	1
1	A	13	DT	C5'-C4'-O4'	5.73	120.19	109.30	11	3
1	A	17	DC	O3'-P-O5'	5.71	114.86	104.00	5	1
1	A	1	DC	O3'-P-O5'	5.71	114.84	104.00	4	1
1	A	10	DC	P-O3'-C3'	5.67	126.51	119.70	14	1
1	A	10	DC	C3'-C2'-C1'	-5.67	95.70	102.50	13	1
1	A	21	DG	O4'-C4'-C3'	-5.56	102.28	104.50	7	1
1	A	17	DC	C5'-C4'-O4'	-5.44	98.97	109.30	2	1
1	A	11	DC	OP1-P-O3'	5.43	117.15	105.20	11	2
1	A	21	DG	N9-C1'-C2'	-5.42	102.30	112.60	7	1
1	A	11	DC	C2'-C3'-O3'	-5.33	95.01	112.60	13	1
1	A	2	DG	OP1-P-O3'	5.28	116.81	105.20	8	1
1	A	8	DG	OP1-P-O3'	5.25	116.74	105.20	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	13	DT	OP1-P-O3'	5.24	116.72	105.20	4	1
1	A	19	DG	C5-N7-C8	-5.17	101.72	104.30	2	7
1	A	16	DG	O5'-P-OP2	-5.15	101.06	105.70	15	1
1	A	12	DT	C6-C5-C7	-5.12	119.83	122.90	11	8
1	A	16	DG	C1'-O4'-C4'	5.11	115.21	110.10	5	1
1	A	13	DT	C6-C5-C7	-5.10	119.84	122.90	11	14
1	A	14	DG	C5-N7-C8	-5.10	101.75	104.30	9	4
1	A	22	DT	C6-C5-C7	-5.07	119.86	122.90	13	5
1	A	12	DT	O5'-C5'-C4'	5.05	123.63	111.00	1	1

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	460	247	247	2±1
2	A	27	15	0	0±0
All	All	7305	3930	3705	23

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:DG:H4'	1:A:17:DC:O5'	0.66	1.91	7	8
1:A:11:DC:H4'	1:A:12:DT:OP2	0.56	2.00	10	1
1:A:13:DT:H2'	1:A:13:DT:O2	0.55	2.01	5	2
1:A:13:DT:H2'	1:A:14:DG:C8	0.51	2.40	9	1
1:A:12:DT:H2''	1:A:13:DT:OP1	0.51	2.06	11	1
1:A:11:DC:H2''	1:A:12:DT:OP1	0.46	2.11	15	2
1:A:13:DT:H3'	1:A:14:DG:H5''	0.45	1.89	2	1
1:A:12:DT:C2'	1:A:13:DT:OP1	0.45	2.65	6	1
1:A:13:DT:O2	1:A:13:DT:H2'	0.43	2.14	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:DG:H2''	1:A:16:DG:O5'	0.43	2.12	14	1
1:A:10:DC:C2	2:A:101:EL9:C19	0.43	3.02	9	1
1:A:13:DT:C4'	1:A:14:DG:OP2	0.43	2.66	11	1
1:A:10:DC:C6	2:A:101:EL9:C19	0.41	3.03	9	1
1:A:13:DT:C2'	1:A:13:DT:O2	0.41	2.69	5	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](#)

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	Counts	Bond lengths	
						RMSZ	#Z>2
2	EL9	A	101	-	25,32,32	4.56±0.00	14±0 (56±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	Counts	Bond angles	
						RMSZ	#Z>2
2	EL9	A	101	-	25,51,51	3.27±0.00	15±0 (60±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	EL9	A	101	-	-	-	0±0,6,6,6

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	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	101	EL9	C17-C16	13.43	1.40	1.52	6	15
2	A	101	EL9	C8-C7	11.99	1.42	1.53	6	15
2	A	101	EL9	C6-C5	6.19	1.45	1.38	6	15
2	A	101	EL9	PT1-N4	5.82	2.41	2.04	6	15
2	A	101	EL9	C9-C8	5.34	1.39	1.53	6	15
2	A	101	EL9	C18-C17	5.03	1.40	1.53	6	15
2	A	101	EL9	C10-C9	3.31	1.38	1.51	6	15
2	A	101	EL9	C11-C10	3.25	1.39	1.51	6	15
2	A	101	EL9	C6-C7	3.00	1.47	1.51	6	15
2	A	101	EL9	C20-C19	2.91	1.40	1.51	6	15
2	A	101	EL9	C18-C19	2.81	1.40	1.51	6	15
2	A	101	EL9	C20-N4	2.75	1.40	1.49	6	15
2	A	101	EL9	C11-N1	2.37	1.41	1.49	6	15
2	A	101	EL9	C13-N2	2.17	1.34	1.38	6	15

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

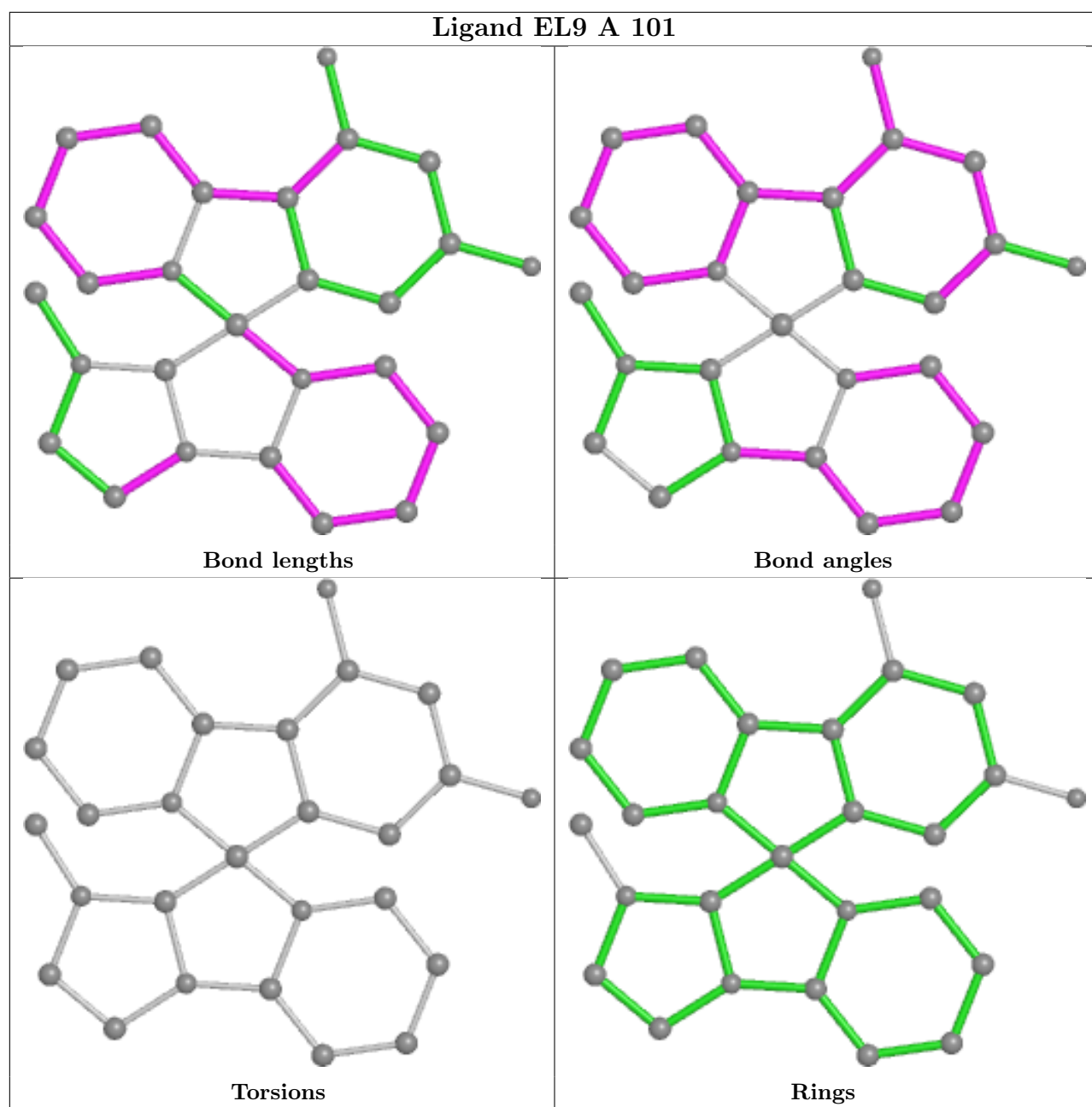
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	101	EL9	C8-C7-N1	6.20	119.47	111.03	6	15
2	A	101	EL9	C11-C10-C9	5.25	120.33	111.44	6	15
2	A	101	EL9	C17-C16-N2	4.59	126.35	112.77	6	15
2	A	101	EL9	C9-C8-C7	4.47	120.44	111.45	6	15
2	A	101	EL9	C10-C9-C8	4.34	120.26	111.42	6	15
2	A	101	EL9	C20-C19-C18	4.31	118.74	111.44	6	15
2	A	101	EL9	C18-C17-C16	4.12	118.25	110.39	6	15
2	A	101	EL9	F2-C5-C6	3.99	122.03	118.13	6	15
2	A	101	EL9	C4-C5-C6	3.95	119.66	124.63	6	15
2	A	101	EL9	C8-C7-C6	3.83	127.20	116.17	6	15
2	A	101	EL9	C19-C18-C17	3.51	118.58	111.42	6	15
2	A	101	EL9	C5-C4-C3	3.35	120.14	116.62	6	15
2	A	101	EL9	C10-C11-N1	3.22	120.95	112.57	6	15
2	A	101	EL9	C4-C3-C2	2.50	120.36	123.52	6	15
2	A	101	EL9	C19-C20-N4	2.32	118.60	112.57	6	15

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 [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 46% for the well-defined parts and 46% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: 1-1-chemicalshifts\_str.txt

#### 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	230
Number of shifts mapped to atoms	230
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

#### 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 46%, i.e. 206 atoms were assigned a chemical shift out of a possible 448. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> 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	206/448 (46%)	206/272 (76%)	0/140 (0%)	0/36 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 206 atoms were assigned a chemical shift out of a possible 448. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
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	206/448 (46%)	206/272 (76%)	0/140 (0%)	0/36 (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, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
1	A	22	DT	H2'	0.75	3.17 – 1.07	-6.5
1	A	16	DG	H5'	2.79	5.12 – 3.02	-6.1
1	A	17	DC	H2'	3.40	3.21 – 1.01	5.9

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (1-1-chemicalshifts\_str.txt). RCI is only applicable to proteins.