Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2LOA
Title	:	Structural Basis for Bifunctional Zn(II) Macrocyclic Complex Recognition of Thymine Bulges in DNA
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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
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:

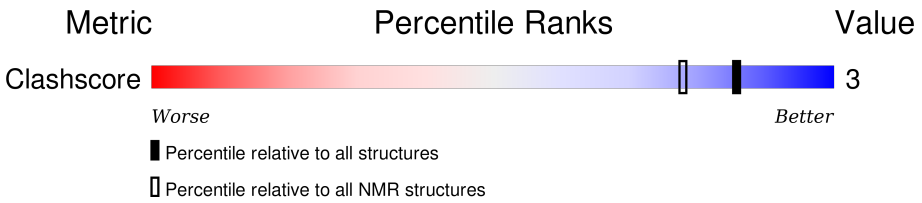
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 22%.

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	10	40% 50% 10%

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

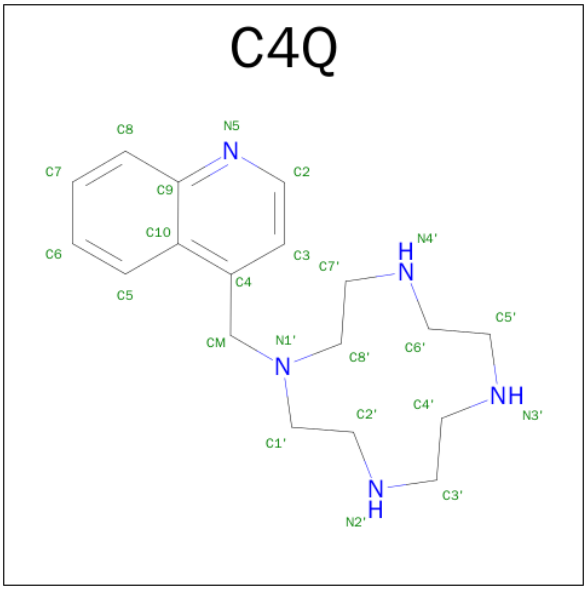
3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 365 atoms, of which 139 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	10	314	96	112	39	58	9	0

- Molecule 2 is 4-(1,4,7,10-TETRAAZACYCLODODECAN-1-YLMETHYL)QUINOLINE (three-letter code: C4Q) (formula: $C_{18}H_{27}N_5$).



Mol	Chain	Residues	Atoms			
			Total	C	H	N
2	A	1	50	18	27	5

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	A	1	1	1

4 Residue-property plots (i)

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*CP*GP*CP*AP*GP*TP*GP*C)-3')

Chain A:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DGSA-distance geometry simulated annealing, Docking with energy minimization.*

Of the 1 calculated structures, 1 were deposited, based on the following criterion: *structures with acceptable covalent geometry.*

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

Software name	Classification	Version
CYANA	geometry optimization	2.1
HYPERCHEM	refinement	6
CYANA	refinement	2.1

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)	2loa_cs.str
Number of chemical shift lists	1
Total number of shifts	55
Number of shifts mapped to atoms	55
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	22%

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: ZN, C4Q

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	1.98	3/226 (1.3%)	3.35	32/347 (9.2%)
All	All	1.98	3/226 (1.3%)	3.35	32/347 (9.2%)

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	1
All	All	0	1

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	DT	C4-O4	-11.91	1.12	1.23
1	A	8	DG	C4'-O4'	-7.09	1.38	1.45
1	A	9	DT	C4'-O4'	-6.90	1.38	1.45

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	9	DT	O4'-C4'-C3'	-18.50	94.90	106.00
1	A	8	DG	O4'-C4'-C3'	-13.45	97.93	106.00
1	A	5	DG	C5-C6-N1	11.88	117.44	111.50
1	A	2	DG	C5-C6-N1	11.81	117.40	111.50
1	A	7	DA	O4'-C4'-C3'	-11.71	98.98	106.00
1	A	8	DG	C5-C6-N1	11.70	117.35	111.50
1	A	10	DG	C5-C6-N1	11.69	117.35	111.50
1	A	9	DT	N3-C4-O4	-11.30	113.12	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	DG	C6-N1-C2	-11.07	118.46	125.10
1	A	2	DG	C6-N1-C2	-11.00	118.50	125.10
1	A	10	DG	C6-N1-C2	-10.96	118.52	125.10
1	A	8	DG	C6-N1-C2	-10.92	118.55	125.10
1	A	5	DG	N1-C2-N3	8.71	129.13	123.90
1	A	2	DG	N1-C2-N3	8.68	129.11	123.90
1	A	10	DG	N1-C2-N3	8.68	129.11	123.90
1	A	8	DG	N1-C2-N3	8.64	129.08	123.90
1	A	7	DA	C1'-O4'-C4'	7.22	117.32	110.10
1	A	9	DT	C1'-O4'-C4'	6.75	116.85	110.10
1	A	2	DG	O4'-C4'-C3'	-6.17	102.03	104.50
1	A	9	DT	C2-N3-C4	-6.00	123.60	127.20
1	A	9	DT	C5'-C4'-O4'	5.93	120.56	109.30
1	A	5	DG	O4'-C4'-C3'	-5.84	102.16	104.50
1	A	8	DG	C1'-O4'-C4'	-5.78	104.32	110.10
1	A	5	DG	N1-C2-N2	-5.51	111.24	116.20
1	A	2	DG	N1-C2-N2	-5.45	111.29	116.20
1	A	10	DG	N1-C2-N2	-5.44	111.31	116.20
1	A	8	DG	N1-C2-N2	-5.40	111.34	116.20
1	A	2	DG	C5-C6-O6	-5.40	125.36	128.60
1	A	5	DG	C5-C6-O6	-5.37	125.38	128.60
1	A	8	DG	C5-C6-O6	-5.28	125.43	128.60
1	A	10	DG	C5-C6-O6	-5.26	125.44	128.60
1	A	5	DG	C1'-O4'-C4'	5.11	115.20	110.10

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	9	DT	Sidechain

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
2	A	23	27	27	1
All	All	226	139	140	1

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:A:101:C4Q:H3	2:A:101:C4Q:H8'	0.41	1.93

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 carbohydrates in this entry.

6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	C4Q	A	101	3	25,25,25	1.30	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	C4Q	A	101	3	29,31,31	2.25	2 (6%)

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	C4Q	A	101	3	-	0,18,18,18	0,3,3,3

There are no bond-length outliers.

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	101	C4Q	C10-C9-N5	6.28	116.03	122.83
2	A	101	C4Q	C2-N5-C9	5.76	126.79	116.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 22% for the well-defined parts and 22% for the entire structure.

7.1 Chemical shift list 1

File name: 2loa_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	55
Number of shifts mapped to atoms	55
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

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

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 22%, i.e. 45 atoms were assigned a chemical shift out of a possible 202. 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	45/202 (22%)	45/122 (37%)	0/66 (0%)	0/14 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 22%, i.e. 45 atoms were assigned a chemical shift out of a possible 202. 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	45/202 (22%)	45/122 (37%)	0/66 (0%)	0/14 (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_1). RCI is only applicable to proteins.