wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2LLJ
BMRB ID	:	18050
Title	:	Structure of a bis-naphthalene bound to a thymine-thymine DNA mismatch
Authors	:	Jourdan, M.; Granzhan, A.; Guillot, R.; Dumy, P.; Teulade-Fichou, M.
Deposited on	:	2011-11-10

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 (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 (i)) were used in the production of this report:

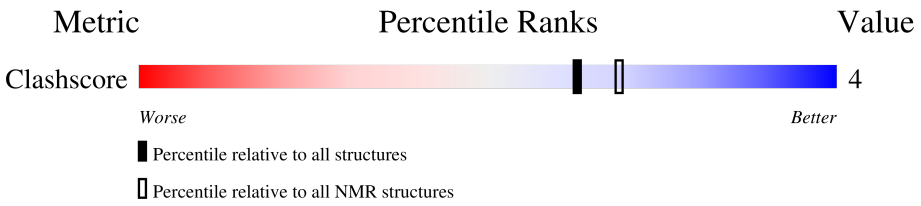
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 38%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	11	18% 64% 18%
2	B	11	36% 36% 27%

2 Ensemble composition and analysis (i)

This entry contains 5 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. 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 4 unique types of molecules in this entry. The entry contains 828 atoms, of which 295 are hydrogens and 0 are deuteriums.

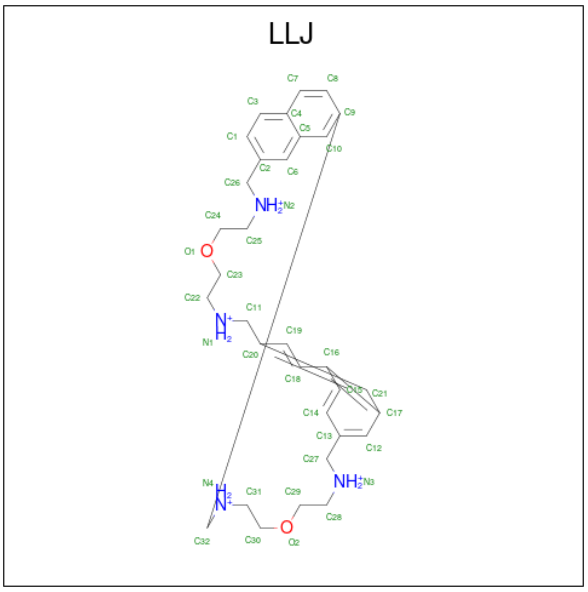
- Molecule 1 is a DNA chain called DNA (5'-D(*CP*GP*TP*CP*GP*TP*AP*GP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	11	349	107	126	40	66	10	0

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	11	346	106	125	41	64	10	0

- Molecule 3 is 6,22-dioxa-3,9,19,25-tetraazoniapentacyclo[25.5.3.3 11,17 .0 14,37 .0 30,34]octatriaconta-1(33),11(38),12,14(37),15,17(36),27,29,31,34-decaene (three-letter code: LLJ) (formula: $C_{32}H_{44}N_4O_2$).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
3	B	1	82	32	44	4	2

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	
			Total	O
4	A	19	19	19
			Total	O
4	B	32	32	32

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 (5'-D(*CP*GP*TP*CP*GP*TP*AP*GP*TP*GP*C)-3')

Chain A: 18% 64% 18%

C1 G2 T3 C4 G5 T6 A7 G8 T9 G10 C11

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

Chain B: 36% 36% 27%

G12 C13 A14 C15 T16 T17 C18 G19 A20 C21 G22

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: DNA (5'-D(*CP*GP*TP*CP*GP*TP*AP*GP*TP*GP*C)-3')

Chain A: 27% 55% 18%

C1 G2 T3 C4 G5 T6 A7 G8 T9 G10 C11

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

Chain B: 45% 27% 27%

G12 C13 A14 C15 T16 T17 C18 G19 A20 C21 G22

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 5 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	structure solution	10.1
Amber	refinement	10.1

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	178
Number of shifts mapped to atoms	178
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

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: LLJ

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	1.63±0.02	0±0/249 (0.0± 0.0%)	2.63±0.02	25±2/383 (6.4± 0.5%)
2	B	1.75±0.03	1±0/247 (0.5± 0.2%)	3.56±0.02	36±2/379 (9.6± 0.5%)
All	All	1.69	6/2480 (0.2%)	3.13	305/3810 (8.0%)

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	7.0±0.0
2	B	0.0±0.0	6.6±0.5
All	All	0	68

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	B	20	DA	N9-C8	-6.03	1.32	1.37	3	5
2	B	17	DT	N1-C2	5.55	1.42	1.38	1	1

5 of 77 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	16	DT	O4'-C1'-N1	37.48	134.24	108.00	2	5
2	B	16	DT	C6-C5-C7	-13.66	114.70	122.90	5	5
1	A	9	DT	C6-C5-C7	-13.39	114.87	122.90	4	5
2	B	20	DA	O4'-C1'-N9	11.81	116.27	108.00	4	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	14	DA	N1-C6-N6	-11.49	111.70	118.60	1	5

There are no chirality outliers.

5 of 14 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	5	DG	Sidechain	5
1	A	6	DT	Sidechain	5
1	A	7	DA	Sidechain	5
1	A	8	DG	Sidechain	5
1	A	9	DT	Sidechain	5

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	223	126	126	2±0
2	B	221	125	125	2±0
3	B	38	44	37	1±0
All	All	2665	1475	1440	18

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:16:DT:C6	3:B:101:LLJ:C7	0.63	2.81	3	5
2:B:12:DG:C8	2:B:13:DC:C5	0.44	3.06	2	5
1:A:2:DG:H1'	1:A:3:DT:C6	0.43	2.48	1	5
1:A:8:DG:C8	1:A:9:DT:C5	0.42	3.07	1	3

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
3	LLJ	B	101	-	42,42,42	76.65±0.07	4±0 (10±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.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	LLJ	B	101	-	54,54,54	8.07±0.00	10±0 (18±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
3	LLJ	B	101	-	-	0±0,24,24,24	0±0,4,5,5

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
3	B	101	LLJ	C25-N2	298.64	11.41	1.46	5	5
3	B	101	LLJ	C28-N3	294.15	11.26	1.46	5	5
3	B	101	LLJ	C26-N2	196.15	10.59	1.46	5	5
3	B	101	LLJ	C27-N3	182.61	9.96	1.46	3	5
3	B	101	LLJ	C15-C14	2.25	1.41	1.36	1	2

5 of 10 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	101	LLJ	C13-C27-N3	30.27	34.39	112.80	3	5
3	B	101	LLJ	C27-N3-C28	29.84	11.21	113.41	4	5
3	B	101	LLJ	C26-N2-C25	29.59	12.08	113.41	5	5
3	B	101	LLJ	C2-C26-N2	25.12	47.72	112.80	3	5
3	B	101	LLJ	C24-C25-N2	11.06	84.34	111.44	2	5

There are no chirality outliers.

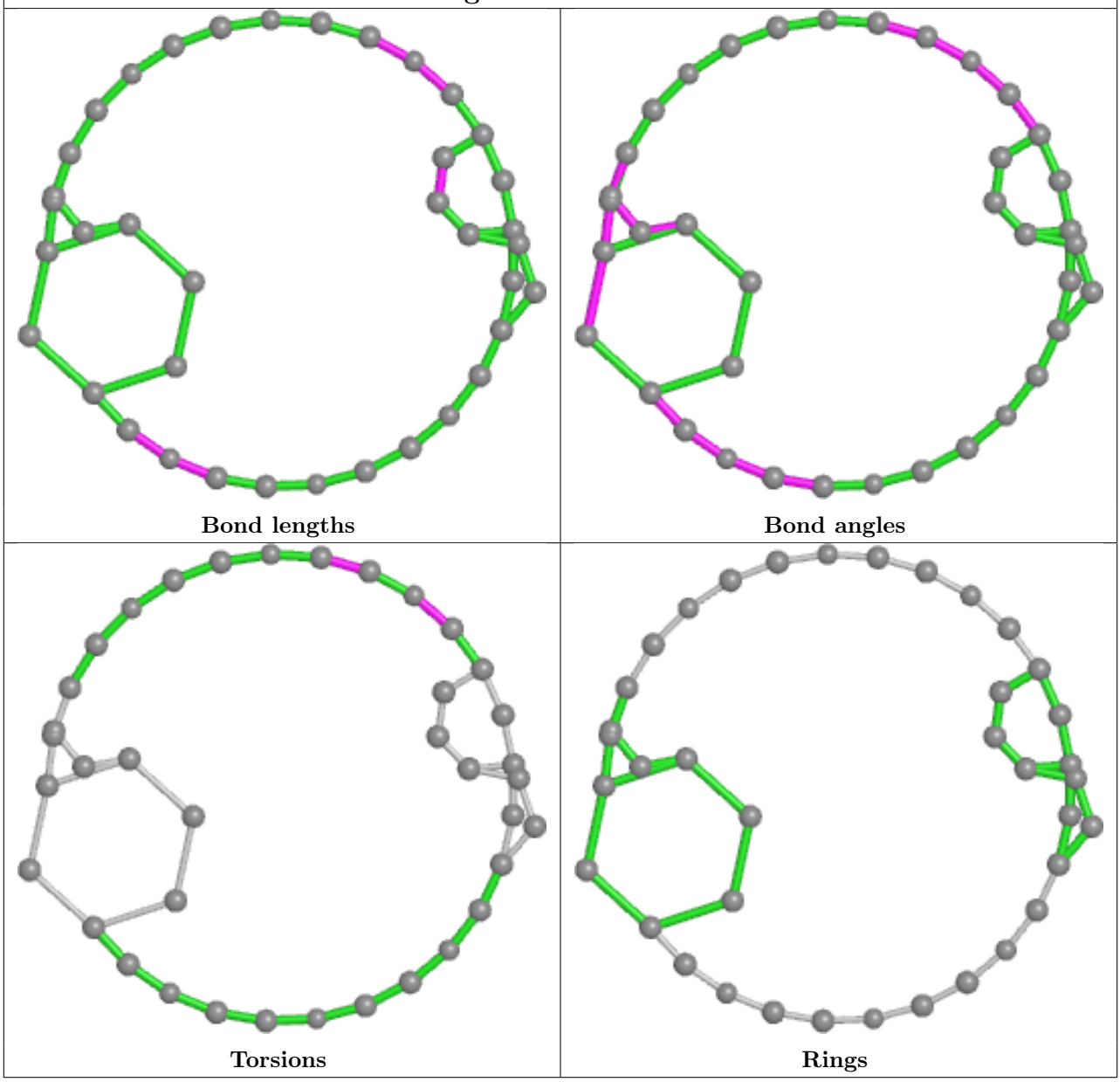
There are no torsion outliers.

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 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.

Ligand LLJ B 101



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 38% for the well-defined parts and 38% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	178
Number of shifts mapped to atoms	178
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 38%, i.e. 164 atoms were assigned a chemical shift out of a possible 437. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Sugar	109/264 (41%)	109/154 (71%)	0/110 (0%)	0/0 (—%)
Base	55/173 (32%)	55/107 (51%)	0/37 (0%)	0/29 (0%)
Overall	164/437 (38%)	164/261 (63%)	0/147 (0%)	0/29 (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. RCI is only applicable to proteins