wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1B0S
Title	:	BINDING OF AR-1-144, A TRI-IMIDAZOLE DNA MINOR GROOVE BINDER, TO CCGG SEQUENCE ANALYZED BY NMR SPECTROSCOPY
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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
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:

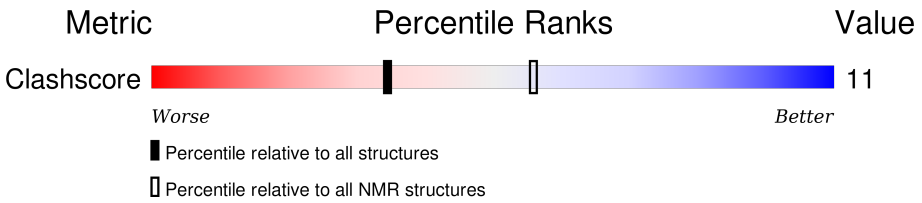
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 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	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	10% 50% 20% 20%
1	B	10	10% 50% 30% 10%

2 Ensemble composition and analysis (i)

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

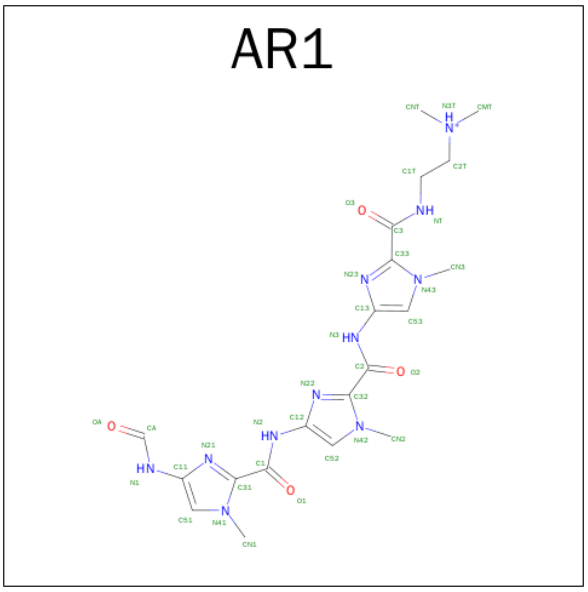
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 758 atoms, of which 284 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	10	316	97	114	38	58	9	0
1	B	10	316	97	114	38	58	9	0

- Molecule 2 is (2-{[4-({4-[(4-FORMYLAMINO-1-METHYL-1H-IMIDAZOLE-2-CARBONYL)-AMINO]-1-METHYL-1H-IMIDAZOLE-2-CARBONYL}-AMINO)-1-METHYL-1H-IMIDAZOLE-2-CARBONYL]-AMINO}-ETHYL)-DIMETHYL-AMMONIUM (three-letter code: AR1) (formula: $C_{20}H_{28}N_{11}O_4$).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	A	1	63	20	28	11	4
2	B	1	63	20	28	11	4

4 Residue-property plots (i)

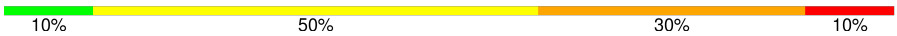
These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain 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*AP*AP*CP*CP*GP*GP*TP*TP*C)-3')

Chain A:

- Molecule 1: DNA (5'-D(*GP*AP*AP*CP*CP*GP*GP*TP*TP*C)-3')

Chain B:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *NOE-RMD*.

Of the 11 calculated structures, 1 were deposited, based on the following criterion: *REFINED AVERAGE STRUCTURE*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	3.1
SPEDREF	structure solution	

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)	BMRB entry 4392
Number of chemical shift lists	3
Total number of shifts	195
Number of shifts mapped to atoms	182
Number of unparsed shifts	0
Number of shifts with mapping errors	13
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

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: AR1

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	1.49	5/226 (2.2%)	2.42	21/347 (6.1%)
1	B	1.48	5/226 (2.2%)	2.42	21/347 (6.1%)
All	All	1.49	10/452 (2.2%)	2.42	42/694 (6.1%)

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	2
1	B	0	1
All	All	0	3

5 of 10 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	C5-C7	8.26	1.55	1.50
1	B	19	DT	C5-C7	8.10	1.54	1.50
1	A	8	DT	C5-C7	7.98	1.54	1.50
1	B	18	DT	C5-C7	7.97	1.54	1.50
1	B	20	DC	C5-C6	6.23	1.39	1.34

5 of 42 angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	18	DT	O4'-C1'-N1	9.38	114.56	108.00
1	A	8	DT	O4'-C1'-N1	9.35	114.55	108.00
1	A	5	DC	O4'-C1'-N1	9.04	114.33	108.00
1	B	15	DC	O4'-C1'-N1	9.03	114.32	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	13	DA	O4'-C1'-N9	9.00	114.30	108.00

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	8	DT	Sidechain
1	B	19	DT	Sidechain
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
1	A	202	114	114	4
1	B	202	114	114	4
2	A	35	28	25	3
2	B	35	28	25	3
All	All	474	284	278	8

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 11.

5 of 8 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:15:DC:O4'	2:B:2:AR1:HA	0.49	2.07
1:A:9:DT:H4'	2:A:11:AR1:O3	0.49	2.07
1:B:19:DT:H4'	2:B:2:AR1:O3	0.49	2.07
1:A:5:DC:O4'	2:A:11:AR1:HA	0.49	2.07
1:B:18:DT:H4'	2:B:2:AR1:C13	0.41	2.45

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)

2 ligands are 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	AR1	A	11	-	31,37,37	3.91	3 (9%)
2	AR1	B	2	-	31,37,37	3.92	3 (9%)

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	AR1	A	11	-	27,52,52	1.16	0 (0%)
2	AR1	B	2	-	27,52,52	1.16	0 (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	AR1	A	11	-	-	0,11,29,29	0,3,3,3
2	AR1	B	2	-	-	0,11,29,29	0,3,3,3

5 of 6 bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	11	AR1	C33-C3	12.93	1.45	1.53
2	B	2	AR1	C33-C3	12.83	1.45	1.53
2	B	2	AR1	C31-C1	12.58	1.45	1.53
2	A	11	AR1	C31-C1	12.51	1.45	1.53
2	B	2	AR1	C32-C2	11.56	1.46	1.53

There are no bond-angle outliers.

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

7.1 Chemical shift list 1

File name: BMRB entry 4392

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	162
Number of shifts mapped to atoms	162
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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. 150 atoms were assigned a chemical shift out of a possible 398. 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	150/398 (38%)	150/238 (63%)	0/134 (0%)	0/26 (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, *ppm*	Expected range, *ppm*	Z-score
1	B	18	DT	H4'	2.04	5.65 – 2.55	-6.6
1	A	8	DT	H4'	2.04	5.65 – 2.55	-6.6
1	B	16	DG	H4'	3.27	5.22 – 3.42	-5.8
1	A	6	DG	H4'	3.27	5.22 – 3.42	-5.8

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.

7.2 Chemical shift list 2

File name: BMRB entry 4392

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	20
Number of shifts mapped to atoms	20
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

7.2.2 Chemical shift referencing (i)

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

7.2.3 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 5%, i.e. 20 atoms were assigned a chemical

shift out of a possible 398. 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	20/398 (5%)	20/238 (8%)	0/134 (0%)	0/26 (0%)

7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 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_2). RCI is only applicable to proteins.

7.3 Chemical shift list 3

File name: BMRB entry 4392

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 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	13
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	13
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.

- Chain not found in structure. First 5 (of 13) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	AR1	3MIM_H5	7.626	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	AR1	TAI_H22	3.34	-1.0	1
UNMAPPED	1	AR1	4MIM_HNA	4.062	-1.0	1
UNMAPPED	1	AR1	TAI_H11	3.474	-1.0	1
UNMAPPED	1	AR1	TAI_H12	3.431	-1.0	1

7.3.2 Chemical shift referencing (i)

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

7.3.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 398. 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	0/398 (0%)	0/238 (0%)	0/134 (0%)	0/26 (0%)

7.3.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.3.5 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_3). RCI is only applicable to proteins.