



wwPDB NMR Structure Validation Summary Report ⓘ

Feb 12, 2017 – 11:57 pm GMT

PDB ID : 2LEF
Title : LEF1 HMG DOMAIN (FROM MOUSE), COMPLEXED WITH DNA
(15BP), NMR, 12 STRUCTURES
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Deposited on : 1998-10-13

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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

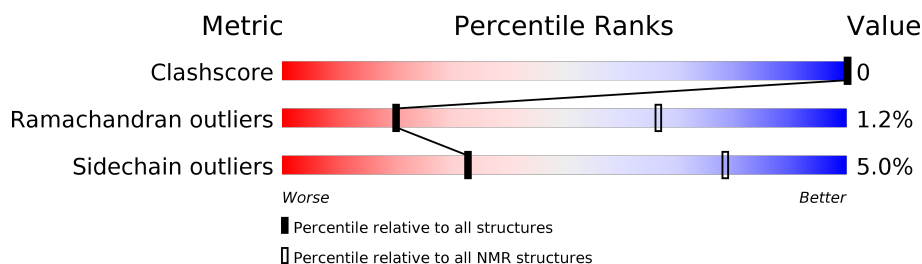
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 55%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	B	15	<div> <div>20%</div> <div>67%</div> <div>13%</div> </div>
2	C	15	<div> <div>27%</div> <div>67%</div> <div>7%</div> </div>
3	A	86	<div> <div>52%</div> <div>5%</div> <div>43%</div> </div>

2 Ensemble composition and analysis

This entry contains 12 models. Model 3 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:56 (49)	0.12	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 1 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 9, 10, 11, 12
Single-model clusters	5; 7; 8

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2398 atoms, of which 1061 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	B	15	Total	C	H	N	O	P	0
			469	144	171	51	89	14	

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

Mol	Chain	Residues	Atoms						Trace
2	C	15	Total	C	H	N	O	P	0
			481	148	170	62	87	14	

- Molecule 3 is a protein called PROTEIN (LYMPHOID ENHANCER-BINDING FACTOR).

Mol	Chain	Residues	Atoms						Trace
3	A	86	Total	C	H	N	O	S	0
			1448	460	720	141	122	5	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	PRO	CONFLICT	UNP P27782
A	25	SER	CYS	ENGINEERED	UNP P27782

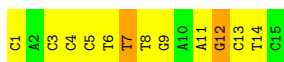
4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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.

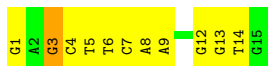
- Molecule 1: DNA (5'-D(*CP*AP*CP*CP*CP*TP*TP*TP*GP*AP*AP*GP*CP*TP*C)-3')

Chain B: 



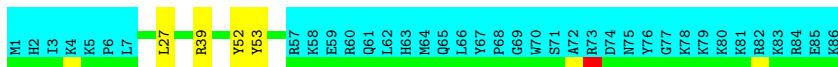
- Molecule 2: DNA (5'-D(*GP*AP*GP*CP*TP*TP*CP*AP*AP*AP*GP*GP*GP*TP*G)-3')

Chain C: 



- Molecule 3: PROTEIN (LYMPHOID ENHANCER-BINDING FACTOR)

Chain A: 

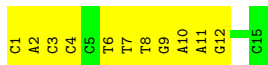


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

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

Chain B: 



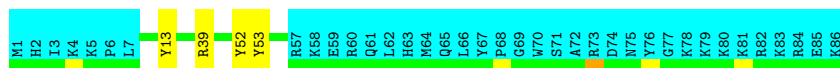
- Molecule 2: DNA (5'-D(*GP*AP*GP*CP*TP*TP*CP*AP*AP*AP*GP*GP*GP*TP*G)-3')

Chain C: 



- Molecule 3: PROTEIN (LYMPHOID ENHANCER-BINDING FACTOR)

Chain A: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DG IN TORSION SPACE (DIANA) AND DYNAMICAL SIMULATED ANNEALING*.

Of the 28 calculated structures, 12 were deposited, based on the following criterion: *CONSTRAINTS VIOLATION, AMBER ENERGIES*.

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

Software name	Classification	Version
AMBER	refinement	
FELIX	structure solution	
DIANA	structure solution	
AMBER	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 4248
Number of chemical shift lists	3
Total number of shifts	1339
Number of shifts mapped to atoms	1151
Number of unparsed shifts	0
Number of shifts with mapping errors	188
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	55%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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	B	1.26±0.01	0±0/332 (0.0±0.0%)	1.89±0.04	11±2/509 (2.1±0.5%)
2	C	1.22±0.01	0±0/350 (0.0±0.0%)	1.93±0.03	8±2/540 (1.5±0.4%)
3	A	0.57±0.01	0±0/408 (0.0±0.0%)	0.86±0.02	0±0/548 (0.0±0.1%)
All	All	1.04	0/13080 (0.0%)	1.63	226/19164 (1.2%)

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	B	0.0±0.0	4.7±1.6
2	C	0.0±0.0	4.5±1.2
3	A	0.0±0.0	2.6±0.9
All	All	0	141

There are no bond-length outliers.

5 of 41 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	C	3	DG	O4'-C1'-N9	11.13	115.79	108.00	6	12
1	B	11	DA	O4'-C1'-N9	10.25	115.17	108.00	12	12
1	B	12	DG	O4'-C4'-C3'	7.73	110.64	106.00	12	10
1	B	6	DT	C6-C5-C7	-7.64	118.31	122.90	1	11
2	C	5	DT	O4'-C1'-N1	7.25	113.08	108.00	6	4

There are no chirality outliers.

5 of 24 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
3	A	52	TYR	Sidechain	12
2	C	9	DA	Sidechain	12
1	B	4	DC	Sidechain	12
3	A	53	TYR	Sidechain	11
2	C	3	DG	Sidechain	9

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	B	298	171	171	0±0
2	C	311	170	170	0±0
3	A	401	373	401	0±0
All	All	12120	8568	8904	-

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](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	49/86 (57%)	43±1 (88±2%)	5±1 (10±2%)	1±0 (1±1%)	20	66
All	All	588/1032 (57%)	520 (88%)	61 (10%)	7 (1%)	20	66

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	29	GLU	6

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Mol	Chain	Res	Type	Models (Total)
3	A	31	ALA	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	40/74 (54%)	38±1 (95±2%)	2±1 (5±2%)	33	78
All	All	480/888 (54%)	456 (95%)	24 (5%)	33	78

All 4 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	39	ARG	9
3	A	27	LEU	9
3	A	51	LYS	3
3	A	46	ARG	3

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](#)

There are no ligands in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 55% for the well-defined parts and 63% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4248

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	973
Number of shifts mapped to atoms	973
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	86	2.08 ± 0.12	Should be applied
$^{13}\text{C}_\beta$	83	2.59 ± 0.10	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	82	0.08 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 42%, i.e. 517 atoms were assigned a chemical shift out of a possible 1232. 2 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	196/245 (80%)	98/98 (100%)	49/98 (50%)	49/49 (100%)
Sidechain	279/340 (82%)	173/200 (86%)	104/120 (87%)	2/20 (10%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	42/53 (79%)	23/27 (85%)	18/23 (78%)	1/3 (33%)
Overall	517/1232 (42%)	294/679 (43%)	171/443 (39%)	52/110 (47%)

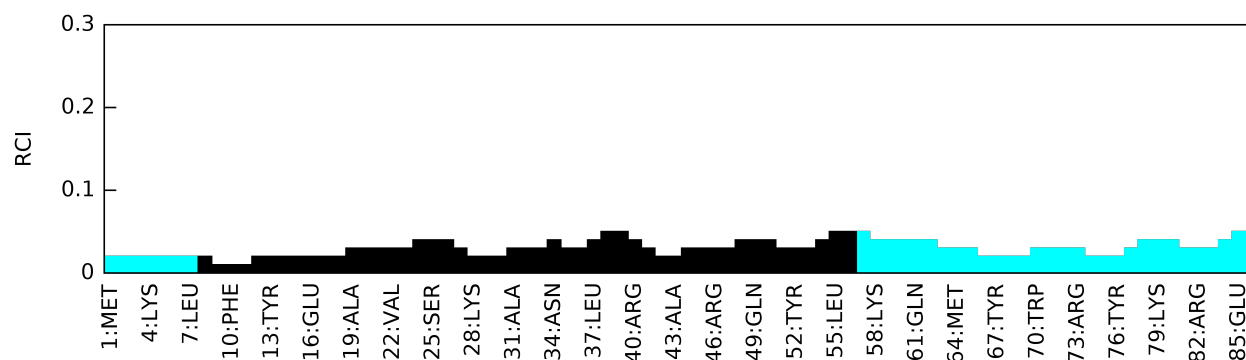
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: BMRB entry 4248

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	254
Number of shifts mapped to atoms	178
Number of unparsed shifts	0

Number of shifts with mapping errors	76
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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

- Residue not found in structure. First 5 (of 76) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
C	9	DG	H4'	3.829	-1.0	1
C	8	DT	H73	1.909	-1.0	1
C	3	DC	H2'	2.501	-1.0	1
C	7	DT	H1'	6.202	-1.0	1
C	13	DC	H5''	3.533	-1.0	2

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 13%, i.e. 160 atoms were assigned a chemical shift out of a possible 1232. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/245 (0%)	0/98 (0%)	0/98 (0%)	0/49 (0%)
Sidechain	0/340 (0%)	0/200 (0%)	0/120 (0%)	0/20 (0%)
Aromatic	0/53 (0%)	0/27 (0%)	0/23 (0%)	0/3 (0%)
Overall	160/1232 (13%)	160/679 (24%)	0/443 (0%)	0/110 (0%)

7.2.4 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
2	B	12	DG	H2''	1.16	3.60 – 1.70	-7.8
3	C	12	DG	H2''	1.16	3.60 – 1.70	-7.8

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
3	C	12	DG	H5'	2.90	5.12 – 3.02	-5.6
2	B	12	DG	H5'	2.90	5.12 – 3.02	-5.6

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 4248

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	112
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	112
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- Chain not found in structure. First 5 (of 112) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	6	DT	H1'	5.8	-1.0	1
UNMAPPED	13	DG	H2''	2.508	-1.0	2
UNMAPPED	11	DG	H4'	4.423	-1.0	1
UNMAPPED	13	DG	H3'	4.938	-1.0	1
UNMAPPED	1	DG	H5'	3.676	-1.0	2

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 1232. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/245 (0%)	0/98 (0%)	0/98 (0%)	0/49 (0%)
Sidechain	0/340 (0%)	0/200 (0%)	0/120 (0%)	0/20 (0%)
Aromatic	0/53 (0%)	0/27 (0%)	0/23 (0%)	0/3 (0%)
Overall	0/1232 (0%)	0/679 (0%)	0/443 (0%)	0/110 (0%)

7.3.4 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
???	UNMAPPED	6	DT	H4'	2.24	5.65 – 2.55	-6.0

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.