



# wwPDB NMR Structure Validation Summary Report ⓘ

Feb 12, 2017 – 05:41 pm GMT

PDB ID : 1C7U  
Title : Complex of the DNA binding core domain of the transcription factor MEF2A  
with a 20mer oligonucleotide  
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Deposited on : 2000-03-17

This is a wwPDB NMR Structure Validation Summary 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

<http://wwpdb.org/validation/2016/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:

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

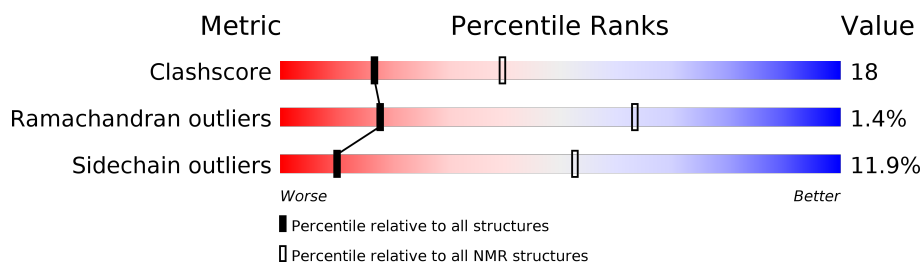
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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  $\geq 3$ , 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	C	20	75% 25%
1	D	20	75% 25%
2	A	85	47% 33% 7% 13%
2	B	85	45% 33% 9% 13%

## 2 Ensemble composition and analysis ⓘ

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3772 atoms, of which 1734 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	C	20	Total	C	H	N	O	P	0
			634	195	227	75	118	19	
1	D	20	Total	C	H	N	O	P	0
			634	195	227	75	118	19	

- Molecule 2 is a protein called MYOCYTE-SPECIFIC ENHANCER FACTOR 2A, C4 FORM.

Mol	Chain	Residues	Atoms						Trace
2	A	74	Total	C	H	N	O	S	0
			1252	392	640	105	112	3	
2	B	74	Total	C	H	N	O	S	0
			1252	392	640	105	112	3	

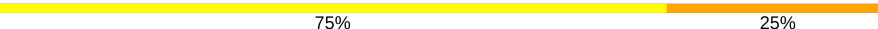
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ALA	CYS	CONFLICT	UNP Q02078
A	40	ALA	CYS	CONFLICT	UNP Q02078
B	138	ALA	CYS	CONFLICT	UNP Q02078
B	140	ALA	CYS	CONFLICT	UNP Q02078

## 4 Residue-property plots


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: 5'-D(\*CP\*TP\*CP\*GP\*GP\*CP\*TP\*AP\*TP\*TP\*AP\*AP\*TP\*AP\*GP\*CP\*CP\*GP\*AP\*G)-3'

Chain C: 

C201 T202 C203 G204 G205 C206 T207 A208 T209 T210 A211 A212 T213 A214 G215 C216 C217 G218 A219 G220

- Molecule 1: 5'-D(\*CP\*TP\*CP\*GP\*GP\*CP\*TP\*AP\*TP\*TP\*AP\*AP\*TP\*AP\*GP\*CP\*CP\*GP\*AP\*G)-3'

Chain D: 

C221 T222 C223 G224 G225 C226 T227 A228 T229 T230 A231 A232 T233 A234 G235 C236 C237 G238 A239 G240

- Molecule 2: MYOCYTE-SPECIFIC ENHANCER FACTOR 2A, C4 FORM

Chain A: 

G1 R2 K3 K4 I5 R14 V18 R23 K24 L27 M28 K29 K30 E33 E34 S35 A38 D39 A40 E41 I42 A43 L44 I45 I46 F47 N48 S49 K52 K53 F54 Q55 S58 T59 D60 M61 D62 K63 V64 K67 Y68 E73 P74 HIS GLU SER ARG THR ASN SER

ASP  
ILE  
VAL  
GLU

- Molecule 2: MYOCYTE-SPECIFIC ENHANCER FACTOR 2A, C4 FORM

Chain B: 

G103 R102 K103 K104 I105 R114 V118 R123 K124 L127 M128 K129 K130 E133 L134 S135 A138 D139 A140 E141 I142 A143 L144 I145 I146 F147 N148 S149 K152 K153 F154 Q155 S158 T159 D160 M161 D162 K163 Y164 L165 L166 K167 Y168 T169 E173 P174 HIS GLU SER ARG THR

ASN  
SER  
ASP  
ILE  
VAL  
GLU

## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 35 calculated structures, 1 were deposited, based on the following criterion: *REGULARIZED MEAN STRUCTURE*.

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

Software name	Classification	Version
X-PLOR/CNS	refinement	
CNS/X-PLOR	structure solution	

No chemical shift data was provided. 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](#)

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	C	1.44	5/456 (1.1%)	2.23	36/702 (5.1%)
1	D	1.44	5/456 (1.1%)	2.22	35/702 (5.0%)
2	A	1.08	0/620 (0.0%)	0.90	0/828 (0.0%)
2	B	1.09	0/620 (0.0%)	0.90	0/828 (0.0%)
All	All	1.25	10/2152 (0.5%)	1.65	71/3060 (2.3%)

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	D	229	DT	C5-C7	6.29	1.53	1.50
1	C	209	DT	C5-C7	6.29	1.53	1.50
1	D	230	DT	C5-C7	6.20	1.53	1.50
1	C	210	DT	C5-C7	6.10	1.53	1.50
1	C	202	DT	C5-C7	5.67	1.53	1.50

5 of 71 angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	231	DA	C4'-C3'-C2'	9.46	111.61	103.10
1	C	211	DA	C4'-C3'-C2'	9.34	111.50	103.10
1	C	210	DT	C4'-C3'-C2'	8.86	111.07	103.10
1	D	230	DT	C4'-C3'-C2'	8.85	111.06	103.10
1	D	232	DA	C4'-C3'-C2'	8.71	110.94	103.10

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	C	407	227	227	8
1	D	407	227	227	8
2	A	612	640	640	29
2	B	612	640	637	32
All	All	2038	1734	1731	66

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 18.

5 of 66 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:C:214:DA:H5''	2:B:105:ILE:HG21	0.63	1.71
1:D:234:DA:H5''	2:A:5:ILE:HG21	0.63	1.71
2:B:155:GLN:NE2	2:B:161:MET:SD	0.62	2.73
2:A:55:GLN:NE2	2:A:61:MET:SD	0.61	2.73
2:B:114:ARG:HH11	2:B:114:ARG:HG2	0.60	1.56

## 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	
2	A	72/85 (85%)	67 (93%)	4 (6%)	1 (1%)	18	63
2	B	72/85 (85%)	64 (89%)	7 (10%)	1 (1%)	18	63
All	All	144/170 (85%)	131 (91%)	11 (8%)	2 (1%)	18	63

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

Mol	Chain	Res	Type
2	B	160	ASP
2	A	60	ASP



### 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	
2	A	67/78 (86%)	59 (88%)	8 (12%)	10	52
2	B	67/78 (86%)	59 (88%)	8 (12%)	10	52
All	All	134/156 (86%)	118 (88%)	16 (12%)	10	52

5 of 16 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	B	124	LYS
2	A	24	LYS
2	B	173	GLU
2	A	73	GLU
2	A	41	GLU

### 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

No chemical shift data were provided