

Full wwPDB NMR Structure Validation Report (i)

Aug 20, 2022 – 08:06 AM EDT

PDB ID : 1C7U

Title: Complex of the DNA binding core domain of the transcription factor MEF2A

with a 20mer oligonucleotide

Authors: Clore, G.M.; Huang, K.

Deposited on : 2000-03-17

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
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

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

ShiftChecker : 2.29

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.29

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 was not calculated.

There are no overall percentile quality scores available for this entry.

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 | С | 20 | 100% | | | | |
| 1 | D | 20 | 100% | | | | |
| 2 | A | 85 | 87% | 13% | | | |
| 2 | В | 85 | 87% | 13% | | | |



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 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*AP*AP*AP*AP*AP*GP*CP*CP*GP*AP*G)-3'.

| Mol | Chain | Residues | | Atoms | | | | | Trace |
|-----|-------|----------|-------|-------|-----|-----|-----|----|-------|
| 1 | С | 20 | Total | С | Н | N | О | Р | 0 |
| | 20 | 634 | 195 | 227 | 75 | 118 | 19 | 0 | |
| 1 | D | 20 | Total | С | Н | N | О | Р | 0 |
| | ט | 20 | 634 | 195 | 227 | 75 | 118 | 19 | U |

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

| Mol | Chain | Residues | | Atoms | | | | | Trace |
|---|-------|----------|-------|-------|-----|-----|---|---|-------|
| 9 | Λ | 74 | Total | С | Н | N | О | S | 0 |
| $\begin{array}{ c c c c c } \hline Z & A \\ \hline \end{array}$ | 74 | 1252 | 392 | 640 | 105 | 112 | 3 | | |
| 9 | D | 74 | Total | С | Н | N | О | S | 0 |
| $\begin{vmatrix} 2 & B \end{vmatrix}$ | /4 | 1252 | 392 | 640 | 105 | 112 | 3 | U | |

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 |
| В | 138 | ALA | CYS | conflict | UNP Q02078 |
| В | 140 | ALA | CYS | conflict | UNP Q02078 |



4 Residue-property plots (i)

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

| Chain C: 100% 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 | , | | |
|--|--|--|--|
| ● Molecule 1: 5'-D(*CP*TP*CP*GP*GP*CP*TP*AP*TP*AP*AP*TP*AP*GP*CFP*AP*G)-3' Chain D: 100% Nolecule 2: MYOCYTE-SPECIFIC ENHANCER FACTOR 2A, C4 FORM Chain A: 87% 13% B 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 | Chain C: | 100% | |
| P*AP*G)-3' Chain D: 100% Note the content of the | C201 T202 C203 G204 G206 C206 T20 A208 T210 A211 A211 A211 G215 G215 G215 | 6220 6220 | |
| • Molecule 2: MYOCYTE-SPECIFIC ENHANCER FACTOR 2A, C4 FORM Chain A: 87% 13% *** | | *TP*CP*GP*GP*CP*TP*AP | *TP*TP*AP*AP*TP*AP*GP*Cl |
| • Molecule 2: MYOCYTE-SPECIFIC ENHANCER FACTOR 2A, C4 FORM Chain A: 87% 13% 13% 13% 13% Molecule 2: MYOCYTE-SPECIFIC ENHANCER FACTOR 2A, C4 FORM | Chain D: | 100% | |
| Chain A: 87% 13% 22222222222222222222222222222222 | 7221 7222 7223 7224 7226 7226 7226 7236 7231 7233 7233 7233 7235 7235 | 0240 0240 | |
| • Molecule 2: MYOCYTE-SPECIFIC ENHANCER FACTOR 2A, C4 FORM | • Molecule 2: MYOCY | ΓΕ-SPECIFIC ENHANCER FA | ACTOR 2A, C4 FORM |
| • Molecule 2: MYOCYTE-SPECIFIC ENHANCER FACTOR 2A, C4 FORM | Chain A: | 87% | 13% |
| • Molecule 2: MYOCYTE-SPECIFIC ENHANCER FACTOR 2A, C4 FORM | 01 | 119 121 121 122 123 124 127 127 128 130 131 132 134 138 138 138 138 138 138 138 138 | 142 143 144 145 145 146 148 148 148 148 148 148 148 148 148 148 |
| | M61 D62 C63 C63 C63 C65 C66 C66 C67 M72 M72 M72 M72 M72 M72 M72 M72 M72 M7 | THE ASN SER ASN ASP ASN ASP | |
| Chain B: 87% 13% Chain B: 87% 2511 2511 2511 2511 2511 2511 2511 251 | • Molecule 2: MYOCY | ΓΕ-SPECIFIC ENHANCER FA | ACTOR 2A, C4 FORM |
| M. M | Chain B: | 87% | 13% |
| M 161 K165 K166 K167 K167 K167 K167 K167 K167 K167 | R102 R103 R104 R104 R106 R107 R110 M111 D112 R114 R114 R115 | H119 H121 H123 H123 H124 H128 H128 H128 H139 H131 H131 H132 H133 H134 H134 H134 H135 H136 H137 H138 | 1142 1142 1144 1146 1146 1146 1146 1146 |
| | M161 M163 M163 M164 M165 M167 M172 M172 M172 M172 M172 M173 M174 M174 M175 M176 M177 | THR SER SER ASP ILE VAL GLU | |



Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: simulated annealing.

Of the 35 calculated structures, 1 were deposited, based on the following criterion: REGULAR-IZED 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.



6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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 | С | 0 | 0 | 0 | 0 |
| 1 | D | 0 | 0 | 0 | 0 |
| 2 | A | 0 | 0 | 0 | 0 |
| 2 | В | 0 | 0 | 0 | 0 |
| All | All | 0 | 0 | 0 | - |

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 |
|-----|-------|----------|----------|---------|----------|-------------|
| 2 | A | 0 | - | - | - | - |
| 2 | В | 0 | - | - | = | - |
| All | All | 0 | - | - | - | - |



There are no Ramachandran outliers.

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 | 0 | - | - | - |
| 2 | В | 0 | - | - | - |
| All | All | 0 | - | - | - |

There are no protein residues with a non-rotameric sidechain to report.

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)

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 (i)

No chemical shift data were provided

