Full wwPDB NMR Structure Validation Report (i)

May 7, 2024 – 01:07 pm BST

PDB ID	:	2VRG
Title	:	Structure of human MCFD2
Authors	:	Guy, J.E.; Wigren, E.; Svard, M.; Hard, T.; Lindqvist, Y.
Deposited on	:	2008-04-04

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	:	FAILED
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 was not calculated.

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

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 2 as representative.

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:67-A:101, A:109-A:145 (72)	0.50	17

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20
2	6, 15

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1243 atoms, of which 599 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	80	1241	398	599	104	137	3	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	2	2	2

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: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.2 Score per residue for model 2

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.3 Score per residue for model 3

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.4 Score per residue for model 4

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.5 Score per residue for model 5

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.6 Score per residue for model 6

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.7 Score per residue for model 7

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.8 Score per residue for model 8

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.9 Score per residue for model 9

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.10 Score per residue for model 10

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.11 Score per residue for model 11

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.12 Score per residue for model 12

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.13 Score per residue for model 13

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.14 Score per residue for model 14

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.15 Score per residue for model 15

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.16 Score per residue for model 16

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.17 Score per residue for model 17 (medoid)

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

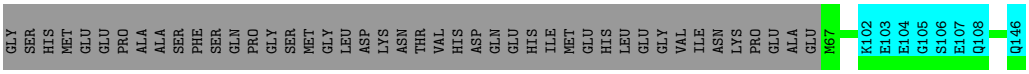
Chain A: 58% 6% 35%

GLY SER HIS MET GLU GLU PRO ALA ALA SER PHE SER GLN PRO GLY SER MET GLY LEU ASP LYS ASN THR VAL HIS ASP GLN GLU HIS ILE MET GLU HIS LEU GLU GLY VAL ILE ASN LYS PRO GLU ALA GLU M67 K102 E103 E104 G105 S106 E107 Q108 Q146

4.2.18 Score per residue for model 18

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

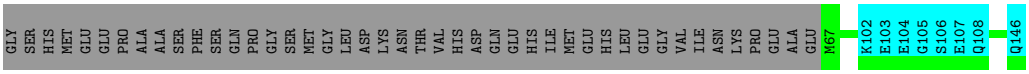
Chain A: 58% 6% 35%



4.2.19 Score per residue for model 19

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

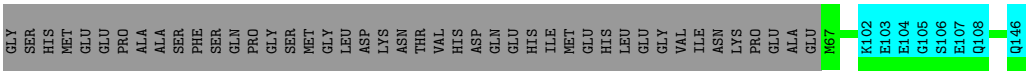
Chain A: 58% 6% 35%



4.2.20 Score per residue for model 20

• Molecule 1: MULTIPLE COAGULATION FACTOR DEFICIENCY PROTEIN 2

Chain A: 58% 6% 35%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *AB INITIO SIMULATED ANNEALING IN ARIA2*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *TOTAL ENERGY AND RESTRAINT VIOLATION STATISTICS*.

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

Software name	Classification	Version
ARIA	refinement	
NMRPipe	structure solution	
CcpNmr Analysis	structure solution	ANALYSIS
TALOS	structure solution	
ARIA	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts (i)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA (i)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates (i)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry (i)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers (i)

MolProbity failed to run properly - this section will have to be empty.

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