wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1LM0
Title	:	Solution structure and characterization of the heme chaperone CcmE
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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
https://www.wwpdb.org/validation/2017/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:

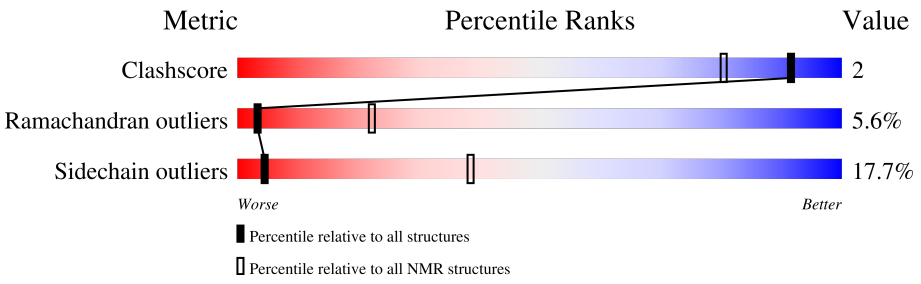
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	136	56% 12% 6% 26%

2 Ensemble composition and analysis (i)

This entry contains 35 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:36-A:86, A:90-A:131 (93)	0.45	8

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 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 6, 7, 8, 9, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 23, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35
2	5, 22
3	4, 10
Single-model clusters	24

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1504 atoms, of which 749 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called cytochrome c maturation protein E.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	101	1504	472	749	131	150	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	PHE	-	cloning artifact	UNP O52690
A	27	ALA	-	cloning artifact	UNP O52690
A	28	ALA	-	cloning artifact	UNP O52690
A	29	ASP	-	cloning artifact	UNP O52690

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: cytochrome c maturation protein E

Chain A: 56% 12% 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 I43 K47 T50 K53 T67 R73 L78 S87 L88 G89 I92 Y96 P101 D102 L103 F104 R105 Q113 K121 L128 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA MET

GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

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

The representative model is number 8. Colouring as in section 4.1 above.

• Molecule 1: cytochrome c maturation protein E

Chain A: 53% 13% •• 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 L36 F37 Y38 E42 I43 D49 K53 R59 M65 V66 R73 L78 H85 D86 S87 L88 G89 I92 Y96 F104 Q113 L116 G117 L122 T125 L128 D132 GLU ASN TYR MET PRO PRO

GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, torsion angle dyanamics, restrained energy minimization.*

Of the 400 calculated structures, 35 were deposited, based on the following criterion: *the submitted conformer models are the 35 structures with the lowest target function.*

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

Software name	Classification	Version
DYANA	structure solution	1.5
Amber	refinement	5.0

No chemical shift data was provided.

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	A	0.52±0.01	0±0/711 (0.0± 0.0%)	0.94±0.04	0±1/965 (0.0± 0.1%)
All	All	0.52	0/24885 (0.0%)	0.94	13/33775 (0.0%)

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	0.0±0.2	1.8±1.1
All	All	1	64

There are no bond-length outliers.

5 of 9 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	96	TYR	CB-CG-CD2	-6.60	117.04	121.00	2	4
1	A	86	ASP	CB-CG-OD2	-5.77	113.11	118.30	15	1
1	A	105	ARG	NE-CZ-NH2	-5.62	117.49	120.30	29	2
1	A	73	ARG	NE-CZ-NH2	-5.61	117.50	120.30	27	1
1	A	93	LEU	CB-CA-C	-5.41	99.92	110.20	3	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	40	PRO	CA	1

5 of 10 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	96	TYR	Sidechain	16
1	A	104	PHE	Sidechain,Peptide	13
1	A	105	ARG	Peptide,Sidechain	11
1	A	38	TYR	Sidechain	9
1	A	59	ARG	Sidechain	4

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	699	698	698	2±2
All	All	24465	24430	24430	75

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 2.

5 of 62 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:HD22	1:A:122:LEU:HD22	0.81	1.48	23	2
1:A:43:ILE:HD13	1:A:43:ILE:H	0.63	1.52	35	1
1:A:96:TYR:OH	1:A:127:VAL:HG13	0.61	1.94	23	2
1:A:48:THR:HG23	1:A:116:LEU:HD11	0.61	1.72	21	1
1:A:38:TYR:OH	1:A:43:ILE:HD12	0.60	1.96	35	1

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
1	A	93/136 (68%)	74±3 (79±3%)	14±3 (15±3%)	5±2 (6±2%)	3 22
All	All	3255/4760 (68%)	2585 (79%)	489 (15%)	181 (6%)	3 22

5 of 27 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	104	PHE	22
1	A	101	PRO	20
1	A	53	LYS	19
1	A	103	LEU	16
1	A	119	ASP	15

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
1	A	75/111 (68%)	62±3 (82±4%)	13±3 (18±4%)	4 38
All	All	2625/3885 (68%)	2161 (82%)	464 (18%)	4 38

5 of 56 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)
1	A	38	TYR	30
1	A	78	LEU	29
1	A	103	LEU	27
1	A	121	LYS	25
1	A	128	LEU	24

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