



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Sep 17, 2017 – 11:34 AM EDT

PDB ID : 5TTP  
EMDB ID: : EMD-8467  
Title : Cryo-EM structure of MsbA-nanodisc with ADP-vanadate  
Authors : Mi, W.; Walz, T.; Liao, M.  
Deposited on : unknown  
Resolution : 4.80 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

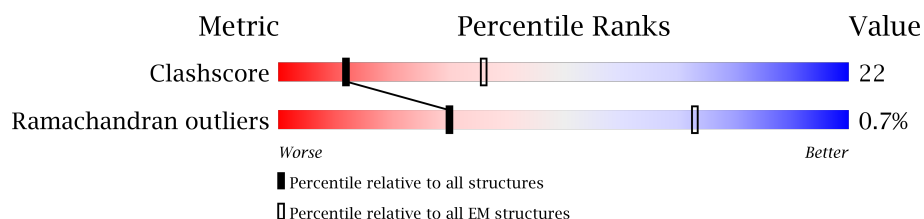
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 Å.

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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A	605	
1	B	605	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5616 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lipid A export ATP-binding/permease protein MsbA.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	569	Total	C	N	O	0	0
			2808	1670	569	569		
1	B	569	Total	C	N	O	0	0
			2808	1670	569	569		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P60753
A	-21	GLY	-	expression tag	UNP P60753
A	-20	HIS	-	expression tag	UNP P60753
A	-19	HIS	-	expression tag	UNP P60753
A	-18	HIS	-	expression tag	UNP P60753
A	-17	HIS	-	expression tag	UNP P60753
A	-16	HIS	-	expression tag	UNP P60753
A	-15	HIS	-	expression tag	UNP P60753
A	-14	HIS	-	expression tag	UNP P60753
A	-13	HIS	-	expression tag	UNP P60753
A	-12	HIS	-	expression tag	UNP P60753
A	-11	HIS	-	expression tag	UNP P60753
A	-10	SER	-	expression tag	UNP P60753
A	-9	SER	-	expression tag	UNP P60753
A	-8	GLY	-	expression tag	UNP P60753
A	-7	HIS	-	expression tag	UNP P60753
A	-6	ILE	-	expression tag	UNP P60753
A	-5	ASP	-	expression tag	UNP P60753
A	-4	ASP	-	expression tag	UNP P60753
A	-3	ASP	-	expression tag	UNP P60753
A	-2	ASP	-	expression tag	UNP P60753
A	-1	LYS	-	expression tag	UNP P60753
A	0	HIS	-	expression tag	UNP P60753
B	-22	MET	-	initiating methionine	UNP P60753
B	-21	GLY	-	expression tag	UNP P60753
B	-20	HIS	-	expression tag	UNP P60753

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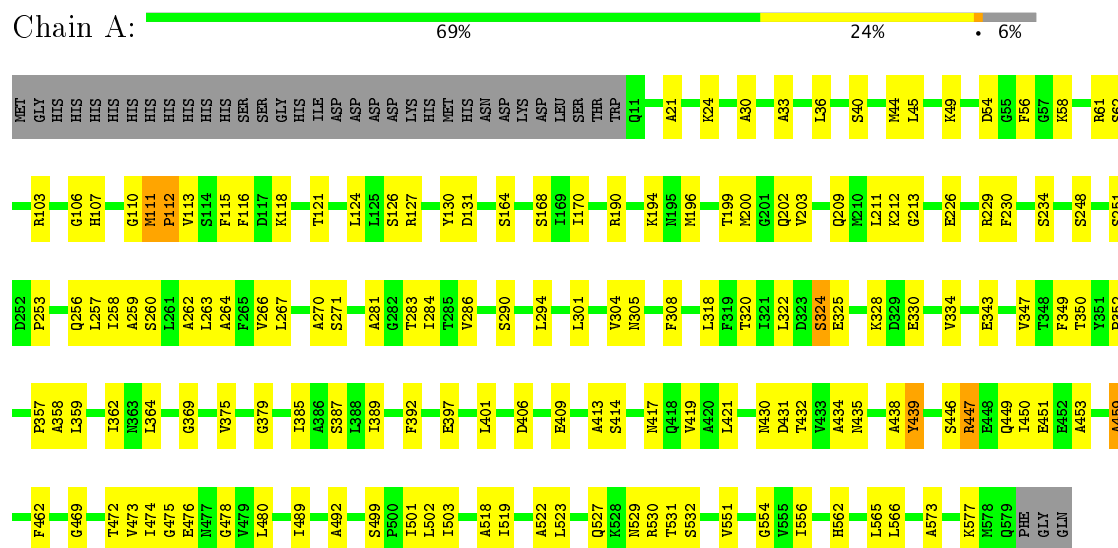
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	HIS	-	expression tag	UNP P60753
B	-18	HIS	-	expression tag	UNP P60753
B	-17	HIS	-	expression tag	UNP P60753
B	-16	HIS	-	expression tag	UNP P60753
B	-15	HIS	-	expression tag	UNP P60753
B	-14	HIS	-	expression tag	UNP P60753
B	-13	HIS	-	expression tag	UNP P60753
B	-12	HIS	-	expression tag	UNP P60753
B	-11	HIS	-	expression tag	UNP P60753
B	-10	SER	-	expression tag	UNP P60753
B	-9	SER	-	expression tag	UNP P60753
B	-8	GLY	-	expression tag	UNP P60753
B	-7	HIS	-	expression tag	UNP P60753
B	-6	ILE	-	expression tag	UNP P60753
B	-5	ASP	-	expression tag	UNP P60753
B	-4	ASP	-	expression tag	UNP P60753
B	-3	ASP	-	expression tag	UNP P60753
B	-2	ASP	-	expression tag	UNP P60753
B	-1	LYS	-	expression tag	UNP P60753
B	0	HIS	-	expression tag	UNP P60753

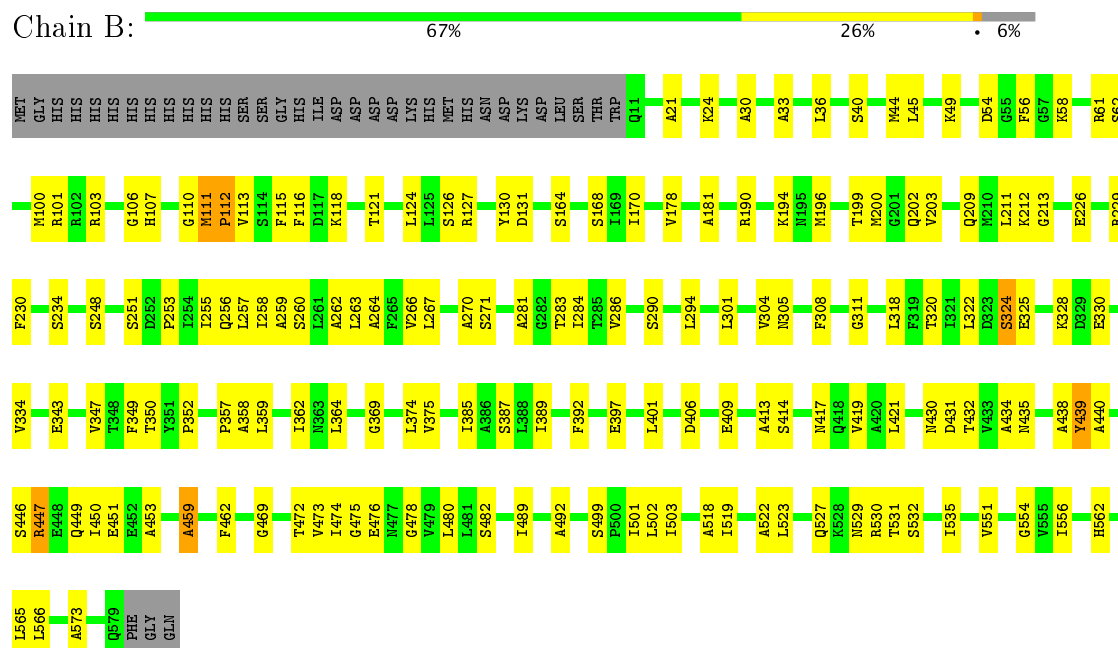
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lipid A export ATP-binding/permease protein MsbA



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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	36732	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 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 root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	A	0.38	0/2807	0.67	1/3906 (0.0%)
1	B	0.38	0/2807	0.67	1/3906 (0.0%)
All	All	0.38	0/5614	0.67	2/7812 (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 outliers	#Planarity outliers
1	A	0	10
1	B	0	10
All	All	0	20

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	GLY	N-CA-C	-5.16	100.21	113.10
1	B	469	GLY	N-CA-C	-5.15	100.23	113.10

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	MET	Peptide
1	A	112	PRO	Peptide
1	A	324	SER	Peptide
1	A	325	GLU	Peptide
1	A	36	LEU	Peptide

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2808	0	1305	88	0
1	B	2808	0	1305	93	0
All	All	5616	0	2610	180	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 22.

The worst 5 of 180 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:GLN:O	1:B:453:ALA:HB2	1.68	0.93
1:A:449:GLN:O	1:A:453:ALA:HB2	1.68	0.91
1:B:446:SER:O	1:B:450:ILE:N	2.04	0.90
1:A:446:SER:O	1:A:450:ILE:N	2.04	0.90
1:A:256:GLN:O	1:A:260:SER:N	2.09	0.86

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 EM 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	567/605 (94%)	483 (85%)	80 (14%)	4 (1%)	25 68
1	B	567/605 (94%)	483 (85%)	80 (14%)	4 (1%)	25 68
All	All	1134/1210 (94%)	966 (85%)	160 (14%)	8 (1%)	30 68



5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	PRO
1	B	112	PRO
1	A	324	SER
1	B	324	SER
1	A	320	THR

### 5.3.2 Protein sidechains ⓘ

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.