



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:42 PM BST

PDB ID : 3J09  
EMDB ID: : EMD-5004  
Title : High resolution helical reconstruction of the bacterial p-type ATPase copper transporter CopA  
Authors : Wu, C.; Allen, G.S.; Cardozo, T.; Stokes, D.L.  
Deposited on : 2011-05-09  
Resolution : 10.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

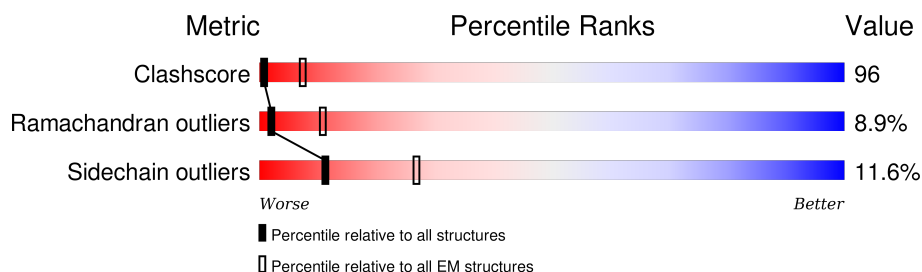
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	723	<div> <div>50%</div> <div>33%</div> <div>11%</div> <div>5%</div> </div>
1	B	723	<div> <div>49%</div> <div>34%</div> <div>11%</div> <div>5%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10932 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 copper-exporting P-type ATPase A.

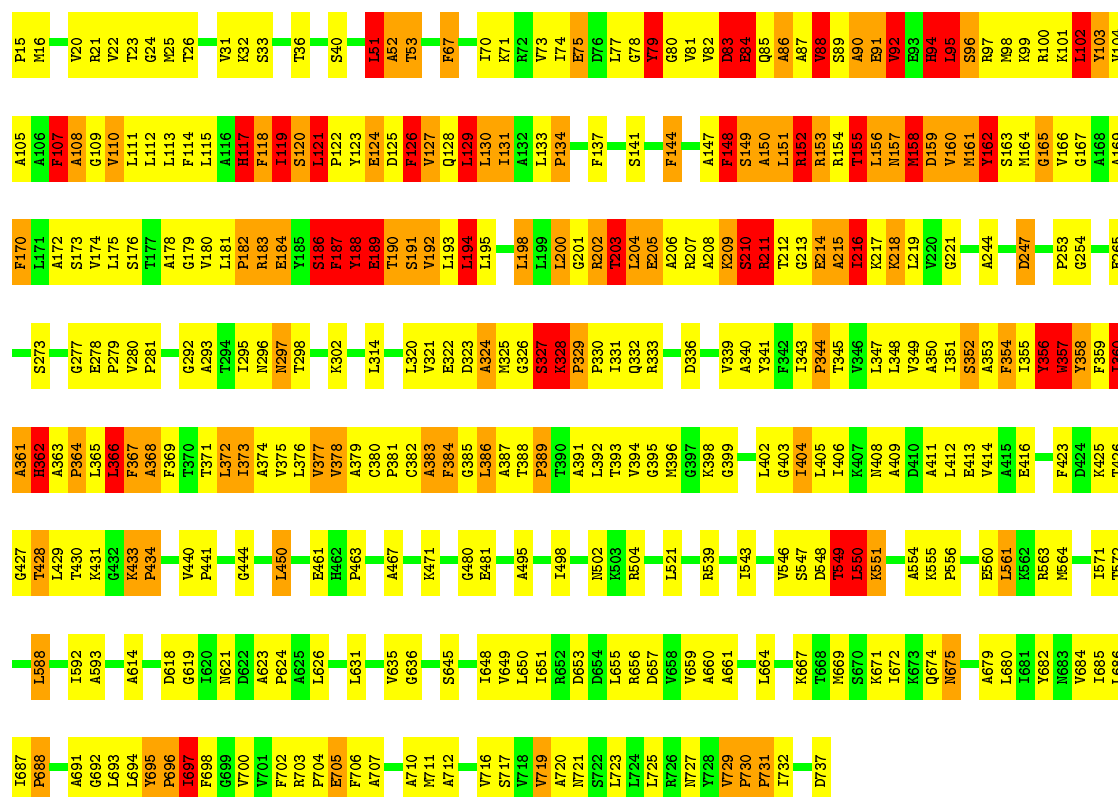
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	723	Total	C	N	O	S	0	0
			5466	3511	920	1015	20		
1	B	723	Total	C	N	O	S	0	0
			5466	3511	920	1015	20		

### 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 errors 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: copper-exporting P-type ATPase A

Chain A: 



A244	A353	V414	E560	A679
F384	F384	A415	L561	L680
D247	I355	E416	R562	I681
	Y356	K417	R563	Y682
P253	Y357		M564	R683
G254	Y358	F423		V684
	F359	D424	I571	I685
E265	I360	K425	T572	L686
	A361	T426		I687
S273	R362	G427	L588	P688
	A363	T428		
G277	P364	L429	I592	A691
E278	L365	T430	A593	G692
F279	L366	K431		L693
V280	F367	G432	A614	L694
V281	A368	P434		V695
	F369		D618	P696
G292	T370	V440	G619	I697
A293	T371	P441	I620	F698
T294	L372		M621	G699
I295	I373	G444	D622	V700
I296	A374		A623	F701
I297	V375	L450	P624	F702
T298	L376	E461	A625	R703
	V377	R462	L626	P704
K302	V378	P463		E705
	A379	L631	V635	F706
L314	C380			A707
	P381	A467		
L320	C382	K471	S639	A710
V321	A383			N711
E322	F384	G480	S645	A712
D323	G385	E481	I648	
A324	L386	A495	V649	V716
I325	T388		L650	S717
G326	T389	I499	I651	V718
S327	T390	N502	L655	V719
I328	A391	R503	R656	A720
P329	L392	R504	V657	N721
P330	T393	L521	V658	S722
I331	V394	R539	V659	L723
Q332	G395		A660	L724
R333	M396	I543	A661	I725
	G397	V546	L664	R726
D336	K398	S547	K667	N727
	G399	D548	T668	Y728
V339	L402	V549	M669	V729
A340	I403	I550	K671	P730
Y341	I404	R551	I672	P731
P342	L405	A554	K673	I732
I343	T345	K555	Q674	
P344	I406	P556	N675	D737
T345	K407			
V346	N408			
I347	A409			
I348	D410			
V349	A411			
A350	L412			
I351	E413			
S352				

## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	two-fold phase residual	Depositor
CTF correction method	each tube-crystal	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	Kodak SO-163	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	1.33	28/5545 (0.5%)	1.28	64/7515 (0.9%)
1	B	1.27	30/5545 (0.5%)	1.29	65/7515 (0.9%)
All	All	1.30	58/11090 (0.5%)	1.28	129/15030 (0.9%)

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	9
1	B	0	9
All	All	0	18

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	356	TYR	CG-CD1	40.18	1.91	1.39
1	A	356	TYR	CG-CD1	38.30	1.89	1.39
1	B	356	TYR	CE1-CZ	33.83	1.82	1.38
1	A	356	TYR	CE1-CZ	33.04	1.81	1.38
1	A	52	ALA	CA-CB	31.50	2.18	1.52

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	SER	O-C-N	16.68	149.39	122.70
1	A	352	SER	O-C-N	16.59	149.24	122.70
1	B	356	TYR	CB-CG-CD2	-16.56	111.06	121.00
1	A	356	TYR	CB-CG-CD2	-14.28	112.43	121.00
1	A	356	TYR	CB-CG-CD1	14.22	129.53	121.00

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	PHE	Peptide
1	A	121	LEU	Peptide
1	A	186	SER	Peptide
1	A	209	LYS	Peptide
1	A	210	SER	Peptide

## 5.2 Too-close contacts ⓘ

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	5466	0	5715	1101	0
1	B	5466	0	5715	1090	0
All	All	10932	0	11430	2148	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 96.

The worst 5 of 2148 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:A:356:TYR:CG	1:A:356:TYR:CD2	1.79	1.64
1:B:356:TYR:CE1	1:B:356:TYR:CZ	1.82	1.62
1:A:354:PHE:N	1:A:356:TYR:CD1	1.68	1.59
1:A:51:LEU:CB	1:A:51:LEU:CA	1.77	1.59
1:B:52:ALA:CB	1:B:52:ALA:CA	1.77	1.59

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	721/723 (100%)	576 (80%)	81 (11%)	64 (9%)	1	17
1	B	721/723 (100%)	576 (80%)	80 (11%)	65 (9%)	1	17
All	All	1442/1446 (100%)	1152 (80%)	161 (11%)	129 (9%)	2	17

5 of 129 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	A	86	ALA
1	A	88	VAL
1	A	102	LEU
1	A	119	ILE

### 5.3.2 Protein sidechains ⓘ

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 EM 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	581/581 (100%)	513 (88%)	68 (12%)	7	32
1	B	581/581 (100%)	514 (88%)	67 (12%)	7	32
All	All	1162/1162 (100%)	1027 (88%)	135 (12%)	11	32

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	588	LEU
1	B	102	LEU
1	B	547	SER
1	A	669	MET
1	B	50	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	721	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.