



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:54 PM BST

PDB ID : 3JCF
EMDB ID: : EMD-6551
Title : Cryo-EM structure of the magnesium channel CorA in the closed symmetric magnesium-bound state
Authors : Matthies, D.; Perozo, E.; Subramaniam, S.
Deposited on : 2015-12-11
Resolution : 3.80 Å(reported)
Based on PDB ID : 4I0U

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

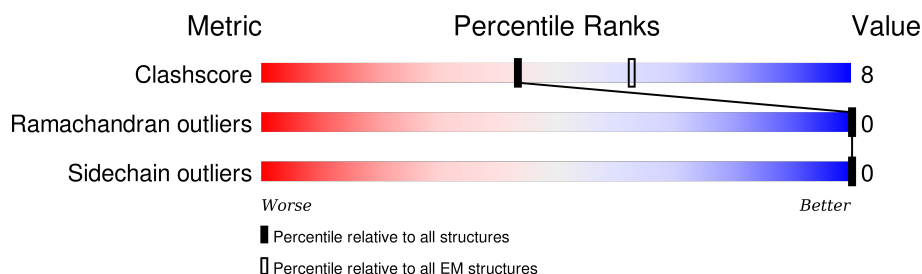
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	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 ≥ 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	351	77% 23% .
1	B	351	77% 22% .
1	C	351	77% 23% .
1	D	351	77% 22% .
1	E	351	77% 22% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14228 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 Magnesium transport protein CorA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	349	Total	C	N	O	S	0	0
			2843	1850	461	524	8		
1	B	349	Total	C	N	O	S	0	0
			2843	1850	461	524	8		
1	C	349	Total	C	N	O	S	0	0
			2843	1850	461	524	8		
1	D	349	Total	C	N	O	S	0	0
			2843	1850	461	524	8		
1	E	349	Total	C	N	O	S	0	0
			2843	1850	461	524	8		

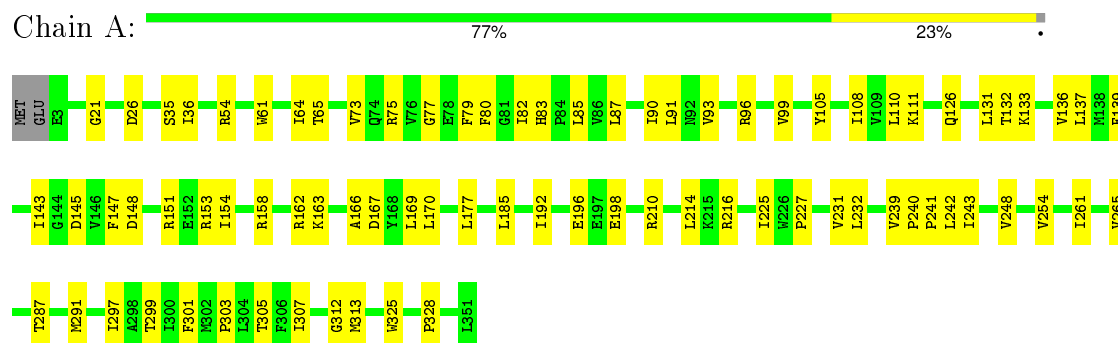
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
2	B	2	Total	Mg	0
			2	2	
2	A	2	Total	Mg	0
			2	2	
2	D	2	Total	Mg	0
			2	2	
2	C	2	Total	Mg	0
			2	2	
2	E	5	Total	Mg	0
			5	5	

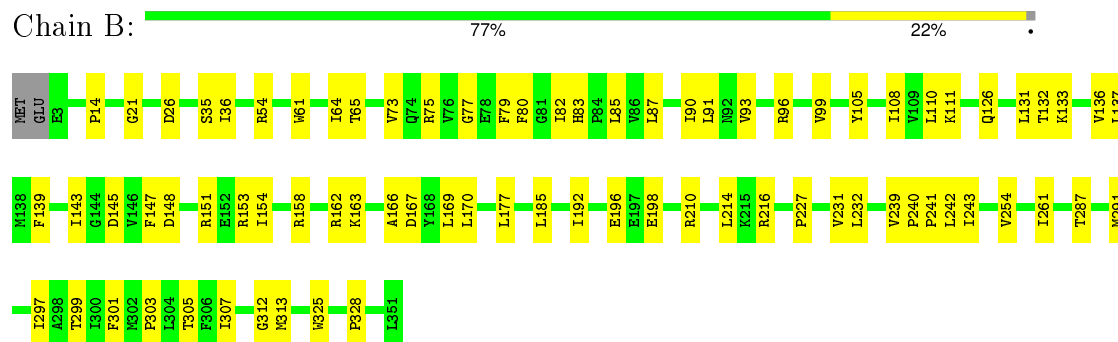
3 Residue-property plots

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.

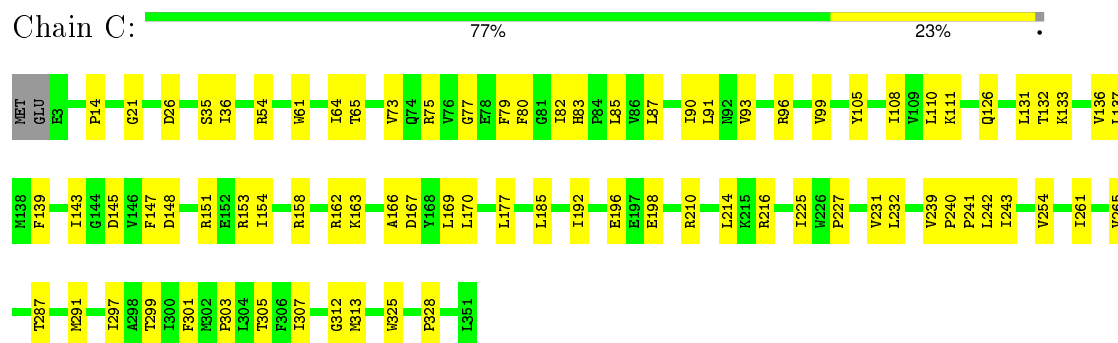
- Molecule 1: Magnesium transport protein CorA



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T299	G144	WET
I300	D145	GLU
F301	V146	E3
K302	F147	
P303	D148	G21
L304		
T305	R151	D26
F306	E152	
I307	R153	S35
	I154	I36
G312	R158	R54
M313		
W325	R162	W61
	K163	
F328	A166	I64
	D167	T65
	Y168	V73
L351	L169	Q74
	L170	R75
		V76
	L177	G77
		E78
	L185	F79
		F80
	I192	G81
		I82
	E196	I83
	E197	F84
	E198	L85
		V86
	R210	L87
	L214	I90
	K215	L91
	R216	I92
		V93
	V231	
	L232	V99
	V239	Y105
	P240	
	P241	I108
	L242	Y109
	I243	L110
		K111
	T247	
	V248	Q126
	V254	L131
		T132
	I261	K133
	T287	V136
		L137
	M291	M138
		F139
	I297	
	V298	T142

- Chain E:  77% 22%

[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	46206	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	CTF parameters obtained from whole micro-graph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	860	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.21	0/2905	0.38	0/3946
1	B	0.21	0/2905	0.38	0/3946
1	C	0.21	0/2905	0.38	0/3946
1	D	0.21	0/2905	0.38	0/3946
1	E	0.21	0/2905	0.38	0/3946
All	All	0.21	0/14525	0.38	0/19730

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2843	0	2837	53	0
1	B	2843	0	2837	53	0
1	C	2843	0	2837	52	0
1	D	2843	0	2837	51	0
1	E	2843	0	2837	52	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	0	0
2	E	5	0	0	0	0
All	All	14228	0	14185	241	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 8.

The worst 5 of 241 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:154:ILE:O	1:A:162:ARG:NH2	2.24	0.70
1:E:154:ILE:O	1:E:162:ARG:NH2	2.24	0.69
1:C:154:ILE:O	1:C:162:ARG:NH2	2.24	0.69
1:B:154:ILE:O	1:B:162:ARG:NH2	2.24	0.68
1:D:154:ILE:O	1:D:162:ARG:NH2	2.24	0.67

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	347/351 (99%)	331 (95%)	16 (5%)	0	100	100
1	B	347/351 (99%)	331 (95%)	16 (5%)	0	100	100
1	C	347/351 (99%)	331 (95%)	16 (5%)	0	100	100
1	D	347/351 (99%)	331 (95%)	16 (5%)	0	100	100
1	E	347/351 (99%)	331 (95%)	16 (5%)	0	100	100
All	All	1735/1755 (99%)	1655 (95%)	80 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	314/330 (95%)	314 (100%)	0	100	100
1	B	314/330 (95%)	314 (100%)	0	100	100
1	C	314/330 (95%)	314 (100%)	0	100	100
1	D	314/330 (95%)	314 (100%)	0	100	100
1	E	314/330 (95%)	314 (100%)	0	100	100
All	All	1570/1650 (95%)	1570 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	140	GLN
1	C	314	ASN
1	D	314	ASN
1	B	314	ASN
1	D	140	GLN

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

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.