wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:53 PM BST

PDB ID	:	3JCG
EMDB ID:	:	EMD-6552
Title	:	Cryo-EM structure of the magnesium channel CorA in the magnesium-free, asymmetric open state I
Authors	:	Matthies, D.; Perozo, E.; Subramaniam, S.
Deposited on	:	2015-12-11
Resolution	:	7.06 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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

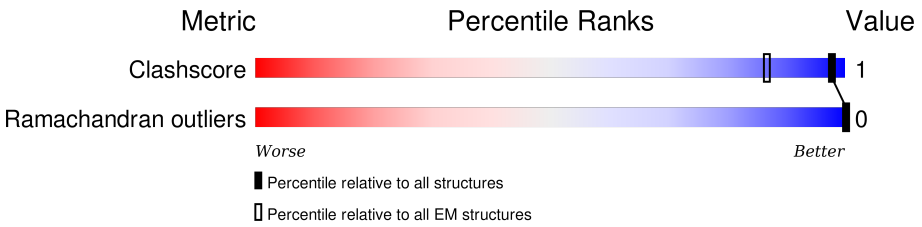
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.06 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

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	351	94% 6%
1	B	351	94% 6%
1	C	351	92% • 6%
1	D	351	93% • 6%
1	E	351	94% • 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6617 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.

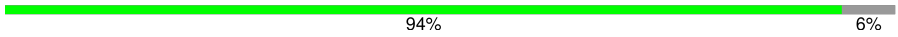
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	331	1325	663	331	331	0	0
1	B	330	1321	661	330	330	0	0
1	C	330	1321	661	330	330	0	0
1	D	331	1325	663	331	331	0	0
1	E	331	1325	663	331	331	0	0

3 Residue-property plots (i)

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.

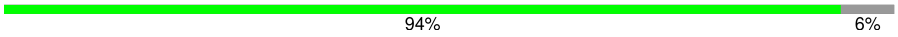
- Molecule 1: Magnesium transport protein CorA

Chain A:



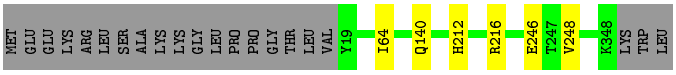
- Molecule 1: Magnesium transport protein CorA

Chain B:



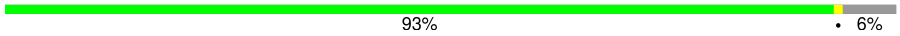
- Molecule 1: Magnesium transport protein CorA

Chain C:



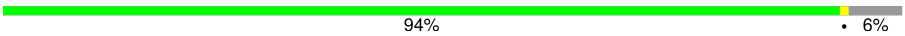
- Molecule 1: Magnesium transport protein CorA

Chain D:



- Molecule 1: Magnesium transport protein CorA

Chain E:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	26271	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	CTF parameters obtained from whole micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	890	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality (i)

5.1 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 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	0.18	0/1324	0.35	0/1654
1	B	0.18	0/1320	0.34	0/1649
1	C	0.18	0/1320	0.35	0/1649
1	D	0.18	0/1324	0.36	0/1654
1	E	0.18	0/1324	0.35	0/1654
All	All	0.18	0/6612	0.35	0/8260

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	1325	0	340	0	0
1	B	1321	0	339	0	0
1	C	1321	0	339	3	0
1	D	1325	0	340	2	0
1	E	1325	0	340	1	0
All	All	6617	0	1698	6	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 1.

All (6) 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:C:212:HIS:O	1:C:216:ARG:N	2.29	0.57
1:D:301:PHE:O	1:D:305:THR:N	2.48	0.45
1:E:207:THR:O	1:E:211:THR:N	2.49	0.45
1:D:192:ILE:O	1:D:196:GLU:N	2.41	0.45
1:C:64:ILE:O	1:C:140:GLN:N	2.47	0.45
1:C:246:GLU:C	1:C:248:VAL:H	2.22	0.42

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	329/351 (94%)	304 (92%)	25 (8%)	0	100	100
1	B	328/351 (93%)	307 (94%)	21 (6%)	0	100	100
1	C	328/351 (93%)	300 (92%)	28 (8%)	0	100	100
1	D	329/351 (94%)	312 (95%)	17 (5%)	0	100	100
1	E	329/351 (94%)	313 (95%)	16 (5%)	0	100	100
All	All	1643/1755 (94%)	1536 (94%)	107 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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.