wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 20, 2017 – 11:11 AM EDT

|		
PDB ID	:	4CY4
EMDB ID:	:	EMD-2626
Title	:	The Cryo-Electron Microscopy Structure of the CorA channel from Methanocaldococcus jannaschii at 21.6 Angstrom in low magnesium.
Authors	:	Cleverley, R.M.; Kean, J.; Shintre, C.A.; Baldock, C.; Derrick, J.P.; Ford, R.C.; Prince, S.M.
Deposited on	:	unknown
Resolution	:	21.60 Å(reported)
Based on PDB ID	:	4EV6

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 21.60 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	Percentile Ranks	Value
Clashscore		7

Worse   *Better*

▮ Percentile relative to all structures

〖 Percentile relative to all EM structures
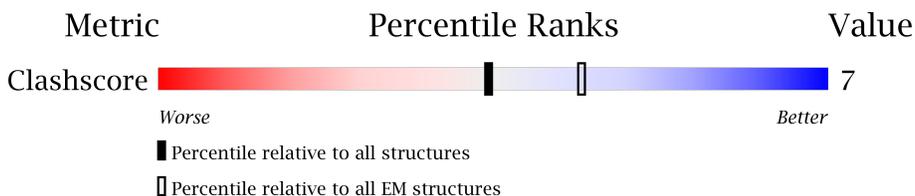
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336

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	317	97%
1	B	317	98%
1	C	317	97%
1	D	317	98%
1	E	317	99%
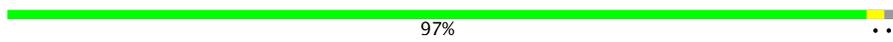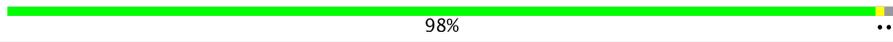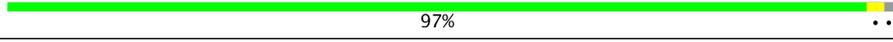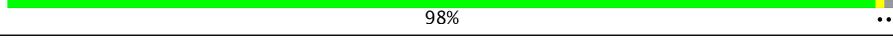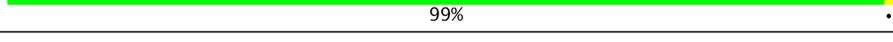
2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 1575 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	315	Total 315	C 315	0	315
1	B	314	Total 314	C 314	0	314
1	C	314	Total 314	C 314	0	314
1	D	314	Total 314	C 314	0	314
1	E	317	Total 318	C 318	1	317

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: MAGNESIUM TRANSPORT PROTEIN CORA

Chain A:
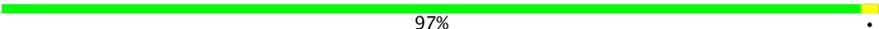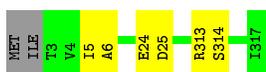
• Molecule 1: MAGNESIUM TRANSPORT PROTEIN CORA

Chain B:
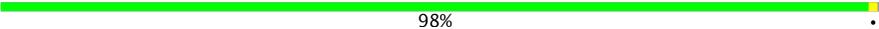
• Molecule 1: MAGNESIUM TRANSPORT PROTEIN CORA

Chain C:
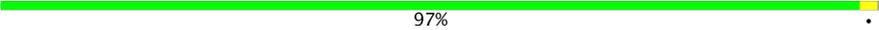
• Molecule 1: MAGNESIUM TRANSPORT PROTEIN CORA

Chain D:
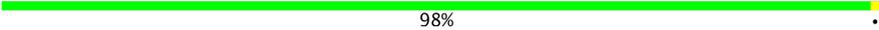
• Molecule 1: MAGNESIUM TRANSPORT PROTEIN CORA

Chain E:

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44064	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	WITH REFERENCE TO X-RAY SCATTERING CURVE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	Not provided	Depositor
Minimum defocus (nm)	3300	Depositor
Maximum defocus (nm)	4800	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN ULTRASCAN 4000 (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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	315	0	0	3	0
1	B	314	0	0	2	0
1	C	314	0	0	3	0
1	D	314	0	0	2	0
1	E	318	0	0	1	0
All	All	1575	0	0	11	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 7.

The worst 5 of 11 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:24:GLU:CA	1:A:25:ASP:CA	2.76	0.63
1:E:1:MET:CA	1:E:2:ILE:CA	2.81	0.59
1:B:122:LYS:CA	1:B:123:LYS:CA	2.83	0.57
1:D:313:ARG:CA	1:D:314:SER:CA	2.85	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:PRO:CA	1:D:125:ARG:CA	2.90	0.50

There are no symmetry-related clashes.

5.3   Torsion angles (i)

5.3.1   Protein backbone (i)

There are no protein backbone outliers to report in this entry.

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.