



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 3, 2018 – 10:51 AM EST

PDB ID : 5OYG
EMDB ID: : EMD-3861
Title : Structure of calcium-free mTMEM16A chloride channel at 4.06 Å resolution
Authors : Paulino, C.; Kalienkova, V.; Lam, K.M.; Neldner, Y.; Dutzler, R.
Deposited on : 2017-09-08
Resolution : 4.06 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at 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.

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-20030736

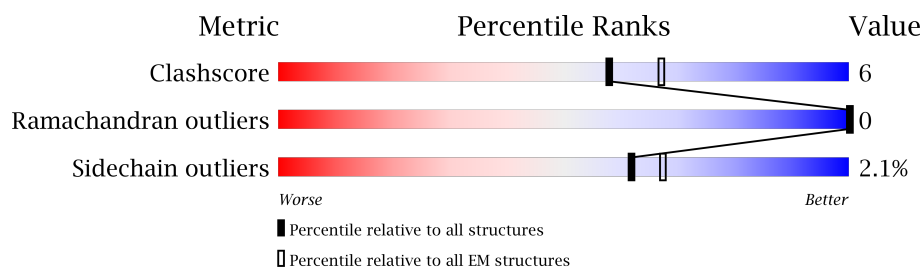
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.06 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	960	 62% 11% • 26%
1	B	960	 62% 11% • 26%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11596 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 Anoctamin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	709	Total	C	N	O	S	0	0
			5798	3783	953	1026	36		
1	B	709	Total	C	N	O	S	0	0
			5798	3783	953	1026	36		

GLU	LYS	VAL	TYR	K588	P380	V197
PRO	LYS	LYS	LYS	S592	L381	L198
ARG	R683	ARG	ARG	K603	C386	Q206
ASP	D690	ASP	ASP	R609	K390	P207
VAL	PRO	VAL	VAL	P610	A210	A210
PRO	CYS	CYS	CYS	G611	R429	L220
ASN	ASN	ASN	ASN	F617	R455	L234
ASN	HIS	HIS	HIS	R618	E459	R246
SER	SER	SER	SER	F618	L463	I249
PRO	PRO	PRO	PRO	A718	S466	L254
THR	THR	THR	THR	M622	LEU	T258
THR	THR	THR	THR	E623	LYS	T259
HIS	HIS	HIS	HIS	E624	GLU	THR
PRO	PRO	PRO	PRO	C625	SER	LYS
GLU	GLU	GLU	GLU	A626	ALA	ALA
ALA	ALA	ALA	ALA	E633	ARG	LYS
GLY	GLY	GLY	GLY	Q645	THR	LYS
ASP	ASP	ASP	ASP	S639	GLU	THR
GLY	GLY	GLY	GLY	I640	SER	LYS
SER	SER	SER	SER	I641	ALA	ALA
PRO	PRO	PRO	PRO	M642	LYS	LYS
VAL	VAL	VAL	VAL	L643	TYR	TYR
PRO	PRO	PRO	PRO	G644	GLU	SER
SER	SER	SER	SER	K645	THR	MET
GLU	GLU	GLU	GLU	Q649	ASP	C267
TYR	TYR	TYR	TYR	N650	LYS	L268
THR	THR	THR	THR	H651	VAL	T269
HIS	HIS	HIS	HIS	L652	LYS	S270
GLY	GLY	GLY	GLY	F653	LEU	N274
ASP	ASP	ASP	ASP	E654	THR	S278
ALA	ALA	ALA	ALA	I655	TTP	ARG
LEU	LEU	LEU	LEU	G656	ASP	L283
				I657	PHE	D287
				P658	ARG	T288
				K659	P483	E289
				MET	V495	K299
				LYS	LYS	V293
				LYS	L498	
				PHE		
				ILE	F505	N296
				ARG	V508	
				TYR	LEU	
				LEU	LYS	
				LYS	R515	V305
				LEU	M524	P316
				ARG	ARG	E326
				GLN	GLN	L330
				LEU	R535	
				LEU	SER	
				ASP	PRO	
				THR	SER	
				TRP	ASP	I343
				MET	ARG	
				GLU	GLU	N375
				LYS	LYS	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	195465	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The contrast transfer function (CTF) parameters were estimated on the movie frames by ctffind4.1	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	36630	Depositor
Image detector	GATAN K2 SUMMIT (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	0.41	0/5945	0.62	0/8047
1	B	0.41	0/5945	0.62	0/8047
All	All	0.41	0/11890	0.62	0/16094

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	5798	0	5797	65	0
1	B	5798	0	5797	67	0
All	All	11596	0	11594	132	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 6.

All (132) 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:380:PRO:O	1:A:381:LEU:HG	1.62	0.98
1:B:380:PRO:O	1:B:381:LEU:HG	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:THR:O	1:B:198:LEU:HB3	1.75	0.86
1:A:187:THR:O	1:A:198:LEU:HB3	1.75	0.85
1:A:258:THR:HG1	1:A:267:GLY:N	1.76	0.83
1:A:169:ALA:O	1:A:173:LYS:HB2	1.87	0.74
1:B:169:ALA:O	1:B:173:LYS:HB2	1.87	0.74
1:B:258:THR:HG1	1:B:267:GLY:N	1.85	0.74
1:B:653:PHE:O	1:B:658:PRO:CG	2.39	0.71
1:A:649:GLN:O	1:A:653:PHE:HB2	1.91	0.71
1:A:653:PHE:O	1:A:658:PRO:CG	2.39	0.70
1:B:649:GLN:O	1:B:653:PHE:HB2	1.91	0.69
1:A:459:GLU:O	1:A:463:LEU:HB2	1.95	0.67
1:A:254:LEU:HD12	1:A:268:ILE:HD13	1.77	0.66
1:B:459:GLU:O	1:B:463:LEU:HB2	1.95	0.66
1:A:892:ASP:O	1:A:896:GLN:HB2	1.96	0.65
1:A:343:ILE:HD13	1:A:728:LEU:HD11	1.78	0.65
1:B:254:LEU:HD12	1:B:268:ILE:HD13	1.77	0.65
1:A:653:PHE:O	1:A:658:PRO:HG3	1.97	0.65
1:B:892:ASP:O	1:B:896:GLN:HB2	1.96	0.65
1:B:343:ILE:HD13	1:B:728:LEU:HD11	1.78	0.64
1:A:904:MET:O	1:A:908:PHE:HB2	1.97	0.64
1:B:653:PHE:O	1:B:658:PRO:HG3	1.97	0.64
1:B:904:MET:O	1:B:908:PHE:HB2	1.97	0.64
1:B:903:LEU:O	1:B:907:LEU:HB2	1.99	0.63
1:A:903:LEU:O	1:A:907:LEU:HB2	1.99	0.62
1:B:380:PRO:C	1:B:381:LEU:HG	2.20	0.62
1:A:380:PRO:C	1:A:381:LEU:HG	2.20	0.62
1:A:542:ALA:O	1:A:546:ASN:HB2	2.01	0.61
1:B:505:PHE:HA	1:B:508:VAL:HG12	1.83	0.61
1:B:125:ARG:HB3	1:B:197:VAL:HB	1.82	0.61
1:B:542:ALA:O	1:B:546:ASN:HB2	2.01	0.61
1:A:125:ARG:HB3	1:A:197:VAL:HB	1.82	0.60
1:A:126:PHE:HD2	1:A:278:SER:HB3	1.67	0.60
1:A:505:PHE:HA	1:A:508:VAL:HG12	1.83	0.60
1:B:177:PRO:HA	1:B:180:LYS:HB2	1.84	0.60
1:B:126:PHE:HD2	1:B:278:SER:HB3	1.67	0.59
1:A:177:PRO:HA	1:A:180:LYS:HB2	1.84	0.58
1:A:657:ILE:N	1:A:658:PRO:HD3	2.19	0.58
1:B:657:ILE:N	1:B:658:PRO:HD3	2.19	0.58
1:B:515:ARG:NH2	1:B:622:MET:O	2.33	0.56
1:B:121:GLU:HG3	1:B:198:LEU:HD11	1.88	0.56
1:B:722:LEU:O	1:B:722:LEU:HD23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LEU:HB2	1:B:234:LEU:HB3	1.88	0.56
1:A:220:LEU:HB2	1:A:234:LEU:HB3	1.88	0.56
1:A:722:LEU:HD23	1:A:722:LEU:O	2.05	0.55
1:A:121:GLU:HG3	1:A:198:LEU:HD11	1.87	0.55
1:A:515:ARG:NH2	1:A:622:MET:O	2.33	0.55
1:A:167:ARG:O	1:A:171:PHE:HB2	2.07	0.54
1:B:167:ARG:O	1:B:171:PHE:HB2	2.07	0.54
1:A:270:SER:O	1:A:274:ASN:HB2	2.09	0.53
1:B:811:SER:OG	1:B:837:ARG:NH1	2.43	0.52
1:B:270:SER:O	1:B:274:ASN:HB2	2.09	0.52
1:B:289:GLU:O	1:B:299:LYS:HE2	2.10	0.52
1:A:811:SER:OG	1:A:837:ARG:NH1	2.43	0.52
1:A:289:GLU:O	1:A:299:LYS:HE2	2.10	0.51
1:A:375:ASN:HA	1:A:390:LYS:HE3	1.93	0.51
1:B:690:ASP:HA	1:B:693:LEU:HD23	1.92	0.50
1:B:727:ALA:O	1:B:731:ASN:HB2	2.11	0.50
1:A:727:ALA:O	1:A:731:ASN:HB2	2.11	0.50
1:B:381:LEU:O	1:B:624:GLU:CD	2.49	0.50
1:A:381:LEU:O	1:A:624:GLU:CD	2.49	0.50
1:A:603:LYS:NZ	1:A:633:GLU:OE1	2.45	0.50
1:B:722:LEU:HD21	1:B:726:PHE:CZ	2.47	0.49
1:A:326:GLU:O	1:A:330:LEU:HB2	2.12	0.49
1:A:690:ASP:HA	1:A:693:LEU:HD23	1.92	0.49
1:A:293:VAL:HB	1:A:299:LYS:NZ	2.27	0.49
1:A:722:LEU:HD21	1:A:726:PHE:CZ	2.47	0.49
1:B:375:ASN:HA	1:B:390:LYS:HE3	1.93	0.49
1:A:718:ALA:HB1	1:A:779:ILE:HG13	1.94	0.49
1:B:293:VAL:HB	1:B:299:LYS:NZ	2.27	0.49
1:B:326:GLU:O	1:B:330:LEU:HB2	2.12	0.49
1:B:603:LYS:NZ	1:B:633:GLU:OE1	2.45	0.49
1:B:718:ALA:HB1	1:B:779:ILE:HG13	1.94	0.48
1:A:207:PRO:HA	1:A:210:ALA:HB3	1.97	0.47
1:A:715:LEU:HD22	1:A:774:ILE:HG21	1.97	0.46
1:B:715:LEU:HD22	1:B:774:ILE:HG21	1.98	0.46
1:A:653:PHE:O	1:A:658:PRO:HG2	2.15	0.46
1:A:127:ARG:HH11	1:A:195:ASN:HD22	1.64	0.46
1:A:495:VAL:HG12	1:A:498:ILE:HD12	1.98	0.45
1:B:127:ARG:HH11	1:B:195:ASN:HD22	1.64	0.45
1:B:122:ASP:OD1	1:B:246:ARG:NH1	2.49	0.45
1:A:892:ASP:O	1:A:896:GLN:CB	2.64	0.45
1:B:127:ARG:HB2	1:B:173:LYS:HZ3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:ARG:HG3	1:B:611:GLY:H	1.82	0.45
1:A:122:ASP:OD1	1:A:246:ARG:NH1	2.50	0.45
1:B:206:GLN:HE22	1:B:246:ARG:HG2	1.81	0.45
1:B:609:ARG:HD2	1:B:851:TYR:HB3	1.99	0.45
1:A:287:ASP:N	1:A:296:ASN:OD1	2.50	0.45
1:A:812:PHE:N	1:A:836:CYS:O	2.50	0.45
1:A:609:ARG:HD2	1:A:851:TYR:HB3	1.99	0.45
1:A:609:ARG:HG3	1:A:611:GLY:H	1.82	0.45
1:B:892:ASP:O	1:B:896:GLN:CB	2.64	0.45
1:A:651:ASN:O	1:A:655:ILE:HD12	2.18	0.44
1:A:515:ARG:HD3	1:A:515:ARG:HA	1.71	0.44
1:B:207:PRO:HA	1:B:210:ALA:HB3	1.97	0.44
1:A:206:GLN:HE22	1:A:246:ARG:HG2	1.81	0.44
1:B:287:ASP:N	1:B:296:ASN:OD1	2.50	0.44
1:B:495:VAL:HG12	1:B:498:ILE:HD12	1.99	0.44
1:B:588:LYS:O	1:B:592:SER:HB3	2.18	0.44
1:B:651:ASN:O	1:B:655:ILE:HD12	2.18	0.44
1:B:812:PHE:N	1:B:836:CYS:O	2.50	0.44
1:A:588:LYS:O	1:A:592:SER:HB3	2.18	0.43
1:B:380:PRO:O	1:B:381:LEU:CG	2.51	0.43
1:A:382:CYS:HB2	1:A:386:CYS:HB2	1.47	0.43
1:A:380:PRO:O	1:A:381:LEU:CG	2.51	0.43
1:A:293:VAL:HG11	1:A:296:ASN:HB2	2.01	0.43
1:B:515:ARG:HA	1:B:515:ARG:HD3	1.71	0.43
1:B:179:LYS:NZ	1:B:258:THR:O	2.50	0.43
1:B:495:VAL:HG21	1:B:568:GLU:HG2	2.01	0.43
1:B:659:LYS:HD2	1:B:659:LYS:HA	1.78	0.43
1:A:618:ARG:HH11	1:A:618:ARG:HG2	1.84	0.42
1:B:618:ARG:HH11	1:B:618:ARG:HG2	1.84	0.42
1:B:639:SER:O	1:B:643:LEU:CB	2.67	0.42
1:B:305:TRP:CD1	1:B:316:PRO:HD2	2.54	0.42
1:B:382:CYS:HB2	1:B:386:CYS:HB2	1.46	0.42
1:B:653:PHE:O	1:B:658:PRO:HG2	2.15	0.42
1:A:305:TRP:CD1	1:A:316:PRO:HD2	2.54	0.42
1:B:625:CYS:SG	1:B:626:ALA:N	2.93	0.42
1:A:639:SER:O	1:A:643:LEU:CB	2.67	0.41
1:A:625:CYS:SG	1:A:626:ALA:N	2.93	0.41
1:B:641:ILE:O	1:B:645:LYS:HB2	2.20	0.41
1:A:641:ILE:O	1:A:645:LYS:HB2	2.20	0.41
1:B:293:VAL:HG11	1:B:296:ASN:HB2	2.01	0.41
1:A:175:LYS:O	1:A:178:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:VAL:HG21	1:A:568:GLU:HG2	2.01	0.41
1:A:124:LYS:HE2	1:A:283:LEU:HD22	2.03	0.41
1:A:603:LYS:HE2	1:A:623:GLU:HG2	2.02	0.40
1:B:124:LYS:HE2	1:B:283:LEU:HD22	2.03	0.40
1:A:617:PHE:O	1:A:618:ARG:HG2	2.21	0.40
1:B:603:LYS:HE2	1:B:623:GLU:HG2	2.02	0.40
1:B:617:PHE:O	1:B:618:ARG:HG2	2.21	0.40

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	699/960 (73%)	651 (93%)	48 (7%)	0	100	100
1	B	699/960 (73%)	651 (93%)	48 (7%)	0	100	100
All	All	1398/1920 (73%)	1302 (93%)	96 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	631/853 (74%)	618 (98%)	13 (2%)	59	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	631/853 (74%)	618 (98%)	13 (2%)	59 82
All	All	1262/1706 (74%)	1236 (98%)	26 (2%)	62 82

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ARG
1	A	167	ARG
1	A	249	ILE
1	A	296	ASN
1	A	429	ARG
1	A	455	ARG
1	A	515	ARG
1	A	524	MET
1	A	535	ARG
1	A	683	ARG
1	A	715	LEU
1	A	717	VAL
1	A	731	ASN
1	B	127	ARG
1	B	167	ARG
1	B	249	ILE
1	B	296	ASN
1	B	429	ARG
1	B	455	ARG
1	B	515	ARG
1	B	524	MET
1	B	535	ARG
1	B	683	ARG
1	B	715	LEU
1	B	717	VAL
1	B	731	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	A	646	GLN
1	A	818	GLN
1	B	206	GLN
1	B	646	GLN

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Mol	Chain	Res	Type
1	B	818	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 ⓘ

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.