wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Feb 8, 2018 – 07:23 PM EST

PDB ID	:	6BGJ
EMDB ID:	:	EMD-7096
Title	:	Cryo-EM structure of the TMEM16A calcium-activated chloride channel in LMNG
Authors	:	Dang, S.; Feng, S.; Tien, J.; Peters, C.J.; Bulkley, D.; Lolicato, M.; Zhao, J.; Zuberbuhler, K.; Ye, W.; Qi, L.; Chen, T.; Craik, C.S.; Jan, Y.N.; Minor, D.L.Jr.; Cheng, Y.; Jan, L.Y.
Deposited on	:	2017-10-28
Resolution	:	3.80 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary 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 (i) symbol.

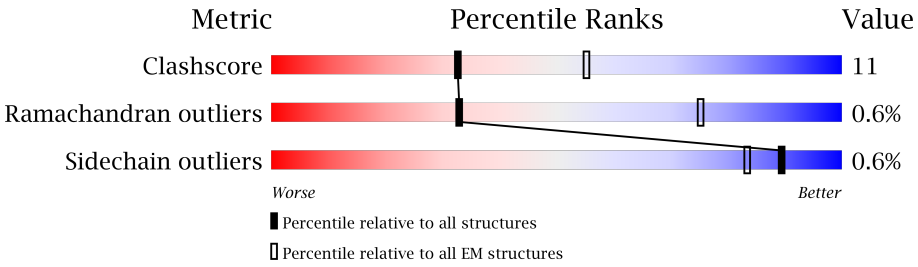
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

1 Overall quality at a glance (i)

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	912	41% 12% • 46%
1	B	912	41% 11% • 46%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7418 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	490	Total 3708	C 2446	N 597	O 641	S 24	0	0
1	B	490	Total 3708	C 2446	N 597	O 641	S 24	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	904	SER	-	expression tag	UNP Q8BHY3
A	905	ASN	-	expression tag	UNP Q8BHY3
A	906	SER	-	expression tag	UNP Q8BHY3
A	907	LEU	-	expression tag	UNP Q8BHY3
A	908	GLU	-	expression tag	UNP Q8BHY3
A	909	VAL	-	expression tag	UNP Q8BHY3
A	910	LEU	-	expression tag	UNP Q8BHY3
A	911	PHE	-	expression tag	UNP Q8BHY3
A	912	GLN	-	expression tag	UNP Q8BHY3
B	904	SER	-	expression tag	UNP Q8BHY3
B	905	ASN	-	expression tag	UNP Q8BHY3
B	906	SER	-	expression tag	UNP Q8BHY3
B	907	LEU	-	expression tag	UNP Q8BHY3
B	908	GLU	-	expression tag	UNP Q8BHY3
B	909	VAL	-	expression tag	UNP Q8BHY3
B	910	LEU	-	expression tag	UNP Q8BHY3
B	911	PHE	-	expression tag	UNP Q8BHY3
B	912	GLN	-	expression tag	UNP Q8BHY3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total 1	Ca 1	0

Continued on next page...

Continued from previous page...

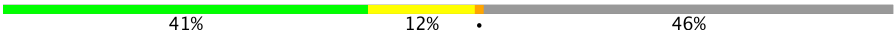
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
2	A	1	1	1	0

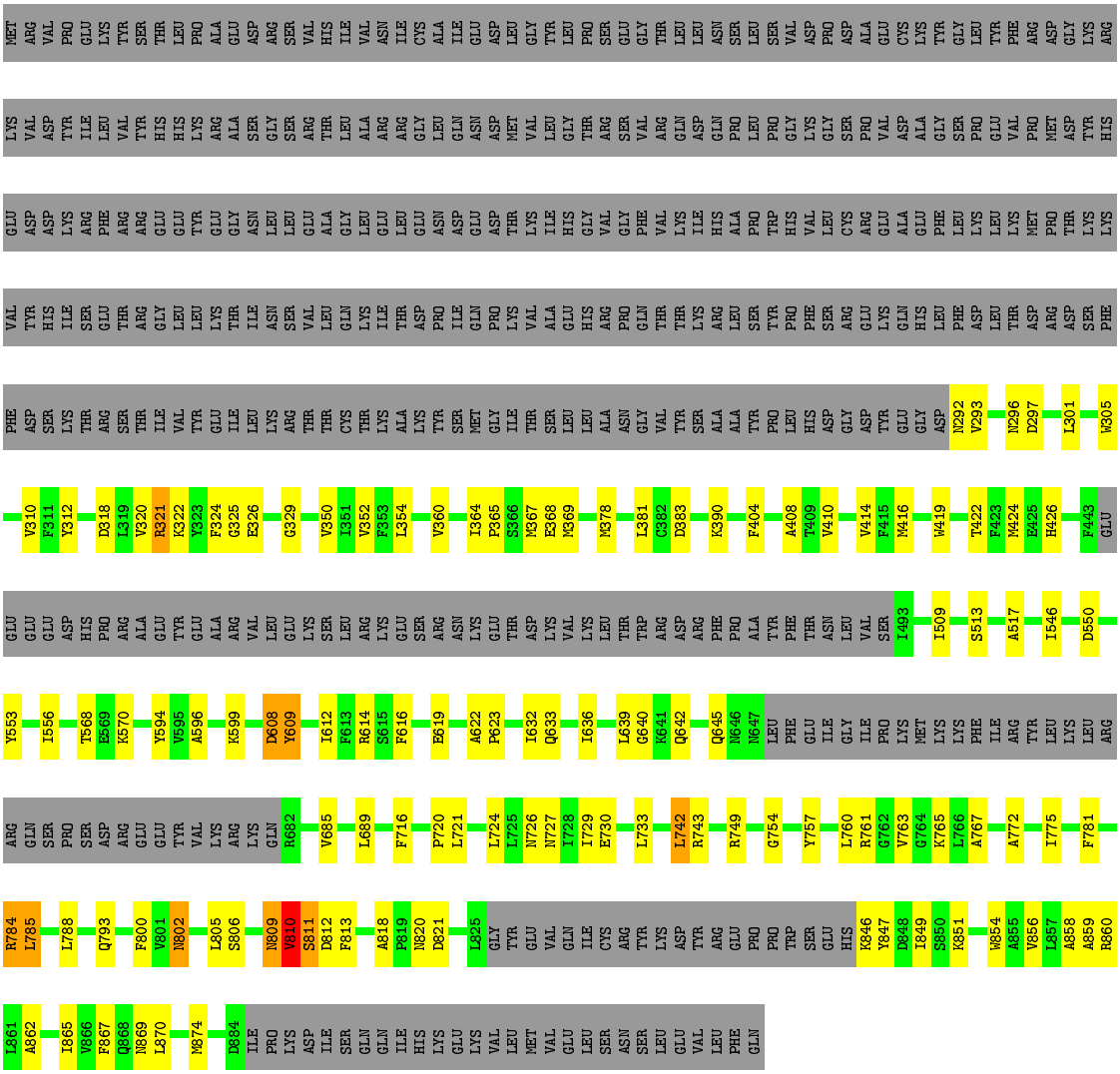
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Anoctamin-1

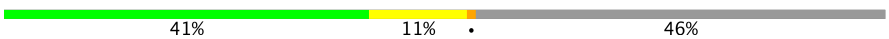
Chain A:

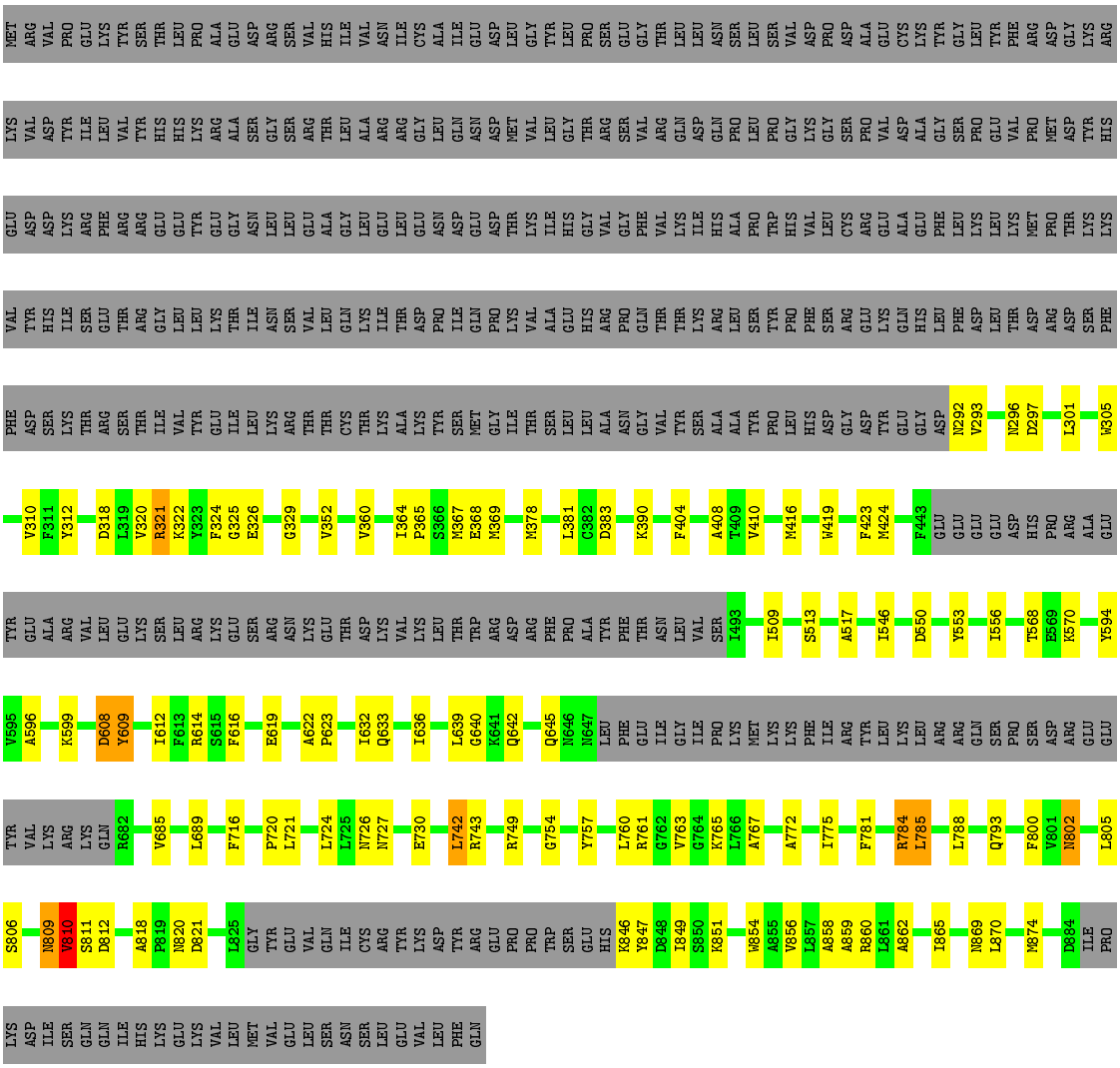




- Molecule 1: Anoctamin-1

Chain B:




MET ARG VAL PRO GLU LYS TYR SER THR LEU PRO ALA GLU ASP ARG SER VAL HIS ILE VAL ASN ILE CYS ALA ILE GLU ASP LEU GLY TYR LEU PRO SER GLU GLY THR LEU LEU ASN SER LEU SER VAL ASP PRO ASP ALA GLU CYS LYS TYR GLY LEU TYR PHE ARG ASP GLY LYS ARG
LYS VAL ASP TYR ILE LEU VAL TYR HIS HIS LYS ARG ALA SER GLY SER ARG THR LEU ALA ARG ARG GLY GLU GLN ASN ASP MET VAL LEU GLY THR ARG SER VAL ARG GLN ASP GLN PRO LEU PRO GLY LYS GLY SER PRO VAL ASP ALA GLY SER PRO GLU VAL PRO MET ASP TYR HIS
GLU ASP ASP LYS ARG PHE ARG ARG GLU GLU TYR GLU GLY ASN LEU LEU GLU ALA GLY LEU GLU LEU GLU GLU ASN ASP ASP GLU ASP THR LYS ILE HIS GLY VAL GLY PHE VAL LYS ILE HIS ALA PRO TRP HIS VAL LEU CYS ARG GLU ALA GLU PHE LEU LYS LEU LYS MET PRO THR LYS LYS
VAL TYR HIS ILE SER GLU THR ARG GLY LEU LEU LYS THR ILE LEU ILE ASN SER VAL LEU GLN LYS ILE THR ASP PRO ILE GLN PRO LYS VAL ALA GLU HIS ARG PRO GLN GLY THR THR LYS ARG LEU SER TYR PRO PHE SER ARG GLU LYS GLN HIS LEU PHE ASP LEU THR ASP ARG ASP SER PHE
PHE ASP SER LYS THR ARG SER THR ILE VAL TYR GLU ILE LEU LYS ARG THR THR CYS THR LYS ALA LYS TYR SER MET GLY ILE THR SER LEU LEU ALA ASN GLY VAL TYR SER ALA ALA TYR PRO LEU HIS ASP GLY ASP TYR GLU GLY ASP N292 V293 N296 D297 L301 W305
V310 F311 Y312 D318 L319 V320 R321 K322 Y323 F324 G325 E326 G329 V352 V360 I364 P365 S366 M367 E368 M369 M378 L381 C382 D383 K390 G390 F404 A408 T409 V410 M416 W419 F423 M424 F443 GLU GLU GLU GLU ASP HIS PRO ARG ALA GLU
TYR GLU ALA ARG VAL LEU GLU LYS SER LEU ARG LYS GLU SER ARG ASN LYS GLU THR ASP LYS VAL LYS LEU THR TRP ARG ASP ARG PHE PRO ALA TYR PHE THR ASN LEU VAL SER T493 I509 S513 A517 I546 D550 Y553 I556 T568 E569 K570 V594
V595 A596 K599 D608 Y609 I612 F613 R614 S615 F616 E619 A622 P623 I632 Q633 I636 L639 G640 K641 Q642 Q645 N646 N647 LEU PHE GLU ILE GLY ILE PRO LYS MET LYS LYS PHE ILE ARG TYR LEU LYS LEU ARG ARG GLN SER PRO SER ASP ARG GLU GLU
TYR VAL LYS ARG LYS GLN R682 V685 L689 F716 P720 L721 L724 L725 N726 N727 E730 L742 R743 R749 G754 Y757 L760 R761 G762 V763 G764 K765 L766 A767 A772 I775 F781 R784 L785 L788 Q793 F800 V801 N802 L805
S806 N809 V810 S811 D812 A818 P819 N820 D821 L825 GLY TYR GLU VAL GLN ILE CYS ARG TYR LYS ASP TYR ARG GLU PRO PRO TRP SER GLU HIS K846 Y847 D848 I849 S850 K851 W854 A855 V856 I857 A858 A859 R860 L861 A862 I865 N869 L870 M874 D884 ILE PRO
LYS ASP ILE SER GLN GLN ILE HIS LYS GLU LYS VAL LEU MET VAL GLU LEU SER ASN SER LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	251851	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.40	0/3801	0.63	1/5180 (0.0%)
1	B	0.40	0/3801	0.63	1/5180 (0.0%)
All	All	0.40	0/7602	0.63	2/10360 (0.0%)

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	11
1	B	0	11
All	All	0	22

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	810	VAL	CG1-CB-CG2	-6.26	100.88	110.90
1	A	810	VAL	CG1-CB-CG2	-6.25	100.91	110.90

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	TRP	Peptide
1	A	404	PHE	Peptide
1	A	608	ASP	Peptide
1	A	622	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	742	LEU	Peptide

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	3708	0	3540	80	0
1	B	3708	0	3540	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	7418	0	7080	154	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 11.

The worst 5 of 154 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:B:383:ASP:OD2	1:B:614:ARG:NH2	2.14	0.80
1:A:383:ASP:OD2	1:A:614:ARG:NH2	2.14	0.80
1:B:424:MET:HE3	1:B:761:ARG:HA	1.64	0.79
1:B:321:ARG:NH2	1:B:326:GLU:OE2	2.19	0.76
1:A:321:ARG:NH2	1:A:326:GLU:OE2	2.19	0.75

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	482/912 (53%)	413 (86%)	66 (14%)	3 (1%)	28	70
1	B	482/912 (53%)	413 (86%)	66 (14%)	3 (1%)	28	70
All	All	964/1824 (53%)	826 (86%)	132 (14%)	6 (1%)	33	70

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	812	ASP
1	B	812	ASP
1	A	609	TYR
1	B	609	TYR
1	A	810	VAL

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	363/812 (45%)	361 (99%)	2 (1%)	89	95
1	B	363/812 (45%)	361 (99%)	2 (1%)	89	95
All	All	726/1624 (45%)	722 (99%)	4 (1%)	89	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	ARG
1	A	784	ARG
1	B	321	ARG
1	B	784	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	809	ASN
1	B	809	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	296	ASN
1	A	794	ASN
1	B	794	ASN

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 2 ligands modelled in this entry, 2 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.