



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Oct 16, 2017 – 11:26 PM EDT

PDB ID : 5WPT
EMDB ID: : EMD-8882
Title : Cryo-EM structure of mammalian endolysosomal TRPML1 channel in nanodiscs in closed II conformation at 3.75 Angstrom resolution
Authors : Chen, Q.; She, J.; Guo, J.; Bai, X.; Jiang, Y.
Deposited on : unknown
Resolution : 3.75 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 ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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-20030345

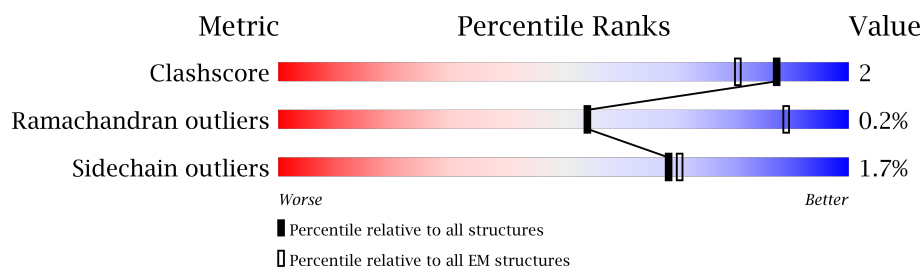
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.75 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	592	70% 6% 23%
1	B	592	70% 6% • 23%
1	C	592	70% 6% • 23%
1	D	592	70% 6% • 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14889 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 Mucolipin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	454	Total	C	N	O	S	0	0
			3694	2427	609	634	24		
1	B	454	Total	C	N	O	S	0	0
			3694	2427	609	634	24		
1	C	454	Total	C	N	O	S	0	0
			3694	2427	609	634	24		
1	D	454	Total	C	N	O	S	0	0
			3694	2427	609	634	24		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	581	VAL	-	expression tag	UNP Q99J21
A	582	ASP	-	expression tag	UNP Q99J21
A	583	GLY	-	expression tag	UNP Q99J21
A	584	GLY	-	expression tag	UNP Q99J21
A	585	SER	-	expression tag	UNP Q99J21
A	586	SER	-	expression tag	UNP Q99J21
A	587	GLY	-	expression tag	UNP Q99J21
A	588	GLY	-	expression tag	UNP Q99J21
A	589	LEU	-	expression tag	UNP Q99J21
A	590	VAL	-	expression tag	UNP Q99J21
A	591	PRO	-	expression tag	UNP Q99J21
A	592	ARG	-	expression tag	UNP Q99J21
B	581	VAL	-	expression tag	UNP Q99J21
B	582	ASP	-	expression tag	UNP Q99J21
B	583	GLY	-	expression tag	UNP Q99J21
B	584	GLY	-	expression tag	UNP Q99J21
B	585	SER	-	expression tag	UNP Q99J21
B	586	SER	-	expression tag	UNP Q99J21
B	587	GLY	-	expression tag	UNP Q99J21
B	588	GLY	-	expression tag	UNP Q99J21
B	589	LEU	-	expression tag	UNP Q99J21
B	590	VAL	-	expression tag	UNP Q99J21

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Chain	Residue	Modelled	Actual	Comment	Reference
B	591	PRO	-	expression tag	UNP Q99J21
B	592	ARG	-	expression tag	UNP Q99J21
C	581	VAL	-	expression tag	UNP Q99J21
C	582	ASP	-	expression tag	UNP Q99J21
C	583	GLY	-	expression tag	UNP Q99J21
C	584	GLY	-	expression tag	UNP Q99J21
C	585	SER	-	expression tag	UNP Q99J21
C	586	SER	-	expression tag	UNP Q99J21
C	587	GLY	-	expression tag	UNP Q99J21
C	588	GLY	-	expression tag	UNP Q99J21
C	589	LEU	-	expression tag	UNP Q99J21
C	590	VAL	-	expression tag	UNP Q99J21
C	591	PRO	-	expression tag	UNP Q99J21
C	592	ARG	-	expression tag	UNP Q99J21
D	581	VAL	-	expression tag	UNP Q99J21
D	582	ASP	-	expression tag	UNP Q99J21
D	583	GLY	-	expression tag	UNP Q99J21
D	584	GLY	-	expression tag	UNP Q99J21
D	585	SER	-	expression tag	UNP Q99J21
D	586	SER	-	expression tag	UNP Q99J21
D	587	GLY	-	expression tag	UNP Q99J21
D	588	GLY	-	expression tag	UNP Q99J21
D	589	LEU	-	expression tag	UNP Q99J21
D	590	VAL	-	expression tag	UNP Q99J21
D	591	PRO	-	expression tag	UNP Q99J21
D	592	ARG	-	expression tag	UNP Q99J21

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

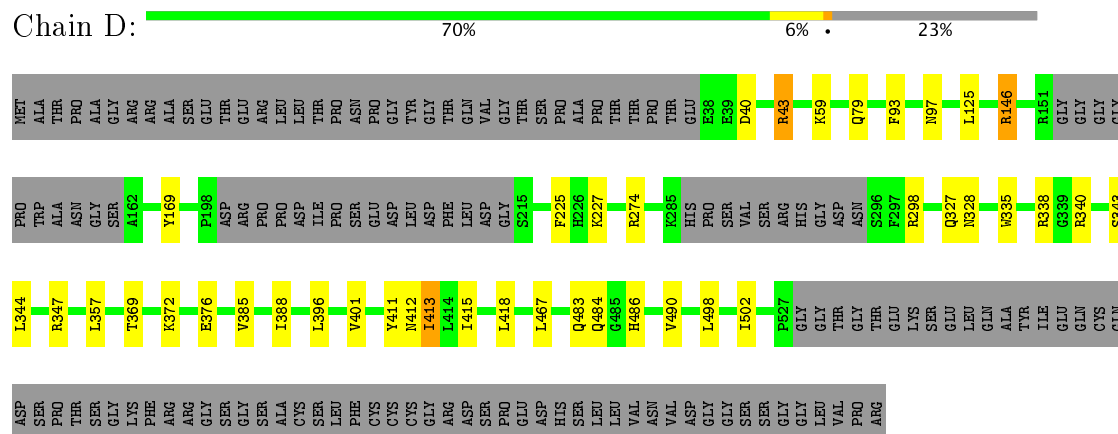


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			28	16	2	10	
2	A	1	Total	C	N	O	0
			28	16	2	10	
2	B	1	Total	C	N	O	0
			28	16	2	10	
2	B	1	Total	C	N	O	0
			28	16	2	10	
2	C	1	Total	C	N	O	0
			28	16	2	10	
2	C	1	Total	C	N	O	0
			28	16	2	10	
2	D	1	Total	C	N	O	0
			28	16	2	10	
2	D	1	Total	C	N	O	0
			28	16	2	10	

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Na	0
			1	1	

- Molecule 1: Mucolipin-1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	2D CRYSTAL, a =Not provided Å, b =Not provided Å, c =Not provided Å, γ =Not provided°, space group=Not provided	Depositor
Number of particles used	11000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The CTF correction was performed during the map refinement in RELION.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	46730	Depositor
Image detector	GATAN K2 SUMMIT (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: NA, NAG

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	0.45	0/3781	0.60	1/5125 (0.0%)
1	B	0.44	0/3781	0.60	1/5125 (0.0%)
1	C	0.44	0/3781	0.59	1/5125 (0.0%)
1	D	0.45	0/3781	0.59	1/5125 (0.0%)
All	All	0.45	0/15124	0.60	4/20500 (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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	418	LEU	CA-CB-CG	5.13	127.11	115.30
1	B	418	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	418	LEU	CA-CB-CG	5.11	127.05	115.30
1	C	418	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	411	TYR	Peptide
1	A	412	ASN	Peptide
1	B	411	TYR	Peptide
1	B	412	ASN	Peptide
1	C	411	TYR	Peptide

5.2 Too-close contacts

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	3694	0	3765	17	0
1	B	3694	0	3765	17	0
1	C	3694	0	3765	19	0
1	D	3694	0	3765	19	0
2	A	28	0	25	0	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	1	0	0	0	0
All	All	14889	0	15160	69	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 2.

The worst 5 of 69 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:D:335:TRP:O	1:D:338:ARG:HG3	1.57	1.04
1:A:335:TRP:O	1:A:338:ARG:HG3	1.57	1.04
1:C:335:TRP:O	1:C:338:ARG:HG3	1.57	1.04
1:B:335:TRP:O	1:B:338:ARG:HG3	1.57	1.02
1:D:335:TRP:O	1:D:338:ARG:CG	2.28	0.81

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	446/592 (75%)	409 (92%)	36 (8%)	1 (0%)	51	85
1	B	446/592 (75%)	409 (92%)	36 (8%)	1 (0%)	51	85
1	C	446/592 (75%)	409 (92%)	36 (8%)	1 (0%)	51	85
1	D	446/592 (75%)	409 (92%)	36 (8%)	1 (0%)	51	85
All	All	1784/2368 (75%)	1636 (92%)	144 (8%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	ILE
1	B	413	ILE
1	C	413	ILE
1	D	413	ILE

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	411/520 (79%)	404 (98%)	7 (2%)	66	86
1	B	411/520 (79%)	404 (98%)	7 (2%)	66	86
1	C	411/520 (79%)	404 (98%)	7 (2%)	66	86
1	D	411/520 (79%)	404 (98%)	7 (2%)	66	86
All	All	1644/2080 (79%)	1616 (98%)	28 (2%)	68	86

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	340	ARG
1	C	59	LYS
1	D	328	ASN
1	B	401	VAL
1	C	43	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	486	HIS
1	C	243	GLN
1	D	243	GLN
1	B	484	GLN
1	D	328	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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	601	1,2	14,14,15	0.16	0	15,19,21	0.78	1 (6%)
2	NAG	A	602	2	14,14,15	0.23	0	15,19,21	0.75	1 (6%)
2	NAG	B	601	1,2	14,14,15	0.16	0	15,19,21	0.77	1 (6%)
2	NAG	B	602	2	14,14,15	0.22	0	15,19,21	0.74	1 (6%)
2	NAG	C	601	1,2	14,14,15	0.17	0	15,19,21	0.80	1 (6%)
2	NAG	C	602	2	14,14,15	0.21	0	15,19,21	0.73	1 (6%)
2	NAG	D	601	1,2	14,14,15	0.17	0	15,19,21	0.78	1 (6%)
2	NAG	D	602	2	14,14,15	0.21	0	15,19,21	0.73	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	602	2	-	0/6/23/26	0/1/1/1
2	NAG	C	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	602	2	-	0/6/23/26	0/1/1/1
2	NAG	D	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	602	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	602	NAG	C1-O5-C5	2.07	115.02	112.17
2	D	602	NAG	C1-O5-C5	2.08	115.03	112.17
2	B	602	NAG	C1-O5-C5	2.12	115.08	112.17
2	A	602	NAG	C1-O5-C5	2.18	115.17	112.17
2	B	601	NAG	C1-O5-C5	2.61	115.76	112.17

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.