



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 14, 2017 – 02:08 AM EST

PDB ID : 5YE5
EMDB ID: : EMD-6826
Title : structure of endo-lysosomal TRPML1 channel inserting into nanodisc
Authors : Yang, M.; Gao, N.
Deposited on : unknown
Resolution : 5.80 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 ⓘ 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

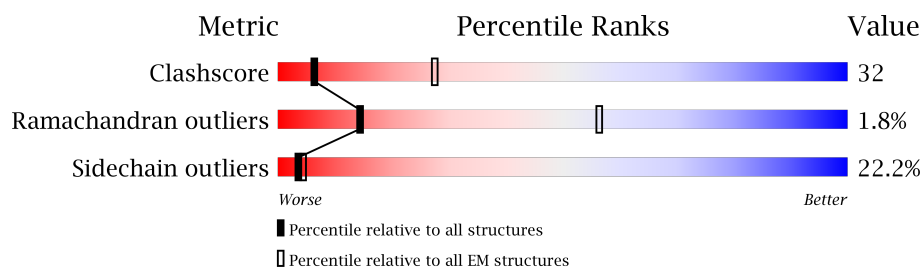
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.80 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	580	63% 16% • 20%
1	B	580	63% 16% • 20%
1	C	580	63% 16% • 20%
1	D	580	63% 16% • 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	602	-	-	X	-
2	NAG	B	602	-	-	X	-
2	NAG	C	602	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	602	-	-	X	-

2 Entry composition [i](#)

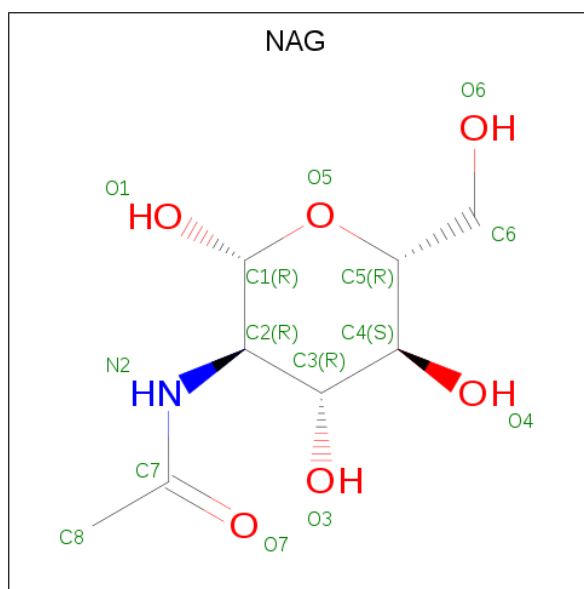
There are 2 unique types of molecules in this entry. The entry contains 7852 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 mammalian endo-lysosomal TRPML1 channel.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	464	Total	C	N	O	0	0
			1935	994	468	473		
1	B	464	Total	C	N	O	0	0
			1935	994	468	473		
1	C	464	Total	C	N	O	0	0
			1935	994	468	473		
1	D	464	Total	C	N	O	0	0
			1935	994	468	473		

- 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	

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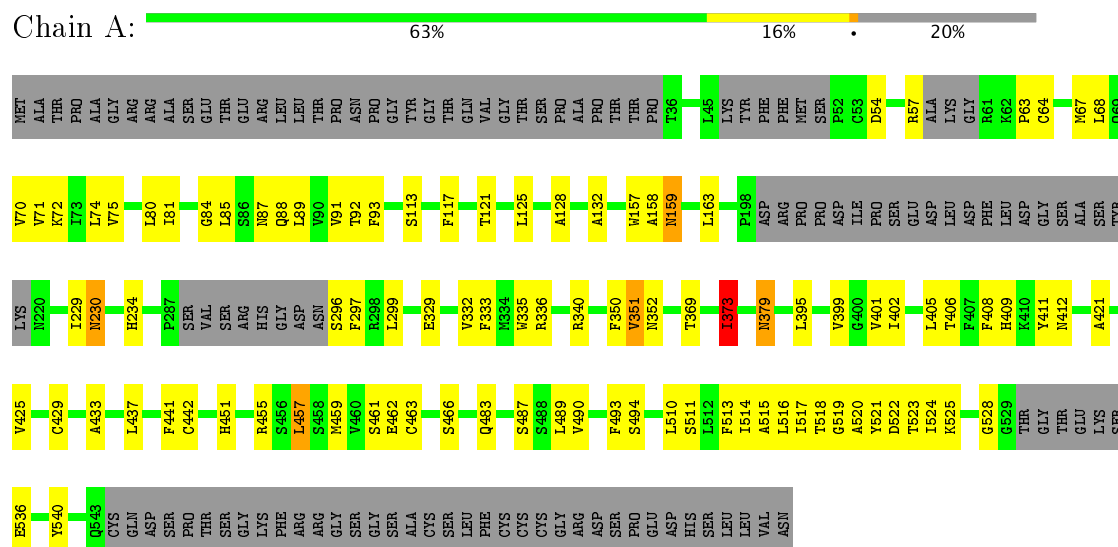
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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			28	16	2	10	
2	C	1	Total	C	N	O	0
			28	16	2	10	
2	C	1	Total	C	N	O	0
			28	16	2	10	
2	D	1	Total	C	N	O	0
			28	16	2	10	
2	D	1	Total	C	N	O	0
			28	16	2	10	

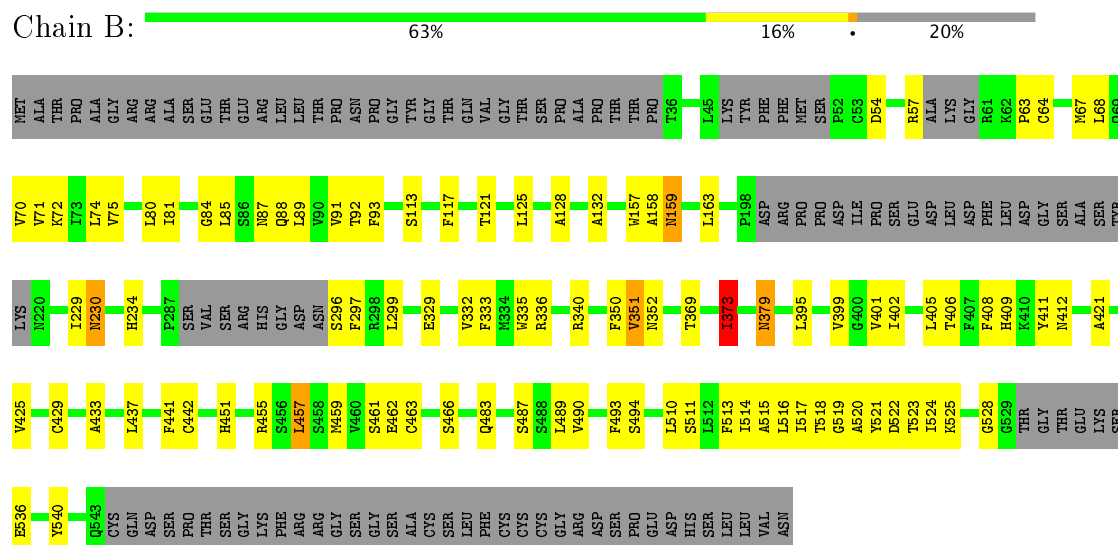
3 Residue-property plots

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: mammalian endo-lysosomal TRPML1 channel



- Molecule 1: mammalian endo-lysosomal TRPML1 channel



- Molecule 1: mammalian endo-lysosomal TRPML1 channel

Chain D: 

E536	V425	LYS	V70	MET
Y540	Q429	N220	K72	ALA
Q543	A433	I229	I73	PRO
CYS	L437	N230	I74	ALA
ASP	L437	H234	V75	GLY
SER	F441	S287	L80	ARG
THR	Q442	VAL	I81	ALA
SER	H451	SER	G84	GLU
GLY	R455	ARG	S86	THR
LYS	S456	HIS	N87	GLU
PHE	L457	GLY	Q88	LEU
ARG	S458	ASP	L89	LEU
ARG	H459	ASN	V90	THR
GLY	V460	S296	V91	PRO
SER	S461	F297	T92	ASN
GLY	E462	R298	F93	PRO
ALA	Q463	L299	S113	GLY
CYS	S466	E329	F117	TYR
SER	Q483	V332	T121	GLY
PHE	CYS	M334	L126	GLN
CYS	S487	W335	A128	GLY
CYS	S488	R336	A132	THR
GLY	L489	R340	W157	SER
ASP	V490	V351	A158	PRO
ASP	F493	N352	N159	ALA
PRO	S494	T369	L163	PRO
GLU	L510	I373	P198	THR
ASP	S511	N379	ASP	THR
HIS	L512	L395	ANG	PRO
SER	F513	V399	PRO	SER
LEU	T514	G400	ILE	P52
LEU	A515	V401	PRO	C53
VAL	L516	I402	SER	D54
ASN	T517	L405	GLU	R57
	T518	T406	ASP	ALA
	A519	F407	LEU	LYS
	A520	H408	ASP	GLY
	A521	H409	LEU	R61
	B522	R410	ASP	K62
	T523	N412	GLY	P63
	B524		SER	C64
	B525		ALA	M67
	G528		LYS	L68
	G529		GLY	G69
	THR		THR	
	GLY		THR	
	THR		GLU	
	LYS		SER	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	167000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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:
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	0.37	0/1930	0.79	1/2437 (0.0%)
1	B	0.37	0/1930	0.79	1/2437 (0.0%)
1	C	0.37	0/1930	0.79	1/2437 (0.0%)
1	D	0.37	0/1930	0.79	1/2437 (0.0%)
All	All	0.37	0/7720	0.79	4/9748 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	373	ILE	N-CA-C	6.86	129.52	111.00
1	A	373	ILE	N-CA-C	6.86	129.51	111.00
1	C	373	ILE	N-CA-C	6.85	129.50	111.00
1	D	373	ILE	N-CA-C	6.85	129.50	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	379	ASN	Peptide
1	A	457	LEU	Peptide
1	A	483	GLN	Peptide
1	B	379	ASN	Peptide
1	B	457	LEU	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	1935	0	598	82	0
1	B	1935	0	598	84	0
1	C	1935	0	598	80	0
1	D	1935	0	598	82	0
2	A	28	0	26	11	0
2	B	28	0	26	11	0
2	C	28	0	26	11	0
2	D	28	0	26	11	0
All	All	7852	0	2496	328	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 32.

The worst 5 of 328 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:159:ASN:CB	2:B:602:NAG:O7	1.73	1.35
1:D:159:ASN:CB	2:D:602:NAG:O7	1.73	1.35
1:A:159:ASN:CB	2:A:602:NAG:O7	1.73	1.33
1:C:159:ASN:CB	2:C:602:NAG:O7	1.73	1.33
1:D:70:VAL:O	1:D:74:LEU:N	1.65	1.28

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	452/580 (78%)	430 (95%)	14 (3%)	8 (2%)	10	49
1	B	452/580 (78%)	430 (95%)	14 (3%)	8 (2%)	10	49
1	C	452/580 (78%)	430 (95%)	14 (3%)	8 (2%)	10	49
1	D	452/580 (78%)	430 (95%)	14 (3%)	8 (2%)	10	49
All	All	1808/2320 (78%)	1720 (95%)	56 (3%)	32 (2%)	14	49

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	PHE
1	A	379	ASN
1	B	297	PHE
1	B	379	ASN
1	C	297	PHE

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	9/512 (2%)	7 (78%)	2 (22%)	1	7
1	B	9/512 (2%)	7 (78%)	2 (22%)	1	7
1	C	9/512 (2%)	7 (78%)	2 (22%)	1	7
1	D	9/512 (2%)	7 (78%)	2 (22%)	1	7
All	All	36/2048 (2%)	28 (78%)	8 (22%)	3	7

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	230	ASN
1	D	230	ASN
1	C	230	ASN
1	B	159	ASN
1	C	159	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

8 ligands are modelled in this entry.

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	14,14,15	0.41	0	15,19,21	1.17	1 (6%)
2	NAG	A	602	1	14,14,15	0.40	0	15,19,21	1.17	2 (13%)
2	NAG	B	601	1	14,14,15	0.41	0	15,19,21	1.16	1 (6%)
2	NAG	B	602	1	14,14,15	0.40	0	15,19,21	1.17	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	601	1	14,14,15	0.41	0	15,19,21	1.16	1 (6%)
2	NAG	C	602	1	14,14,15	0.40	0	15,19,21	1.16	2 (13%)
2	NAG	D	601	1	14,14,15	0.41	0	15,19,21	1.16	2 (13%)
2	NAG	D	602	1	14,14,15	0.41	0	15,19,21	1.17	2 (13%)

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	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1	-	0/6/23/26	0/1/1/1
2	NAG	C	601	1	-	0/6/23/26	0/1/1/1
2	NAG	C	602	1	-	0/6/23/26	0/1/1/1
2	NAG	D	601	1	-	0/6/23/26	0/1/1/1
2	NAG	D	602	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	NAG	C2-N2-C7	-2.05	119.96	122.94
2	B	602	NAG	C2-N2-C7	-2.04	119.97	122.94
2	D	601	NAG	C2-N2-C7	-2.03	119.97	122.94
2	C	602	NAG	C2-N2-C7	-2.03	119.98	122.94
2	A	602	NAG	C2-N2-C7	-2.02	119.99	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	NAG	11	0
2	B	602	NAG	11	0
2	C	602	NAG	11	0
2	D	602	NAG	11	0

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.