wwPDB EM Validation Summary Report

Oct 28, 2024 – 12:07 PM JST

PDB ID	:	8H8D
EMDB ID	:	EMD-34543
Title	:	Structure of Xenopus tropicalis acid-sensitive outwardly rectifying channel ASOR trimer bound with tRNA (intermediate state)
Authors	:	Chi, P.; Wang, X.; Li, J.; Li, K.; Zhang, Y.; Geng, J.; Wu, J.; Deng, D.
Deposited on	:	2022-10-22
Resolution	:	4.26 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

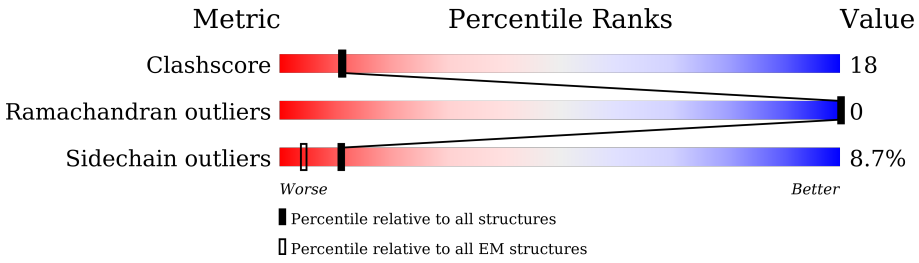
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.26 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	352	50% 29% • 18%
1	B	352	43% 31% 5% • 20%
1	C	352	50% 29% • 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7054 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 Proton-activated chloride channel.

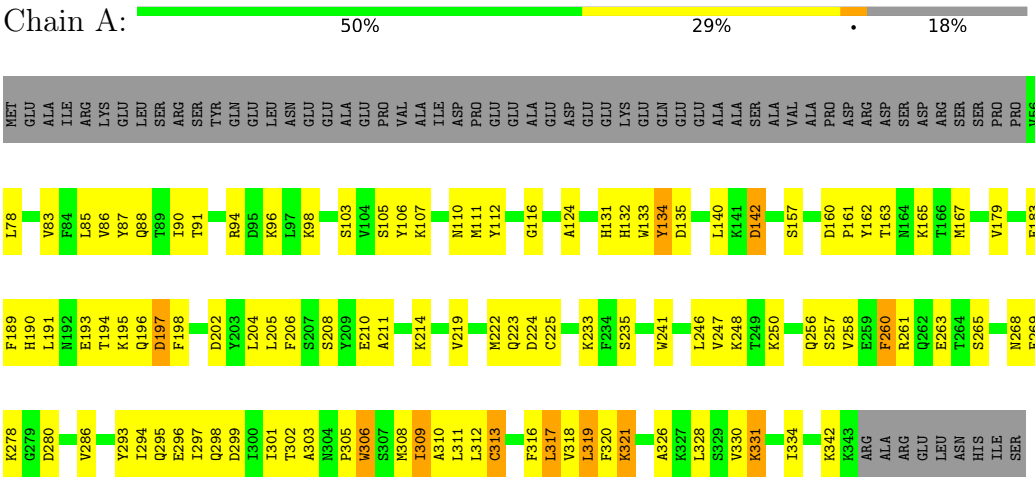
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	288	Total	C	N	O	S	0	0
			2366	1536	398	419	13		
1	B	283	Total	C	N	O	S	0	0
			2337	1521	389	414	13		
1	C	285	Total	C	N	O	S	0	0
			2351	1530	392	416	13		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

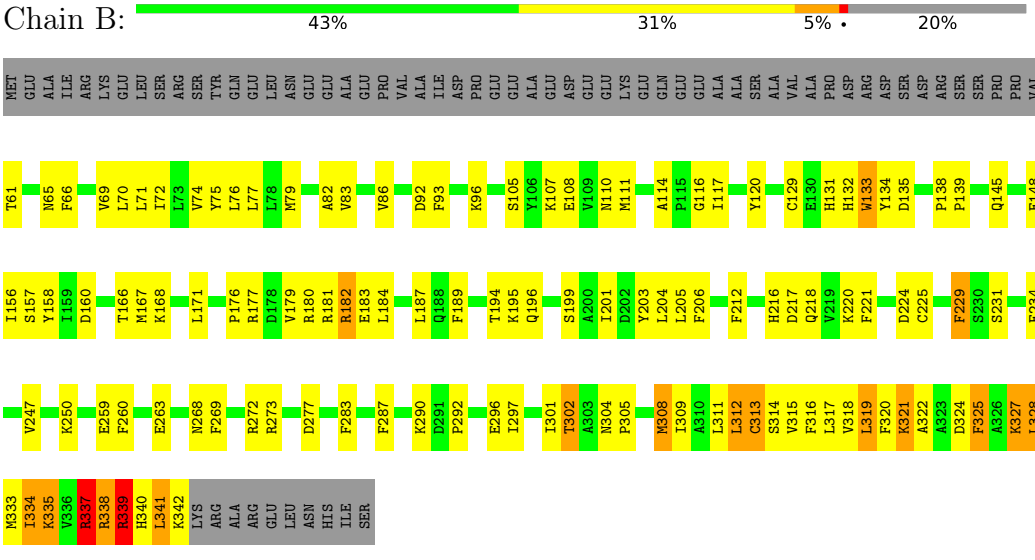
- Molecule 1: Proton-activated chloride channel

Chain A:



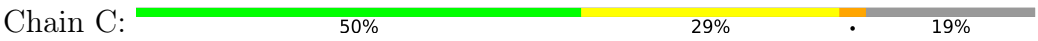
- Molecule 1: Proton-activated chloride channel

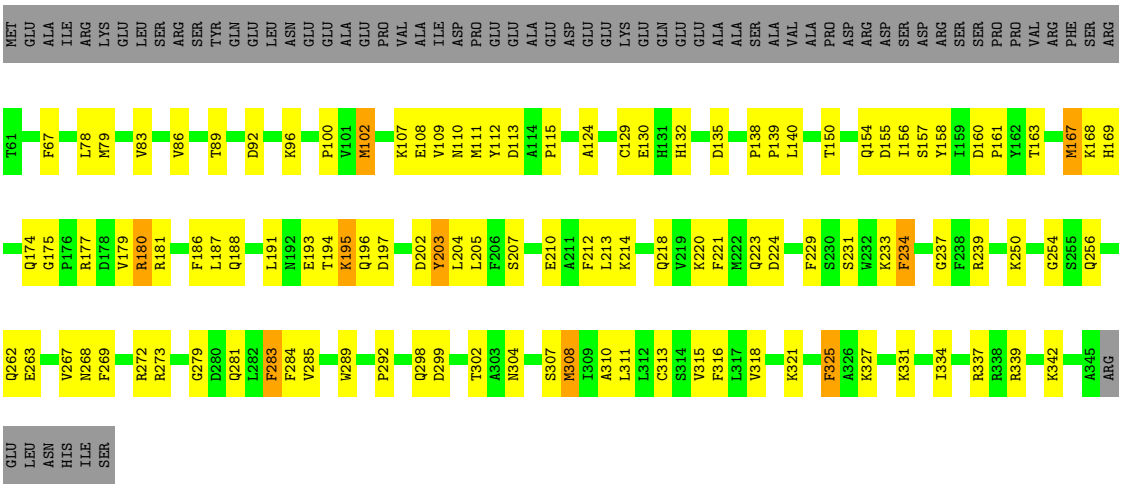
Chain B:



- Molecule 1: Proton-activated chloride channel

Chain C:




MET GLU ALA ILE ARG LYS GLU LEU SER ARG SER TYR GLN GLU LEU ASN GLU GLU ALA GLU PRO VAL ALA ILE ASP PRO GLU GLU ALA GLU ASP GLU GLU LYS GLU GLN GLU GLU ALA ALA SER ALA VAL ALA PRO ASP ARG ASP SER ASP ARG SER SER PRO PRO VAL ARG PHE SER ARG
T61 F67 L78 M79 V83 V86 T89 D92 K96 P100 V101 M102 K107 E108 V109 N110 M111 Y112 D113 A114 P115 A124 C129 E130 H131 H132 D135 P138 P139 L140 T150 Q154 D155 I156 S157 Y158 I159 D160 P161 Y162 T163 M167 K168 H169
Q174 G175 P176 R177 D178 V179 R180 R181 F186 L187 Q188 L191 N192 E193 T194 K195 Q196 D197 D202 Y203 L204 L205 F206 S207 E210 A211 F212 L213 K214 Q218 V219 K220 F221 M222 Q223 D224 F229 S230 S231 W232 K233 F234 G237 F238 R239 K250 G254 S255 Q256
Q262 E263 V267 N268 F269 R272 R273 G279 D280 Q281 L282 F283 F284 V285 W289 P292 Q298 D299 T302 A303 N304 S307 M308 I309 A310 L311 L312 C313 S314 V315 F316 L317 V318 K321 F325 A326 K327 K331 I334 R337 R338 R339 K342 A345 ARG
GLU LEU ASN HIS ILE SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53188	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.30	0/2429	0.56	0/3283
1	B	0.35	0/2400	0.57	0/3246
1	C	0.27	0/2414	0.55	1/3264 (0.0%)
All	All	0.31	0/7243	0.56	1/9793 (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	B	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	78	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	337	ARG	Sidechain
1	B	339	ARG	Sidechain

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	2366	0	2348	80	0
1	B	2337	0	2331	108	0
1	C	2351	0	2349	77	0
All	All	7054	0	7028	252	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 18.

The worst 5 of 252 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:334:ILE:HG23	1:B:338:ARG:HE	1.37	0.88
1:A:316:PHE:HA	1:A:319:LEU:HD23	1.56	0.88
1:B:339:ARG:HA	1:B:342:LYS:HD2	1.60	0.84
1:A:197:ASP:OD2	1:A:198:PHE:N	2.15	0.79
1:A:222:MET:SD	1:A:223:GLN:NE2	2.57	0.78

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	286/352 (81%)	275 (96%)	11 (4%)	0	100	100
1	B	281/352 (80%)	269 (96%)	12 (4%)	0	100	100
1	C	283/352 (80%)	267 (94%)	16 (6%)	0	100	100
All	All	850/1056 (80%)	811 (95%)	39 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	262/321 (82%)	242 (92%)	20 (8%)	11 31
1	B	261/321 (81%)	229 (88%)	32 (12%)	4 17
1	C	262/321 (82%)	246 (94%)	16 (6%)	15 38
All	All	785/963 (82%)	717 (91%)	68 (9%)	11 26

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	203	TYR
1	C	212	PHE
1	C	313	CYS
1	B	199	SER
1	B	182	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	340	HIS

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 oligosaccharides 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.