



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 16, 2019 – 01:43 PM EDT

PDB ID : 5A6F
EMDB ID: : EMD-3063
Title : Cryo-EM structure of the Slo2.2 Na-activated K channel
Authors : Hite, R.K.; Yuan, P.; Li, Z.; Hsuing, Y.; Walz, T.; MacKinnon, R.
Deposited on : 2015-06-25
Resolution : 4.20 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

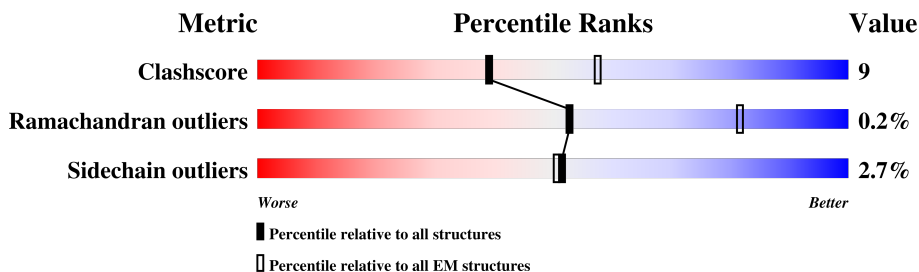
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	C	700	
2	D	43	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9095 atoms, of which 4544 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 GATING RING OF POTASSIUM CHANNEL SUBFAMILY T MEMBER 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	540	Total	C	H	N	O	S	0	0
			8666	2778	4330	729	794	35		

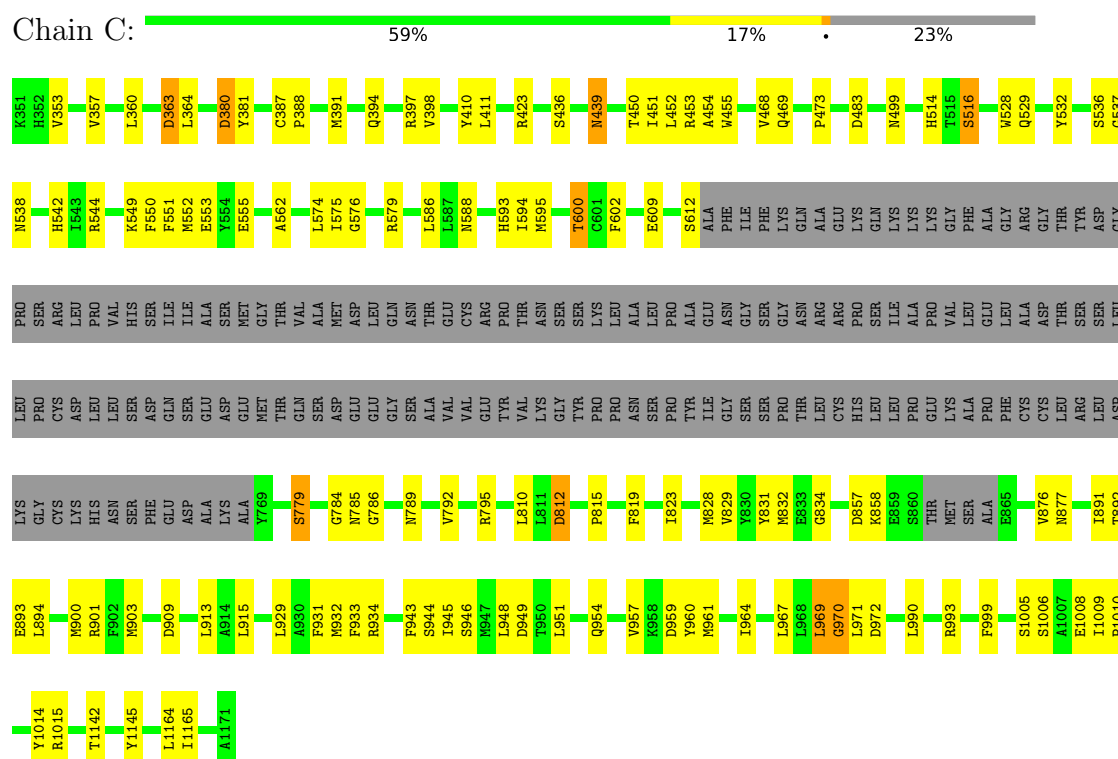
- Molecule 2 is a protein called RCK2 ELABORATION OF POTASSIUM CHANNEL SUBFAMILY T MEMBER 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	43	Total	C	H	N	O	0	0
			429	129	214	43	43		

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: GATING RING OF POTASSIUM CHANNEL SUBFAMILY T MEMBER 1



- Molecule 2: RCK2 ELABORATION OF POTASSIUM CHANNEL SUBFAMILY T MEMBER 1



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	24231	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 (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	C	0.56	0/4428	0.66	1/5988 (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	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	970	GLY	N-CA-C	-5.46	99.44	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	969	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	C	4336	4330	4331	76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	215	214	48	0	0
All	All	4551	4544	4379	76	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 9.

All (76) 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:C:549:LYS:NZ	1:C:612:SER:O	2.11	0.83
1:C:894:LEU:HD12	1:C:900:MET:HE2	1.75	0.67
1:C:550:PHE:N	1:C:609:GLU:OE2	2.22	0.58
1:C:528:TRP:CE3	1:C:1145:TYR:HE1	2.23	0.57
1:C:439:ASN:OD1	1:C:439:ASN:N	2.37	0.56
1:C:542:HIS:HB2	1:C:960:TYR:CZ	2.41	0.56
1:C:931:PHE:HA	1:C:934:ARG:NE	2.20	0.55
1:C:451:ILE:O	1:C:455:TRP:CD1	2.62	0.53
1:C:514:HIS:CG	1:C:929:LEU:HD21	2.44	0.53
1:C:353:VAL:HG23	1:C:381:TYR:CD1	2.43	0.53
1:C:528:TRP:HB2	1:C:1145:TYR:CE1	2.45	0.52
1:C:1006:SER:OG	1:C:1008:GLU:OE1	2.28	0.51
1:C:588:ASN:ND2	1:C:1165:ILE:O	2.46	0.49
1:C:357:VAL:HG11	1:C:360:LEU:HG	1.95	0.48
1:C:1009:ILE:O	1:C:1164:LEU:HA	2.14	0.48
1:C:831:TYR:O	1:C:832:MET:SD	2.71	0.48
1:C:909:ASP:O	1:C:913:LEU:HG	2.15	0.46
1:C:1015:ARG:HB2	1:C:1145:TYR:CD2	2.50	0.46
1:C:550:PHE:CG	1:C:550:PHE:O	2.69	0.46
1:C:612:SER:OG	1:C:612:SER:O	2.26	0.46
1:C:380:ASP:O	1:C:381:TYR:CD2	2.69	0.45
1:C:993:ARG:HD2	1:C:993:ARG:N	2.31	0.45
1:C:815:PRO:HG2	1:C:831:TYR:CD1	2.52	0.45
1:C:810:LEU:HA	1:C:832:MET:O	2.16	0.45
1:C:473:PRO:HG2	1:C:785:ASN:HB3	1.97	0.45
1:C:828:MET:O	1:C:829:VAL:HG13	2.16	0.45
1:C:819:PHE:O	1:C:823:ILE:HG22	2.16	0.45
1:C:943:PHE:CZ	1:C:944:SER:O	2.70	0.45
1:C:542:HIS:HB2	1:C:960:TYR:CE1	2.52	0.45
1:C:784:GLY:C	1:C:786:GLY:N	2.70	0.45
1:C:594:ILE:HG22	1:C:595:MET:N	2.33	0.44
1:C:516:SER:HB2	1:C:537:GLY:HA2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:GLY:HA3	1:C:586:LEU:O	2.17	0.44
1:C:779:SER:HA	1:C:810:LEU:O	2.17	0.44
1:C:552:MET:O	1:C:553:GLU:C	2.56	0.44
1:C:943:PHE:CG	1:C:944:SER:N	2.86	0.44
1:C:967:LEU:HD23	1:C:972:ASP:O	2.17	0.44
1:C:468:VAL:HG22	1:C:469:GLN:N	2.32	0.44
1:C:452:LEU:O	1:C:453:ARG:C	2.56	0.44
1:C:961:MET:O	1:C:964:ILE:HG22	2.18	0.44
1:C:579:ARG:HD3	1:C:593:HIS:HE1	1.81	0.43
1:C:901:ARG:C	1:C:903:MET:H	2.20	0.43
1:C:575:ILE:N	1:C:602:PHE:O	2.38	0.43
1:C:876:VAL:O	1:C:877:ASN:C	2.57	0.43
1:C:812:ASP:N	1:C:812:ASP:OD1	2.51	0.43
1:C:857:ASP:O	1:C:858:LYS:HB2	2.17	0.42
1:C:891:ILE:HD12	1:C:891:ILE:C	2.40	0.42
1:C:398:VAL:O	1:C:398:VAL:HG12	2.19	0.42
1:C:954:GLN:O	1:C:957:VAL:HG12	2.19	0.42
1:C:451:ILE:O	1:C:454:ALA:HB3	2.20	0.42
1:C:945:ILE:O	1:C:948:LEU:HG	2.19	0.42
1:C:562:ALA:HB3	1:C:574:LEU:HD21	2.02	0.41
1:C:959:ASP:N	1:C:959:ASP:OD1	2.53	0.41
1:C:550:PHE:HZ	1:C:574:LEU:HD23	1.85	0.41
1:C:555:GLU:O	1:C:595:MET:O	2.38	0.41
1:C:789:ASN:HA	1:C:792:VAL:HG23	2.02	0.41
1:C:892:THR:HG22	1:C:893:GLU:N	2.35	0.41
1:C:394:GLN:O	1:C:397:ARG:HB3	2.20	0.41
1:C:932:MET:CE	1:C:933:PHE:CD1	3.04	0.41
1:C:948:LEU:O	1:C:951:LEU:CB	2.69	0.41
1:C:544:ARG:O	1:C:551:PHE:CE2	2.74	0.41
1:C:810:LEU:HG	1:C:834:GLY:O	2.21	0.41
1:C:946:SER:O	1:C:949:ASP:HB3	2.21	0.41
1:C:363:ASP:OD1	1:C:364:LEU:N	2.53	0.41
1:C:387:CYS:SG	1:C:388:PRO:HD2	2.61	0.41
1:C:999:PHE:CE2	1:C:1010:PRO:HD2	2.55	0.41
1:C:411:LEU:HD13	1:C:423:ARG:HG2	2.03	0.41
1:C:529:GLN:HA	1:C:532:TYR:HB3	2.03	0.41
1:C:1014:TYR:CD1	1:C:1145:TYR:O	2.74	0.40
1:C:514:HIS:ND1	1:C:929:LEU:HD21	2.36	0.40
1:C:544:ARG:HD3	1:C:600:THR:HG23	2.02	0.40
1:C:436:SER:HB2	1:C:450:THR:HG21	2.03	0.40
1:C:915:LEU:HD13	1:C:934:ARG:HA	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:MET:SD	1:C:410:TYR:CZ	3.15	0.40
1:C:536:SER:C	1:C:538:ASN:N	2.74	0.40
1:C:970:GLY:O	1:C:971:LEU:HB3	2.22	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	C	532/700 (76%)	466 (88%)	65 (12%)	1 (0%)	49 84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	363	ASP

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	C	481/619 (78%)	468 (97%)	13 (3%)	48 72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	380	ASP
1	C	439	ASN
1	C	483	ASP
1	C	499	ASN
1	C	516	SER
1	C	600	THR
1	C	779	SER
1	C	795	ARG
1	C	812	ASP
1	C	969	LEU
1	C	990	LEU
1	C	1005	SER
1	C	1142	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	352	HIS
1	C	593	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 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	1019:HIS	C	1141:ASN	N	7.18