



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 17, 2017 – 01:50 PM EST

PDB ID : 5U6O  
EMDB ID: : EMD-8511  
Title : Structure of the human HCN1 hyperpolarization-activated cyclic nucleotide-gated ion channel  
Authors : Lee, C.-H.; MacKinnon, R.  
Deposited on : 2016-12-08  
Resolution : 3.50 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](mailto: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 : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

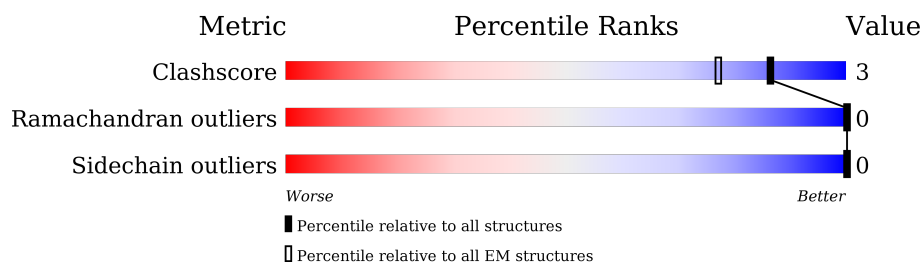
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	660	
1	B	660	
1	C	660	
1	D	660	

## 2 Entry composition

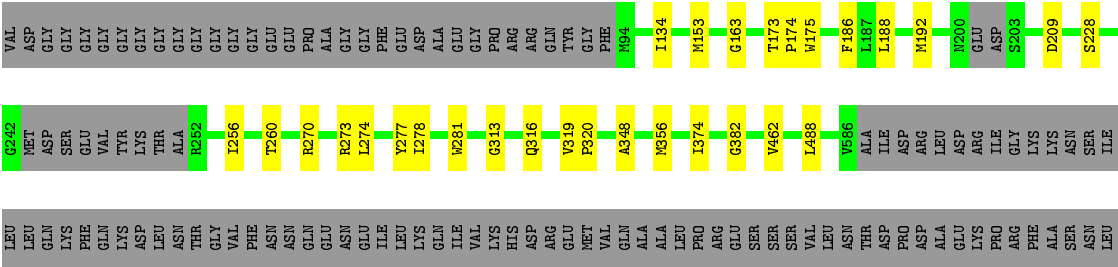
There is only 1 type of molecule in this entry. The entry contains 14480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

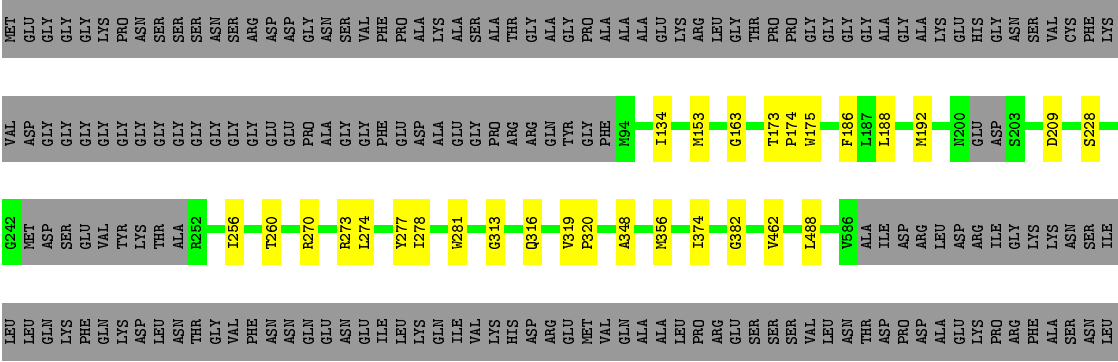
- Molecule 1 is a protein called Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	482	Total	C	N	O	S	0	0
			3620	2358	612	623	27		
1	B	482	Total	C	N	O	S	0	0
			3620	2358	612	623	27		
1	C	482	Total	C	N	O	S	0	0
			3620	2358	612	623	27		
1	D	482	Total	C	N	O	S	0	0
			3620	2358	612	623	27		





● Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 1



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55870	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	A	0.42	0/3710	0.69	0/5046
1	B	0.42	0/3710	0.69	0/5046
1	C	0.42	0/3710	0.69	0/5046
1	D	0.42	0/3710	0.69	0/5046
All	All	0.42	0/14840	0.69	0/20184

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3620	0	3318	18	0
1	B	3620	0	3318	18	0
1	C	3620	0	3318	18	0
1	D	3620	0	3318	18	0
All	All	14480	0	13272	72	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 3.

All (72) 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:A:319:VAL:HG11	1:A:374:ILE:HD11	1.87	0.56
1:C:319:VAL:HG11	1:C:374:ILE:HD11	1.87	0.56
1:B:319:VAL:HG11	1:B:374:ILE:HD11	1.88	0.55
1:D:319:VAL:HG11	1:D:374:ILE:HD11	1.87	0.55
1:A:356:MET:HA	1:A:382:GLY:HA3	1.89	0.54
1:C:356:MET:HA	1:C:382:GLY:HA3	1.89	0.54
1:D:228:SER:HB2	1:D:270:ARG:HG3	1.91	0.53
1:D:356:MET:HA	1:D:382:GLY:HA3	1.89	0.53
1:B:228:SER:HB2	1:B:270:ARG:HG3	1.91	0.53
1:B:356:MET:HA	1:B:382:GLY:HA3	1.89	0.53
1:C:228:SER:HB2	1:C:270:ARG:HG3	1.91	0.53
1:A:228:SER:HB2	1:A:270:ARG:HG3	1.91	0.53
1:A:462:VAL:CG1	1:A:488:LEU:HB3	2.39	0.52
1:D:462:VAL:CG1	1:D:488:LEU:HB3	2.39	0.52
1:C:462:VAL:CG1	1:C:488:LEU:HB3	2.39	0.51
1:B:462:VAL:CG1	1:B:488:LEU:HB3	2.39	0.51
1:C:274:LEU:O	1:C:278:ILE:HG12	2.12	0.50
1:A:163:GLY:HA3	1:A:175:TRP:CH2	2.47	0.49
1:B:274:LEU:O	1:B:278:ILE:HG12	2.12	0.49
1:D:163:GLY:HA3	1:D:175:TRP:CH2	2.47	0.49
1:B:163:GLY:HA3	1:B:175:TRP:CH2	2.47	0.49
1:C:163:GLY:HA3	1:C:175:TRP:CH2	2.47	0.49
1:D:274:LEU:O	1:D:278:ILE:HG12	2.12	0.49
1:A:274:LEU:O	1:A:278:ILE:HG12	2.12	0.49
1:C:134:ILE:HD11	1:C:209:ASP:CB	2.43	0.49
1:B:134:ILE:HD11	1:B:209:ASP:CB	2.43	0.48
1:A:134:ILE:HD11	1:A:209:ASP:CB	2.43	0.48
1:D:134:ILE:HD11	1:D:209:ASP:CB	2.43	0.48
1:D:316:GLN:O	1:D:320:PRO:HD2	2.14	0.47
1:A:316:GLN:O	1:A:320:PRO:HD2	2.14	0.47
1:C:316:GLN:O	1:C:320:PRO:HD2	2.14	0.47
1:B:316:GLN:O	1:B:320:PRO:HD2	2.14	0.47
1:D:277:TYR:O	1:D:281:TRP:CD1	2.68	0.46
1:B:153:MET:HB3	1:B:274:LEU:HD12	1.98	0.46
1:C:277:TYR:O	1:C:281:TRP:CD1	2.68	0.46
1:B:277:TYR:O	1:B:281:TRP:CD1	2.68	0.46
1:C:153:MET:HB3	1:C:274:LEU:HD12	1.98	0.46
1:A:277:TYR:O	1:A:281:TRP:CD1	2.68	0.46
1:A:153:MET:HB3	1:A:274:LEU:HD12	1.98	0.45
1:A:188:LEU:O	1:A:192:MET:HG2	2.17	0.45
1:D:153:MET:HB3	1:D:274:LEU:HD12	1.98	0.45
1:C:188:LEU:O	1:C:192:MET:HG2	2.17	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LEU:O	1:B:192:MET:HG2	2.17	0.44
1:C:356:MET:HA	1:C:382:GLY:CA	2.48	0.44
1:D:356:MET:HA	1:D:382:GLY:CA	2.48	0.44
1:B:356:MET:HA	1:B:382:GLY:CA	2.48	0.44
1:C:462:VAL:HG12	1:C:488:LEU:HB3	2.00	0.44
1:D:188:LEU:O	1:D:192:MET:HG2	2.17	0.44
1:B:173:THR:N	1:B:174:PRO:HD2	2.34	0.43
1:B:228:SER:OG	1:B:273:ARG:NH2	2.51	0.43
1:D:313:GLY:O	1:D:348:ALA:HB1	2.19	0.43
1:A:313:GLY:O	1:A:348:ALA:HB1	2.18	0.43
1:B:462:VAL:HG12	1:B:488:LEU:HB3	2.00	0.43
1:C:313:GLY:O	1:C:348:ALA:HB1	2.19	0.43
1:C:173:THR:N	1:C:174:PRO:HD2	2.34	0.43
1:B:313:GLY:O	1:B:348:ALA:HB1	2.18	0.43
1:A:228:SER:OG	1:A:273:ARG:NH2	2.51	0.43
1:A:356:MET:HA	1:A:382:GLY:CA	2.48	0.43
1:D:186:PHE:CZ	1:D:270:ARG:HD3	2.54	0.43
1:A:186:PHE:CZ	1:A:270:ARG:HD3	2.54	0.42
1:D:173:THR:N	1:D:174:PRO:HD2	2.34	0.42
1:D:228:SER:OG	1:D:273:ARG:NH2	2.51	0.42
1:D:462:VAL:HG12	1:D:488:LEU:HB3	2.00	0.42
1:A:256:ILE:O	1:A:260:THR:HG23	2.20	0.42
1:A:462:VAL:HG12	1:A:488:LEU:HB3	2.00	0.42
1:B:186:PHE:CZ	1:B:270:ARG:HD3	2.54	0.42
1:C:186:PHE:CZ	1:C:270:ARG:HD3	2.54	0.42
1:C:228:SER:OG	1:C:273:ARG:NH2	2.51	0.42
1:A:173:THR:N	1:A:174:PRO:HD2	2.34	0.41
1:B:256:ILE:O	1:B:260:THR:HG23	2.20	0.41
1:C:256:ILE:O	1:C:260:THR:HG23	2.20	0.41
1:D:256:ILE:O	1:D:260:THR:HG23	2.20	0.41

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	476/660 (72%)	454 (95%)	22 (5%)	0	100	100
1	B	476/660 (72%)	454 (95%)	22 (5%)	0	100	100
1	C	476/660 (72%)	454 (95%)	22 (5%)	0	100	100
1	D	476/660 (72%)	454 (95%)	22 (5%)	0	100	100
All	All	1904/2640 (72%)	1816 (95%)	88 (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	335/565 (59%)	335 (100%)	0	100	100
1	B	335/565 (59%)	335 (100%)	0	100	100
1	C	335/565 (59%)	335 (100%)	0	100	100
1	D	335/565 (59%)	335 (100%)	0	100	100
All	All	1340/2260 (59%)	1340 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	GLN
1	A	408	GLN
1	B	398	GLN
1	B	408	GLN
1	C	398	GLN
1	C	408	GLN
1	D	398	GLN
1	D	408	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates 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.