

Integrative Structure Validation Report

March 27, 2025 - 09:59 AM PDT

The following software was used in the production of this report:

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

MolProbity Version 4.5.2

PDB ID	8ZZW
PDB-Dev ID	PDBDEV_00000032
Structure Title	The HCN Channel Voltage Sensor Undergoes A Large Downward Motion During Hyperpolarization
Structure Authors	DiMaio F; Zagotta WN
Deposited on	2019-05-20

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

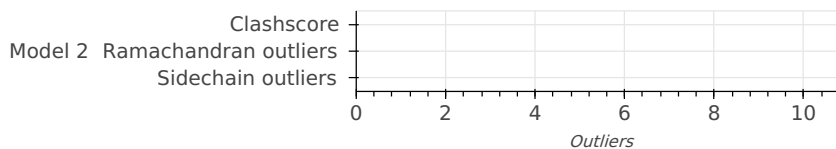
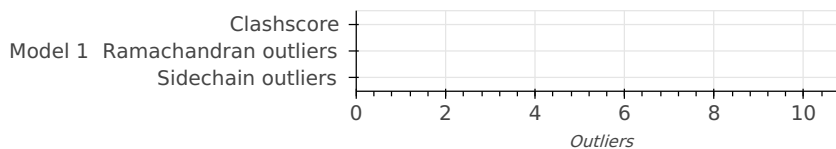
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the  symbol.

List of references used to build this report is available [here](#).

Overall quality

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 2 model(s). A total of 4 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1-2	1	HCN Voltage Gated Ion Channel	1	767	-	167-657	64.02 / 100.00	Atomic
				2					
				3					
				4					

Datasets used for modeling ?

There are 4 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Comparative model	Not available	Not available
2	Single molecule FRET data	Zenodo	10.5281/zenodo.3066494
3	Single molecule FRET data	Zenodo	10.5281/zenodo.3066494
4	Experimental model	PDB	5U6O

Methodology and software ?

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	None	Rosetta Relax	None	None	True	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Rosetta	Rosetta version unknown:5f5eba092eb978ce62ba80b58d7d04cf6a6f9727	RosettaCM/hybridize, Rosetta Relax	https://www.rosettacommons.org/
2	HHpred	website	protein homology detection	https://toolkit.tuebingen.mpg.de/hhpred

Data quality ?

Single molecule FRET

Validation for this section is under development.

Model quality

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

There are 100 bond length outliers in this entry (0.30% of 33168 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
3	186	LEU	CA-CB	11.17	1.75	1.53	2	1
1	186	LEU	CA-CB	11.14	1.75	1.53	2	1
2	186	LEU	CA-CB	11.12	1.75	1.53	2	1
4	186	LEU	CA-CB	11.12	1.75	1.53	2	1
2	213	HIS	CE1-NE2	6.64	1.25	1.32	2	2
1	213	HIS	CE1-NE2	6.60	1.25	1.32	1	2
4	213	HIS	CE1-NE2	6.59	1.26	1.32	2	2
3	213	HIS	CE1-NE2	6.55	1.26	1.32	1	2
3	518	HIS	CB-CG	5.83	1.42	1.50	2	2
1	518	HIS	CB-CG	5.79	1.42	1.50	1	2
2	518	HIS	CB-CG	5.76	1.42	1.50	2	2
4	518	HIS	CB-CG	5.76	1.42	1.50	1	2
2	371	LEU	CB-CG	5.56	1.64	1.53	2	2
1	371	LEU	CB-CG	5.53	1.64	1.53	2	2
3	331	LEU	CG-CD2	5.52	1.34	1.52	2	1
4	371	LEU	CB-CG	5.50	1.64	1.53	2	2
3	371	LEU	CB-CG	5.50	1.64	1.53	2	2
2	331	LEU	CG-CD2	5.49	1.34	1.52	2	1
4	331	LEU	CG-CD2	5.49	1.34	1.52	2	1
1	331	LEU	CG-CD2	5.47	1.34	1.52	2	1
3	341	ARG	CD-NE	5.41	1.38	1.46	2	1
1	356	GLU	CB-CG	5.41	1.36	1.52	2	1
2	341	ARG	CD-NE	5.40	1.38	1.46	2	1
2	356	GLU	CB-CG	5.39	1.36	1.52	2	1
1	341	ARG	CD-NE	5.39	1.38	1.46	2	1
4	356	GLU	CB-CG	5.37	1.36	1.52	2	1
3	356	GLU	CB-CG	5.37	1.36	1.52	2	1
4	341	ARG	CD-NE	5.35	1.38	1.46	2	1
2	199	ARG	NE-CZ	5.26	1.38	1.33	1	2
1	199	ARG	NE-CZ	5.25	1.38	1.33	1	2
3	199	ARG	NE-CZ	5.21	1.38	1.33	2	2
4	199	ARG	NE-CZ	5.21	1.38	1.33	2	2
2	478	ARG	CD-NE	4.72	1.39	1.46	2	1
1	478	ARG	CD-NE	4.72	1.39	1.46	2	1
4	478	ARG	CD-NE	4.71	1.39	1.46	2	1
3	478	ARG	CD-NE	4.69	1.39	1.46	2	1
2	483	GLN	CG-CD	4.61	1.40	1.52	1	2
3	483	GLN	CG-CD	4.60	1.40	1.52	1	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
4	483	GLN	CG-CD	4.60	1.40	1.52	2	2
1	483	GLN	CG-CD	4.59	1.40	1.52	2	2
2	218	TRP	CG-CD2	4.45	1.51	1.43	2	1
3	218	TRP	CG-CD2	4.45	1.51	1.43	2	1
4	370	ASN	CB-CG	4.44	1.41	1.52	1	1
1	370	ASN	CB-CG	4.42	1.41	1.52	1	1
2	370	ASN	CB-CG	4.42	1.41	1.52	1	1
1	218	TRP	CG-CD2	4.42	1.51	1.43	2	1
4	218	TRP	CG-CD2	4.42	1.51	1.43	2	1
1	332	ARG	CG-CD	4.42	1.39	1.52	2	1
4	332	ARG	CG-CD	4.42	1.39	1.52	2	1
3	332	ARG	CG-CD	4.42	1.39	1.52	2	1
1	521	ARG	NE-CZ	4.41	1.37	1.33	1	2
3	370	ASN	CB-CG	4.41	1.41	1.52	1	1
2	332	ARG	CG-CD	4.39	1.39	1.52	2	1
4	521	ARG	NE-CZ	4.39	1.37	1.33	1	2
2	521	ARG	NE-CZ	4.39	1.37	1.33	1	2
3	521	ARG	NE-CZ	4.35	1.37	1.33	2	2
4	444	LEU	CB-CG	4.31	1.62	1.53	2	2
3	444	LEU	CB-CG	4.30	1.62	1.53	1	2
2	444	LEU	CB-CG	4.27	1.62	1.53	2	2
1	444	LEU	CB-CG	4.27	1.62	1.53	1	2
4	341	ARG	CZ-NH2	4.24	1.27	1.33	2	1
3	341	ARG	CZ-NH2	4.19	1.28	1.33	2	1
2	341	ARG	CZ-NH2	4.19	1.28	1.33	2	1
1	341	ARG	CZ-NH2	4.17	1.28	1.33	2	1
1	304	SER	CB-OG	4.15	1.33	1.42	2	1
4	304	SER	CB-OG	4.15	1.33	1.42	2	1
2	304	SER	CB-OG	4.15	1.33	1.42	2	1
2	367	ARG	NE-CZ	4.14	1.37	1.33	1	1
3	367	ARG	NE-CZ	4.14	1.37	1.33	1	1
3	304	SER	CB-OG	4.13	1.33	1.42	2	1
1	367	ARG	NE-CZ	4.09	1.37	1.33	1	1
4	367	ARG	NE-CZ	4.07	1.37	1.33	1	1

Standard geometry: angle outliers ⓘ

There are 227 bond angle outliers in this entry (0.51% of 44872 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
2	640	PHE	CA-CB-CG	8.48	122.28	113.80	1	2
4	459	PHE	CA-CB-CG	8.47	122.27	113.80	1	2
2	459	PHE	CA-CB-CG	8.47	122.27	113.80	1	2
1	640	PHE	CA-CB-CG	8.46	122.26	113.80	1	2
1	459	PHE	CA-CB-CG	8.46	122.26	113.80	1	2
4	640	PHE	CA-CB-CG	8.45	122.25	113.80	1	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
3	459	PHE	CA-CB-CG	8.44	122.24	113.80	1	2
3	640	PHE	CA-CB-CG	8.41	122.21	113.80	1	2
4	346	SER	N-CA-CB	7.23	122.78	110.50	2	1
3	346	SER	N-CA-CB	7.22	122.78	110.50	2	1
2	346	SER	N-CA-CB	7.22	122.77	110.50	2	1
1	346	SER	N-CA-CB	7.18	122.70	110.50	2	1
3	260	PHE	CA-CB-CG	6.90	106.90	113.80	1	2
2	260	PHE	CA-CB-CG	6.90	106.90	113.80	1	2
4	260	PHE	CA-CB-CG	6.90	106.90	113.80	1	2
1	260	PHE	CA-CB-CG	6.88	106.92	113.80	1	2
1	530	ASP	CA-CB-CG	6.79	119.39	112.60	1	2
3	530	ASP	CA-CB-CG	6.79	119.39	112.60	1	2
2	530	ASP	CA-CB-CG	6.78	119.38	112.60	1	2
4	530	ASP	CA-CB-CG	6.77	119.37	112.60	1	2
1	345	LEU	C-N-CA	6.28	110.40	121.70	2	1
3	345	LEU	C-N-CA	6.27	110.42	121.70	2	1
2	345	LEU	C-N-CA	6.25	110.46	121.70	2	1
4	345	LEU	C-N-CA	6.23	110.48	121.70	2	1
2	365	VAL	C-N-CA	6.03	110.85	121.70	2	1
1	359	PHE	C-N-CA	6.01	110.89	121.70	2	1
3	365	VAL	C-N-CA	6.01	110.89	121.70	2	1
4	359	PHE	C-N-CA	6.01	110.89	121.70	2	1
2	359	PHE	C-N-CA	6.00	110.89	121.70	2	1
1	365	VAL	C-N-CA	6.00	110.90	121.70	2	1
3	359	PHE	C-N-CA	6.00	110.91	121.70	2	1
4	365	VAL	C-N-CA	5.99	110.92	121.70	2	1
1	639	HIS	CA-CB-CG	5.77	119.57	113.80	1	2
3	639	HIS	CA-CB-CG	5.76	119.56	113.80	1	2
3	241	HIS	CA-CB-CG	5.71	119.51	113.80	1	1
2	639	HIS	CA-CB-CG	5.71	119.51	113.80	1	2
1	241	HIS	CA-CB-CG	5.69	119.49	113.80	1	1
4	639	HIS	CA-CB-CG	5.68	119.48	113.80	1	2
4	241	HIS	CA-CB-CG	5.66	119.46	113.80	1	1
2	241	HIS	CA-CB-CG	5.65	119.45	113.80	1	2
3	408	HIS	CA-CB-CG	5.47	108.33	113.80	1	2
1	408	HIS	CA-CB-CG	5.44	108.36	113.80	1	2
2	465	ASN	CA-CB-CG	5.43	107.17	112.60	1	2
4	408	HIS	CA-CB-CG	5.43	108.37	113.80	1	2
2	408	HIS	CA-CB-CG	5.42	108.38	113.80	1	2
1	465	ASN	CA-CB-CG	5.38	107.22	112.60	1	2
4	465	ASN	CA-CB-CG	5.37	107.23	112.60	1	2
3	465	ASN	CA-CB-CG	5.36	107.24	112.60	1	2
3	471	ASP	CA-CB-CG	5.21	117.81	112.60	2	2
4	471	ASP	CA-CB-CG	5.18	117.78	112.60	2	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
2	471	ASP	CA-CB-CG	5.18	117.78	112.60	2	2
1	471	ASP	CA-CB-CG	5.18	117.78	112.60	1	2
1	218	TRP	CA-CB-CG	5.17	103.77	113.60	2	1
3	218	TRP	CA-CB-CG	5.15	103.81	113.60	2	1
2	218	TRP	CA-CB-CG	5.15	103.82	113.60	2	1
4	218	TRP	CA-CB-CG	5.15	103.82	113.60	2	1
3	216	PHE	CA-CB-CG	4.93	108.87	113.80	1	1
2	216	PHE	CA-CB-CG	4.90	108.90	113.80	1	1
4	216	PHE	CA-CB-CG	4.89	108.91	113.80	1	1
1	216	PHE	CA-CB-CG	4.88	108.92	113.80	1	1
3	389	VAL	CA-C-N	4.86	124.19	116.90	1	2
1	389	VAL	CA-C-N	4.86	124.19	116.90	1	2
4	641	ASN	CA-CB-CG	4.86	117.46	112.60	2	2
3	641	ASN	CA-CB-CG	4.85	117.45	112.60	2	2
2	641	ASN	CA-CB-CG	4.84	117.44	112.60	2	2
1	641	ASN	CA-CB-CG	4.84	117.44	112.60	1	2
2	389	VAL	CA-C-N	4.83	124.15	116.90	1	2
4	389	VAL	CA-C-N	4.83	124.14	116.90	1	2
2	581	ARG	C-CA-CB	4.82	100.94	110.10	1	1
3	581	ARG	C-CA-CB	4.81	100.97	110.10	1	1
4	581	ARG	C-CA-CB	4.80	100.97	110.10	1	1
1	581	ARG	C-CA-CB	4.80	100.97	110.10	1	1
2	344	ARG	NE-CZ-NH2	4.76	114.92	119.20	1	1
4	320	HIS	CA-CB-CG	4.75	109.05	113.80	1	2
1	344	ARG	NE-CZ-NH2	4.74	114.93	119.20	1	1
3	320	HIS	CA-CB-CG	4.73	109.07	113.80	1	2
3	344	ARG	NE-CZ-NH2	4.72	114.95	119.20	1	1
1	287	GLN	C-N-CA	4.72	113.21	121.70	2	2
2	320	HIS	CA-CB-CG	4.72	109.08	113.80	1	2
4	344	ARG	NE-CZ-NH2	4.71	114.96	119.20	1	1
1	311	PHE	CA-CB-CG	4.71	118.51	113.80	1	1
3	287	GLN	C-N-CA	4.71	113.23	121.70	2	2
4	581	ARG	CA-CB-CG	4.70	123.49	114.10	1	1
1	320	HIS	CA-CB-CG	4.70	109.10	113.80	1	2
2	287	GLN	C-N-CA	4.68	113.27	121.70	2	2
4	287	GLN	C-N-CA	4.68	113.27	121.70	2	2
1	581	ARG	CA-CB-CG	4.68	123.46	114.10	1	1
1	397	ASP	CA-CB-CG	4.68	107.92	112.60	2	2
2	581	ARG	CA-CB-CG	4.68	123.46	114.10	1	1
4	311	PHE	CA-CB-CG	4.68	118.48	113.80	1	1
3	581	ARG	CA-CB-CG	4.67	123.44	114.10	1	1
3	397	ASP	CA-CB-CG	4.67	107.93	112.60	2	2
3	311	PHE	CA-CB-CG	4.65	118.45	113.80	1	1
4	397	ASP	CA-CB-CG	4.65	107.95	112.60	1	2
2	397	ASP	CA-CB-CG	4.64	107.96	112.60	1	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
2	311	PHE	CA-CB-CG	4.64	118.44	113.80	1	1
3	344	ARG	CD-NE-CZ	4.62	130.87	124.40	1	1
4	346	SER	C-CA-CB	4.62	101.32	110.10	2	1
3	346	SER	C-CA-CB	4.61	101.35	110.10	2	1
4	344	ARG	CD-NE-CZ	4.60	130.84	124.40	1	1

Too-close contacts ?

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all atomic models in this entry.

Model ID	Clash score	Number of clashes
1	0.00	0
2	0.00	0

There are no too-close contacts.

Torsion angles: Protein backbone ?

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	1956	1924	32	0
2	1956	1916	40	0

Torsion angles : Protein sidechains ?

In the following table, sidechain rotameric outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	1780	1760	20	0
2	1780	1760	20	0

Fit of model to data used for modeling ?

Single molecule FRET

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

Dr. Jill Trewthella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea

Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.