

Integrative Structure Validation Report ?

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

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

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

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

We welcome your comments at pdb-dev@mail.wwpdb.org

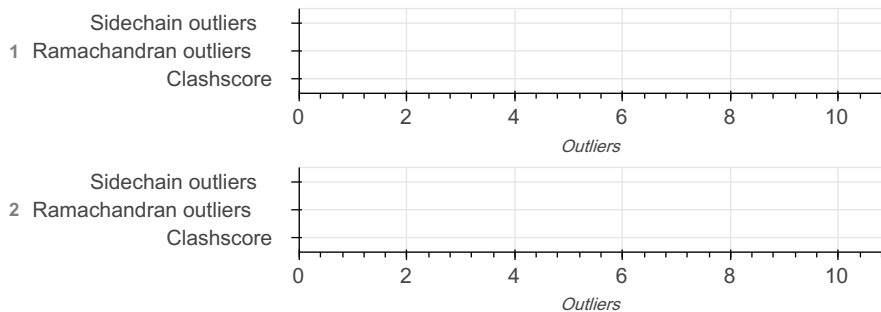
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 assessment for SAS datasets and fit to model assessments for SAS 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 unique models, with 4 subunits in each model. A total of 4 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 4 flexible or non-rigid units.

Entry composition ?

There are 2 unique types of models in this entry. These models are titled HCN 0mV/None, HCN -100mV/None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	HCN Voltage Gated Ion Channel	1	1	491
1	2	1	HCN Voltage Gated Ion Channel	2	2	491
1	3	1	HCN Voltage Gated Ion Channel	3	3	491
1	4	1	HCN Voltage Gated Ion Channel	4	4	491
2	1	1	HCN Voltage Gated Ion Channel	1	1	491
2	2	1	HCN Voltage Gated Ion Channel	2	2	491
2	3	1	HCN Voltage Gated Ion Channel	3	3	491
2	4	1	HCN Voltage Gated Ion Channel	4	4	491

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	File	10.5281/zenodo.3066494
3	Single molecule FRET data	File	10.5281/zenodo.3066494
4	Experimental model	PDB	5U6O

Representation ?

This entry has only one representation and includes 0 rigid bodies and 4 flexible units

Chain ID	Rigid bodies	Non-rigid segments
1	-	167-657

Chain ID	Rigid bodies	Non-rigid segments
2	-	167-657
3	-	167-657
4	-	167-657

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	Rosetta Relax	None	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, molprobtity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers ?

There are 10780 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found [here](#).

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG--2HG	1.05	0.97	8
CE--3HE	1.05	0.97	8
CD--1HD	1.05	0.97	12
CB--2HB	1.05	0.97	33

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CB--1HB	1.05	0.97	18
CB--3HB	1.05	0.97	11
CB--2HB	1.06	0.97	173
CB--1HB	1.06	0.97	130
CB--3HB	1.06	0.97	1
CG--1HG	1.06	0.97	44
CG--2HG	1.06	0.97	59
CE--1HE	1.06	0.97	8
CD--2HD	1.06	0.97	41
CE--3HE	1.06	0.97	8
CD--1HD	1.06	0.97	4
CG--1HG	1.07	0.97	97
CD--2HD	1.07	0.97	59
CB--1HB	1.07	0.97	352
CB--2HB	1.07	0.97	405
CD--1HD	1.07	0.97	52
CG--2HG	1.07	0.97	124
CE--2HE	1.07	0.97	37
CE--1HE	1.07	0.97	16
CB--3HB	1.07	0.97	24
CA--2HA	1.07	0.97	8
NZ--3HZ	0.99	0.89	9
CE--3HE	1.07	0.97	6
CB--1HB	1.08	0.97	726
CD--1HD	1.08	0.97	166
CE--3HE	1.08	0.97	46
CG--2HG	1.08	0.97	280
CG--1HG	1.08	0.97	221

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CB--2HB	1.08	0.97	713
CD--2HD	1.08	0.97	128
CE--2HE	1.08	0.97	99
NZ--3HZ	1.00	0.89	35
NZ--2HZ	1.00	0.89	25
CA--1HA	1.08	0.97	66
CE--1HE	1.08	0.97	48
CB--3HB	1.08	0.97	56
CA--2HA	1.08	0.97	38
NZ--1HZ	1.00	0.89	8
CB--1HB	1.09	0.97	1640
CD--2HD	1.09	0.97	240
CE--2HE	1.09	0.97	168
CB--2HB	1.09	0.97	1497
CD--1HD	1.09	0.97	239
CG--1HG	1.09	0.97	593
CE--1HE	1.09	0.97	215
CA--2HA	1.09	0.97	130
CE--3HE	1.09	0.97	84
CG--2HG	1.09	0.97	492
NZ--2HZ	1.01	0.89	75
CB--3HB	1.09	0.97	98
NZ--1HZ	1.01	0.89	81
CA--1HA	1.09	0.97	110
NZ--3HZ	1.01	0.89	64
N--1H	1.01	0.89	8
N--3H	1.01	0.89	8
CD--1HD	1.10	0.97	35

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG--1HG	1.10	0.97	81
CB--1HB	1.10	0.97	106
NZ--3HZ	1.02	0.89	17
CB--2HB	1.10	0.97	107
CB--3HB	1.10	0.97	2
CE--1HE	1.10	0.97	1
NZ--1HZ	1.02	0.89	23
CG--2HG	1.10	0.97	89
NZ--2HZ	1.02	0.89	41
N--2H	1.02	0.89	8
CD--2HD	1.10	0.97	30
CD--2HD	1.11	0.97	10
NZ--2HZ	1.03	0.89	11
NZ--3HZ	1.03	0.89	19
NZ--1HZ	1.03	0.89	32
CB--2HB	1.11	0.97	8
NZ--3HZ	1.04	0.89	8
NZ--1HZ	1.05	0.89	8

Standard geometry: angle outliers ?

There are 227 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found [here](#).

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	122.28	1
CA-CB-CG	113.80	122.27	2
CA-CB-CG	113.80	122.26	2
CA-CB-CG	113.80	122.25	1
CA-CB-CG	113.80	122.24	2
CA-CB-CG	113.80	122.22	3
CA-CB-CG	113.80	122.21	1
CA-CB-CG	113.80	122.20	3

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	122.19	1
N-CA-CB	110.50	122.78	2
N-CA-CB	110.50	122.77	1
N-CA-CB	110.50	122.70	1
CA-CB-CG	113.80	106.90	3
CA-CB-CG	113.80	106.92	1
CA-CB-CG	112.60	119.39	2
CA-CB-CG	112.60	119.38	1
CA-CB-CG	112.60	119.37	1
CA-CB-CG	112.60	119.35	1
CA-CB-CG	112.60	119.31	2
CA-CB-CG	112.60	119.30	1
C-N-CA	121.70	110.40	1
C-N-CA	121.70	110.42	1
C-N-CA	121.70	110.46	1
C-N-CA	121.70	110.48	1
C-N-CA	121.70	110.85	1
C-N-CA	121.70	110.89	4
C-N-CA	121.70	110.90	1
C-N-CA	121.70	110.91	1
C-N-CA	121.70	110.92	1
CA-CB-CG	113.80	119.57	1
CA-CB-CG	113.80	119.56	1
CA-CB-CG	113.80	119.51	2
CA-CB-CG	113.80	119.49	1
CA-CB-CG	113.80	119.48	1
CA-CB-CG	113.80	119.46	1
CA-CB-CG	113.80	119.45	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	113.80	119.33	1
CA-CB-CG	113.80	119.31	2
CA-CB-CG	113.80	119.27	1
CA-CB-CG	113.80	108.33	1
CA-CB-CG	113.80	108.36	1
CA-CB-CG	112.60	107.17	1
CA-CB-CG	113.80	108.37	2
CA-CB-CG	113.80	108.38	4
CA-CB-CG	112.60	107.22	1
CA-CB-CG	112.60	107.23	2
CA-CB-CG	112.60	107.24	1
CA-CB-CG	112.60	107.26	2
CA-CB-CG	112.60	107.28	1
CA-CB-CG	112.60	117.81	1
CA-CB-CG	112.60	117.78	3
CA-CB-CG	113.60	103.77	1
CA-CB-CG	112.60	117.75	1
CA-CB-CG	113.60	103.81	1
CA-CB-CG	113.60	103.82	2
CA-CB-CG	112.60	117.73	2
CA-CB-CG	112.60	117.68	1
CA-CB-CG	113.80	108.87	1
CA-CB-CG	113.80	108.90	1
CA-CB-CG	113.80	108.91	1
CA-CB-CG	113.80	108.92	1
CA-C-N	116.90	124.19	2
CA-CB-CG	112.60	117.46	1
CA-CB-CG	112.60	117.45	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-C-N	116.90	124.17	1
CA-CB-CG	112.60	117.44	2
CA-C-N	116.90	124.15	1
CA-C-N	116.90	124.14	3
CA-CB-CG	112.60	117.42	3
C-CA-CB	110.10	100.94	1
CA-C-N	116.90	124.13	1
CA-CB-CG	112.60	117.41	1
C-CA-CB	110.10	100.97	3
NE-CZ-NH2	119.20	114.92	1
CA-CB-CG	113.80	109.05	1
NE-CZ-NH2	119.20	114.93	1
CA-CB-CG	113.80	109.07	1
NE-CZ-NH2	119.20	114.95	1
C-N-CA	121.70	113.21	1
CA-CB-CG	113.80	109.08	1
NE-CZ-NH2	119.20	114.96	1
CA-CB-CG	113.80	118.51	1
C-N-CA	121.70	113.23	1
CA-CB-CG	114.10	123.49	1
CA-CB-CG	113.80	109.10	1
C-N-CA	121.70	113.27	2
CA-CB-CG	114.10	123.46	2
CA-CB-CG	112.60	107.92	1
CA-CB-CG	113.80	118.48	1
CA-CB-CG	114.10	123.44	1
CA-CB-CG	112.60	107.93	1
CA-CB-CG	113.80	118.45	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	107.95	1
CA-CB-CG	112.60	107.96	3
CA-CB-CG	113.80	118.44	1
CA-CB-CG	112.60	107.97	1
CD-NE-CZ	124.40	130.87	1
C-CA-CB	110.10	101.32	1
CA-CB-CG	112.60	107.99	1
C-N-CA	121.70	113.41	4
C-CA-CB	110.10	101.35	1
CD-NE-CZ	124.40	130.84	1
C-CA-CB	110.10	101.36	1
C-CA-CB	110.10	101.37	1
CD-NE-CZ	124.40	130.83	1
CD-NE-CZ	124.40	130.81	1
CA-CB-CG	112.60	108.07	2
CA-CB-CG	112.60	108.08	1
C-N-CA	121.70	113.58	1
CA-CB-CG	112.60	108.09	1
CA-CB-CG	113.80	109.29	1
C-N-CA	121.70	113.59	2
C-N-CA	121.70	113.61	3
CA-CB-CG	113.80	118.29	2
C-N-CA	121.70	113.62	1
CA-CB-CG	113.80	109.32	2
CA-CB-CG	113.80	109.33	1
CA-CB-CG	113.80	118.26	1
C-N-CA	121.70	113.67	1
O-C-N	123.00	115.88	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O-C-N	123.00	115.89	1
CA-CB-CG	113.80	118.24	1
O-C-N	123.00	115.92	2
CA-CB-CG	112.60	116.98	1
CA-CB-CG	112.60	116.97	1
CA-CB-CG	112.60	116.96	2
CA-CB-CG	112.60	116.95	1
CA-CB-CG	112.60	116.93	1
CA-CB-CG	112.60	116.92	1
CA-CB-CG	112.60	116.90	1
C-N-CA	121.70	113.97	1
C-N-CA	121.70	114.03	2
C-N-CA	121.70	114.04	1
CA-CB-CG	112.60	116.85	1
CA-CB-CG	112.60	116.83	1
C-CA-CB	110.10	118.12	1
CA-CB-CG	112.60	116.82	1
CA-CB-CG	113.80	109.58	1
CA-CB-CG	112.60	116.81	2
C-CA-CB	110.10	118.10	2
C-CA-CB	110.10	118.09	1
CA-CB-CG	112.60	116.80	1
C-CA-CB	110.10	118.07	1
CA-CB-CG	113.80	109.61	2
C-CA-CB	110.10	118.05	1
CA-CB-CG	113.80	109.62	1
C-CA-CB	110.10	118.04	1
C-CA-CB	110.10	118.03	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-CG	112.60	116.77	1
CA-CB-CG	113.80	109.63	1
NE-CZ-NH2	119.20	115.45	1
NE-CZ-NH1	121.50	125.66	1
CA-CB-CG	112.60	116.76	1
CA-CB-CG	113.80	109.64	2
CA-CB-CG	113.80	109.65	2
CA-CB-CG	113.80	109.66	1
CA-CB-CG	113.80	109.67	2
N-CA-C	111.00	122.51	1
N-CA-C	111.00	122.50	2
NE-CZ-NH1	121.50	125.60	1
NE-CZ-NH1	121.50	125.59	1
N-CA-C	111.00	122.46	1
NE-CZ-NH1	121.50	125.56	1
NE-CZ-NH2	119.20	115.56	3
OE1-CD-NE2	122.60	126.62	2
CA-CB-CG	113.80	117.81	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 the models in this entry.

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

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

Model ID	Analyzed	Favored	Allowed	Outliers
2	1956	1916	40	0

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains ?

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

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

Detailed list of outliers are tabulated below.

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.

Acknowledgements

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