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	9A06
PDB-Dev ID	PDBDEV_00000042
Structure Title	Rosetta docking models of human KCNQ1 channel with KCNE1 auxiliary protein
Structure Authors	Kuenze G; Vanoye CG; Desai RR; Adusumilli S; Sanders CR; George AL Jr; Meiler J

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

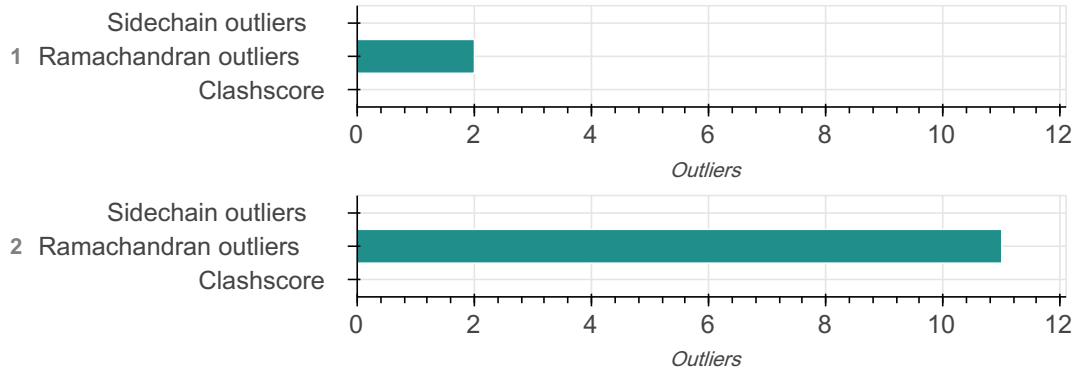
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 6 subunits in each model. A total of 12 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 12 flexible or non-rigid units.

Entry composition

There are 2 unique types of models in this entry.These models are titled Docking model of KCNQ1 in open conformation with KCNE1/Docking model of KCNQ1 in open conformation with KCNE1, Docking model of KCNQ1 in closed conformation with KCNE1/Docking model of KCNQ1 in closed conformation with KCNE1 respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	KCNQ1 channel-forming domain	A	A	267
1	2	1	KCNQ1 channel-forming domain	B	B	267
1	3	1	KCNQ1 channel-forming domain	C	C	267
1	4	1	KCNQ1 channel-forming domain	D	D	267
1	5	2	KCNE1 transmembrane domain	E	E	35

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	6	2	KCNE1 transmembrane domain	F	F	35
2	1	1	KCNQ1 channel-forming domain	A	A	267
2	2	1	KCNQ1 channel-forming domain	B	B	267
2	3	1	KCNQ1 channel-forming domain	C	C	267
2	4	1	KCNQ1 channel-forming domain	D	D	267
2	5	2	KCNE1 transmembrane domain	E	E	35
2	6	2	KCNE1 transmembrane domain	F	F	35

Datasets used for modeling

There are 12 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Comparative model	File	10.5281/zenodo.3598943
2	Comparative model	File	10.5281/zenodo.3598943
3	Comparative model	File	10.5281/zenodo.3598943
4	Crosslinking-MS data	File	10.5281/zenodo.3598943
5	Mutagenesis data	File	10.5281/zenodo.3598943
6	Crosslinking-MS data	File	10.5281/zenodo.3598943
7	Mutagenesis data	File	10.5281/zenodo.3598943
8	Experimental model	PDB	5VMS

ID	Dataset type	Database name	Data access code
9	Experimental model	PDB	2R9R
10	Experimental model	PDB	2K21
11	Experimental model	PDB	4G7Y
12	Experimental model	PDB	5DQQ

Representation

This entry has only one representation and includes 0 rigid bodies and 12 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-2671-267
B	-	1-2671-267
C	-	1-2671-267
D	-	1-2671-267
E	-	1-351-35
F	-	1-351-35

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	RosettaDock	Docking	None	40000	True	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location

ID	Software name	Software version	Software classification	Software location
1	Rosetta	3.10	model building, model validation	https://www.rosettacommons.org/

Data quality

Crosslinking-MS

Validation for this section is under development.

Mutagenesis

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 10800 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
CD--2HD	1.07	0.97	3
CG2--2HG2	1.07	0.97	1
CA--HA	1.07	0.97	2
CG1--2HG1	1.07	0.97	1
CB--2HB	1.08	0.97	56
CG2--2HG2	1.08	0.97	8
CA--HA	1.08	0.97	32
CG1--1HG1	1.08	0.97	24
CG--2HG	1.08	0.97	17
CG--HG	1.08	0.97	13

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG1--2HG1	1.08	0.97	11
CD2--2HD2	1.08	0.97	3
OG--HG	0.95	0.84	3
CD--1HD	1.08	0.97	18
CB--1HB	1.08	0.97	51
CG2--1HG2	1.08	0.97	23
CB--HB	1.08	0.97	14
OG1--HG1	0.95	0.84	10
CD1--3HD1	1.08	0.97	4
CG2--3HG2	1.08	0.97	21
CG--1HG	1.08	0.97	9
CD1--1HD1	1.08	0.97	10
CA--2HA	1.08	0.97	4
CE--2HE	1.08	0.97	6
OH--HH	0.95	0.84	1
CB--3HB	1.08	0.97	12
CD--2HD	1.08	0.97	5
CA--1HA	1.08	0.97	8
CD1--2HD1	1.08	0.97	3
CD2--1HD2	1.08	0.97	2
NZ--2HZ	1.00	0.89	2
NZ--3HZ	1.00	0.89	1
CB--1HB	1.09	0.97	797

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CA--HA	1.09	0.97	1161
CD--1HD	1.09	0.97	114
CB--2HB	1.09	0.97	792
CB--HB	1.09	0.97	330
CG1--1HG1	1.09	0.97	248
CG2--3HG2	1.09	0.97	323
CD1--1HD1	1.09	0.97	230
CG1--2HG1	1.09	0.97	260
CD2--2HD2	1.09	0.97	125
CD--2HD	1.09	0.97	122
OG--HG	0.96	0.84	100
CG--2HG	1.09	0.97	231
CD1--2HD1	1.09	0.97	237
CG2--2HG2	1.09	0.97	335
CG2--1HG2	1.09	0.97	321
CD2--1HD2	1.09	0.97	126
CB--3HB	1.09	0.97	83
CG--HG	1.09	0.97	115
CD1--3HD1	1.09	0.97	236
CG--1HG	1.09	0.97	239
CA--1HA	1.09	0.97	128
CA--2HA	1.09	0.97	132
CE--2HE	1.09	0.97	66

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CG1--3HG1	1.09	0.97	160
CD2--3HD2	1.09	0.97	128
OH--HH	0.96	0.84	37
CE--1HE	1.09	0.97	72
NZ--2HZ	1.01	0.89	54
NZ--3HZ	1.01	0.89	55
OG1--HG1	0.96	0.84	62
NZ--1HZ	1.01	0.89	56
CE--3HE	1.09	0.97	16
OH--HH	0.97	0.84	2
CA--HA	1.10	0.97	13
CB--2HB	1.10	0.97	16
CD--2HD	1.10	0.97	14
OG--HG	0.97	0.84	1
CG--1HG	1.10	0.97	16
SG--HG	1.33	1.20	16
CG--2HG	1.10	0.97	16
CB--1HB	1.10	0.97	16
CD--1HD	1.10	0.97	12
CB--3HB	1.10	0.97	1
ND1--HD1	0.99	0.86	2
NE2--1HE2	0.99	0.86	2
ND1--HD1	1.00	0.86	17

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--2HE2	1.00	0.86	71
NE2--1HE2	1.00	0.86	65
ND2--1HD2	1.00	0.86	16
N--H	1.00	0.86	177
ND2--2HD2	1.00	0.86	16
NH1--2HH1	1.00	0.86	5
NH2--2HH2	1.00	0.86	4
NH1--1HH1	1.00	0.86	2
N--H	1.01	0.86	1114
NE--HE	1.01	0.86	72
NH1--1HH1	1.01	0.86	67
NH2--2HH2	1.01	0.86	68
NE2--1HE2	1.01	0.86	5
NE1--HE1	1.01	0.86	32
NH1--2HH1	1.01	0.86	67
CD2--HD2	1.08	0.93	10
CZ2--HZ2	1.08	0.93	1
NH2--1HH2	1.01	0.86	71
CE1--HE1	1.08	0.93	13
CD1--HD1	1.08	0.93	5
NE2--HE2	1.01	0.86	5
CE2--HE2	1.08	0.93	4
CZ--HZ	1.08	0.93	1

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NE2--2HE2	1.01	0.86	1
N--H	1.02	0.86	37
NH1--1HH1	1.02	0.86	3
CD1--HD1	1.09	0.93	171
NH2--1HH2	1.02	0.86	1
CZ3--HZ3	1.09	0.93	32
CD2--HD2	1.09	0.93	158
CE2--HE2	1.09	0.93	140
CE1--HE1	1.09	0.93	155
CZ--HZ	1.09	0.93	103
CE3--HE3	1.09	0.93	32
CH2--HH2	1.09	0.93	32
CZ2--HZ2	1.09	0.93	31

Standard geometry: angle outliers

There are 13 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-CA-CB-CA-CB-CG	112.60	108.14	1
NE-CZ-NH2	119.20	123.20	1
CA-CB-CG	113.80	118.21	1
C-CA-CB	109.10	99.44	1
CA-CB-CG	113.80	118.18	1
CA-CB-CG	112.60	108.25	1
CA-CB-CA-CB-CG	112.60	108.32	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CA-CB-NE-CZ-NH2	119.20	122.99	1
NE-CZ-NH2	119.20	122.96	1
C-CA-CB	109.10	100.01	1
NE-CZ-NH2	119.20	122.90	1
CA-CB-CG	113.80	117.89	1
CA-CB-CG	113.80	117.88	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	Analyzed	Favored	Allowed	Outliers
1	1126	1073	51	2
2	1126	1072	43	11

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	954	949	5	0
2	954	949	5	0

Detailed list of outliers are tabulated below.

Fit of model to data used for modeling

Crosslinking-MS

Validation for this section is under development.

Mutagenesis

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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