

# Integrative Structure Validation Report ?

March 27, 2025 - 10:00 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	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
Deposited on	2020-02-10

*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](mailto:helpdesk@pdb-ihm.org)*

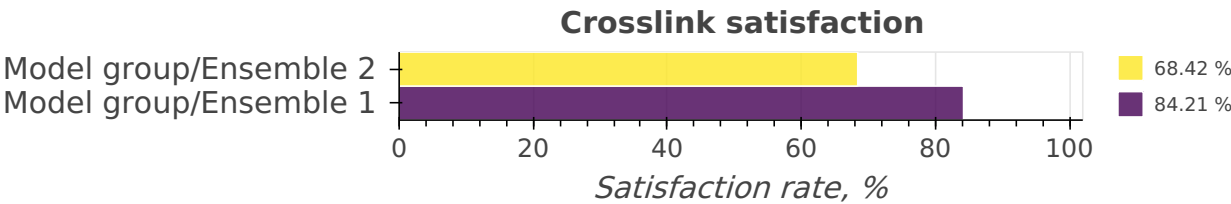
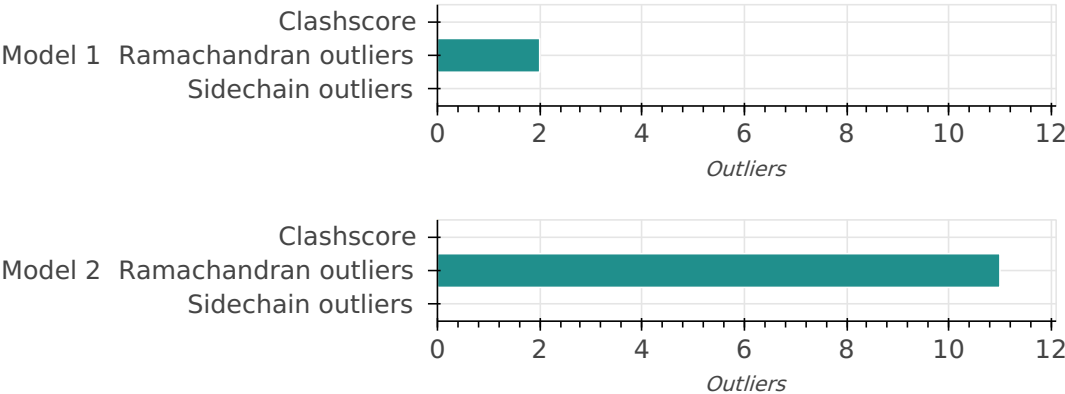
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 12 datasets were used to build this entry.*

Representation ?

*This entry has 2 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	1	KCNQ1 channel-forming domain	A	267	-	1-267	100.00 / 100.00	Atomic
				B					
				C					
				D					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		2	KCNE1 transmembrane domain	E	35	-	1-35	100.00 / 100.00	Atomic
				F					
2	2	1	KCNQ1 channel-forming domain	A	267	-	1-267	100.00 / 100.00	Atomic
				B					
				C					
				D					
		2	KCNE1 transmembrane domain	E	35	-	1-35	100.00 / 100.00	Atomic
				F					

### 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	Zenodo	<a href="https://zenodo.org/record/3598943">10.5281/zenodo.3598943</a>
2	Comparative model	Zenodo	<a href="https://zenodo.org/record/3598943">10.5281/zenodo.3598943</a>
3	Comparative model	Zenodo	<a href="https://zenodo.org/record/3598943">10.5281/zenodo.3598943</a>
4	Crosslinking-MS data	Zenodo	<a href="https://zenodo.org/record/3598943">10.5281/zenodo.3598943</a>
5	Mutagenesis data	Zenodo	<a href="https://zenodo.org/record/3598943">10.5281/zenodo.3598943</a>
6	Crosslinking-MS data	Zenodo	<a href="https://zenodo.org/record/3598943">10.5281/zenodo.3598943</a>
7	Mutagenesis data	Zenodo	<a href="https://zenodo.org/record/3598943">10.5281/zenodo.3598943</a>
8	Experimental model	PDB	<a href="https://www.rcsb.org/structure/5VMS">5VMS</a>
9	Experimental model	PDB	<a href="https://www.rcsb.org/structure/2R9R">2R9R</a>
10	Experimental model	PDB	<a href="https://www.rcsb.org/structure/2K21">2K21</a>
11	Experimental model	PDB	<a href="https://www.rcsb.org/structure/4G7Y">4G7Y</a>
12	Experimental model	PDB	<a href="https://www.rcsb.org/structure/5DQQ">5DQQ</a>

### 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	Docking	RosettaDock	None	40000	True	False

*There is 1 software package reported in this entry.*

ID	Software name	Software version	Software classification	Software location
1	<a href="#">Rosetta</a>	3.10	model building, model validation	<a href="https://www.rosettacommons.org/">https://www.rosettacommons.org/</a>

## Data quality ?

### Crosslinking-MS

*At the moment, data validation is only available for crosslinking-MS data deposited as a fully [compliant](#) dataset in the [PRIDE Crosslinking](#) database. Correspondence between crosslinking-MS and entry entities is established using [pyHMMER](#). Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).*

Crosslinking-MS dataset is not available in the [PRIDE Crosslinking](#) database.

### 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 no bond length outliers.*

### Standard geometry: angle outliers ?

*There are 17 bond angle outliers in this entry (0.07% of 25240 assessed bonds). A summary is provided below.*

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	31	PHE	CA-CB-CG	6.55	120.35	113.80	2	1
D	94	PHE	CA-CB-CG	4.90	108.90	113.80	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	143	ASP	CA-CB-CG	4.46	108.14	112.60	1	1
A	129	ARG	NE-CZ-NH2	4.44	123.20	119.20	1	1
D	133	PHE	CA-CB-CG	4.41	118.21	113.80	2	1
A	213	THR	C-CA-CB	4.39	99.44	109.10	2	1
B	133	PHE	CA-CB-CG	4.38	118.18	113.80	2	1
C	143	ASP	CA-CB-CG	4.35	108.25	112.60	1	1
C	94	PHE	CA-CB-CG	4.30	109.50	113.80	1	1
D	143	ASP	CA-CB-CG	4.28	108.32	112.60	1	1
B	94	PHE	CA-CB-CG	4.22	109.58	113.80	1	1
B	129	ARG	NE-CZ-NH2	4.21	122.99	119.20	1	1
C	129	ARG	NE-CZ-NH2	4.18	122.96	119.20	1	1
C	213	THR	C-CA-CB	4.13	100.01	109.10	2	1
D	129	ARG	NE-CZ-NH2	4.11	122.90	119.20	1	1
B	176	PHE	CA-CB-CG	4.09	117.89	113.80	1	1
D	176	PHE	CA-CB-CG	4.08	117.88	113.80	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	1126	1073	51	2
2	1126	1072	43	11

There are 13 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	18	PRO	1
A	221	PRO	1
B	18	PRO	1

Chain	Res	Type	Models (Total)
B	144	ARG	1
B	195	VAL	1
B	221	PRO	1
C	18	PRO	1
C	221	PRO	1
D	18	PRO	1
D	188	ALA	1
D	195	VAL	1
D	221	PRO	1
F	10	TYR	1

### 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	954	949	5	0
2	954	949	5	0

## Fit of model to data used for modeling ?

### Fit of model(s) to crosslinking-MS data

#### Restraint types

Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*".

*Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

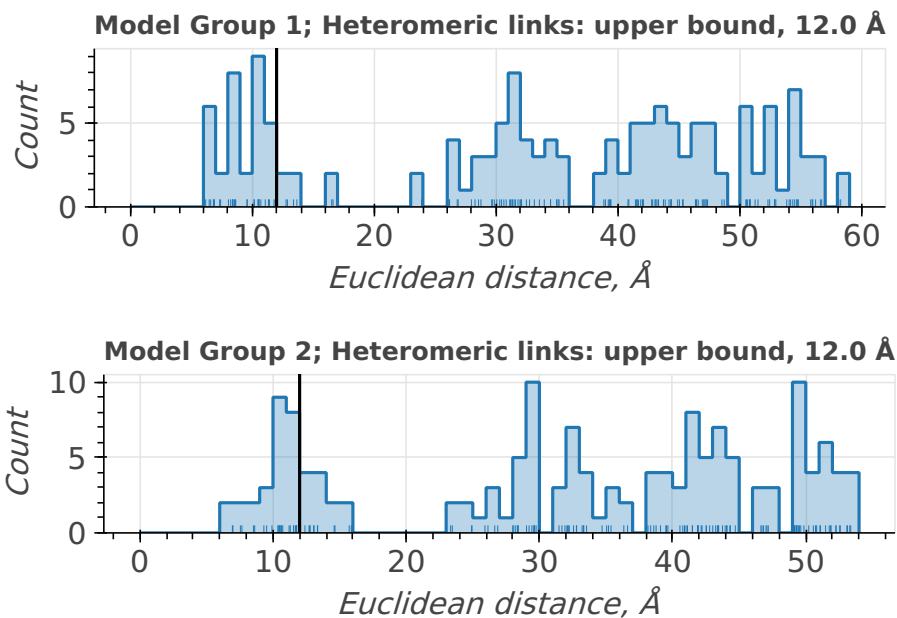
There are 152 crosslinking restraints combined in 19 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
CYS	GLU	CA	VAL	CA	upper bound	12.0	8
CYS	ALA	CA	VAL	CA	upper bound	12.0	8
CYS	GLY	CA	SER	CA	upper bound	12.0	8
CYS	GLY	CA	THR	CA	upper bound	12.0	8
CYS	LYS	CA	THR	CA	upper bound	12.0	8
CYS	GLU	CA	THR	CA	upper bound	12.0	8
CYS	GLY	CA	ILE	CA	upper bound	12.0	8
CYS	ILE	CA	LYS	CA	upper bound	12.0	8

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
CYS	ILE	CA	LEU	CA	upper bound	12.0	8
CYS	GLU	CA	ILE	CA	upper bound	12.0	8
CYS	GLU	CA	GLY	CA	upper bound	12.0	8
CYS	GLU	CA	LYS	CA	upper bound	12.0	8
CYS	GLN	CA	GLY	CA	upper bound	12.0	16
CYS	GLN	CA	LYS	CA	upper bound	12.0	8
CYS	GLU	CA	TRP	CA	upper bound	12.0	8
CYS	LEU	CA	VAL	CA	upper bound	12.0	8
CYS	GLN	CA	SER	CA	upper bound	12.0	8
CYS	LYS	CA	VAL	CA	upper bound	12.0	8

#### Distograms of individual restraints

*Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.*



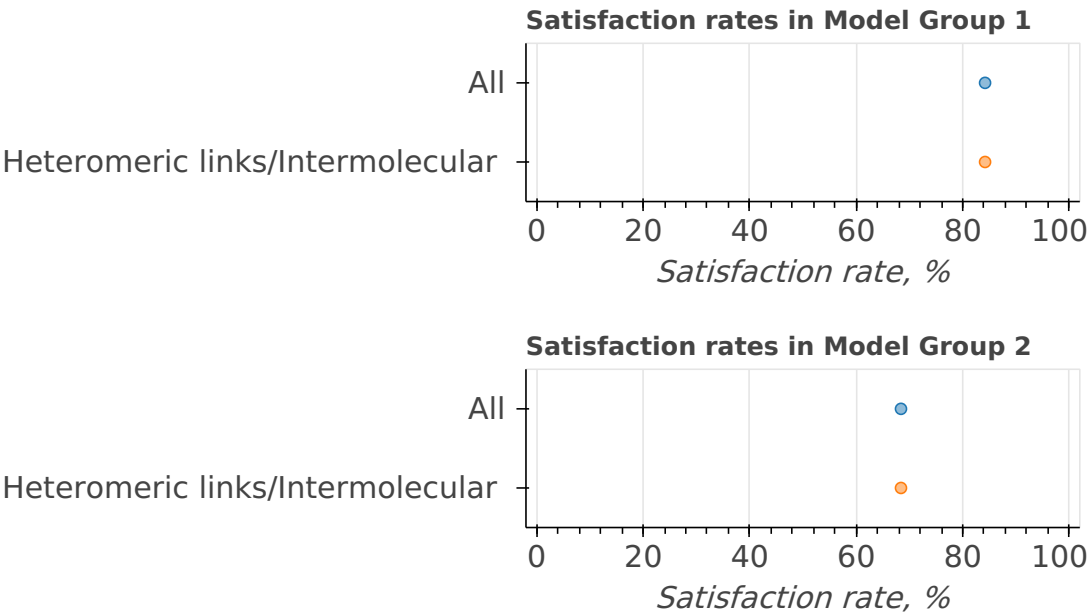
#### Satisfaction of restraints

*Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.*

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=19)
1	1	1	1/1	All	84.21	15.79	19
				Heteromeric links/ Intermolecular	84.21	15.79	19
1	2	2	1/1	All	68.42	31.58	19
				Heteromeric links/ Intermolecular	68.42	31.58	19

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



Mutagenesis

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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