Summary of integrative structure determination of Rosetta docking models of human KCNQ1 channel with KCNE1 auxiliary protein (PDB ID: 9A06, PDB-Dev ID: PDBDEV_00000042)

1. Model Composition	
Entry composition	- KCNE1 transmembrane domain: Chain F (35 residues) - KCNQ1 channel-forming domain: Chain D (267 residues) - KCNQ1 channel-forming domain: Chain A (267 residues) - KCNE1 transmembrane domain: Chain E (35 residues) - KCNQ1 channel-forming domain: Chain C (267 residues) - KCNQ1 channel-forming domain: Chain B (267 residues)
Datasets used for modeling	- Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Crosslinking-MS data, Linker name and number of cross-links: CYS, 17 cross-links - Mutagenesis data, File: 10.5281/zenodo.3598943 - Crosslinking-MS data, Linker name and number of cross-links: CYS, 2 cross-links - Mutagenesis data, File: 10.5281/zenodo.3598943 - Experimental model, PDB ID: 5VMS - Experimental model, PDB ID: 2R9R - Experimental model, PDB ID: 2K21 - Experimental model, PDB ID: 4G7Y - Experimental model, PDB ID: 5DQQ
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 12
Flexible units	- A: 1-2671-267 - B: 1-2671-267 - C: 1-2671-267 - D: 1-2671-267 - E: 1-351-35 - F: 1-351-35
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided

Experimental data	- 1 unique CrossLinkRestraint: CYS, 17 cross-links - 1 unique CrossLinkRestraint: CYS, 2 cross-links - 6 unique DerivedDistanceRestraint: Upper Bound Distance: 12.0 - 3 unique DerivedDistanceRestraint: Upper Bound Distance: 15.0
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	2
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	- Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 2, Number of sidechain outliers = 0 - Model-2: Clashscore = 0.0, Number of Ramachandran outliers = 11, Number of sidechain outliers = 0
Model quality: assessment of excluded volume	Not applicable
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Method	Docking
Name	RosettaDock
Number of computed models	40000
Software	Rosetta (version 3.10)