

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	<ul style="list-style-type: none"> - KCNQ1 channel-forming domain: chain(s) A, B, C, D (267 residues) - KCNE1 transmembrane domain: chain(s) E, F (35 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Comparative model, Zenodo: 10.5281/zenodo.3598943 - Comparative model, Zenodo: 10.5281/zenodo.3598943 - Comparative model, Zenodo: 10.5281/zenodo.3598943 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.3598943 - Mutagenesis data, Zenodo: 10.5281/zenodo.3598943 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.3598943 - Mutagenesis data, Zenodo: 10.5281/zenodo.3598943 - Experimental model, PDB: 5VMS - Experimental model, PDB: 2R9R - Experimental model, PDB: 2K21 - Experimental model, PDB: 4G7Y - Experimental model, PDB: 5DQQ
2. Representation	
Number of representations	2
Scale	<ul style="list-style-type: none"> - Atomic - Atomic
Number of <i>rigid</i> and <i>flexible</i> segments	<ul style="list-style-type: none"> - 0, 6 - 0, 6
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: CYS, 17 crosslinks - 1 unique CrossLinkRestraint: CYS, 2 crosslinks - 6 unique DerivedDistanceRestraint: Upper Bound Distance: 12.0 - 3 unique DerivedDistanceRestraint: Upper Bound Distance: 15.0
4. Validation	

<i>Number of ensembles</i>	0
<i>Number of models in ensembles</i>	Not applicable
<i>Number of deposited models</i>	2
<i>Model precision (uncertainty of models)</i>	Not available
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 0.00-0.00 - Ramachandran outliers: 2-11 - Sidechain outliers: 0-0
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 68.42-84.21%
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Name</i>	Docking
<i>Method</i>	RosettaDock
<i>Number of computed models</i>	40000
<i>Software</i>	Rosetta (version 3.10)