

## Summary of integrative structure determination of Structure of the alpha7nAChR Transmembrane and Intracellular Domains in Complex with the PICK1 PDZ Domain (PDB ID: 9A49, PDB-Dev ID: PDBDEV\_00000230)

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- CHRNA7-FAM7A fusion protein: chain(s) A, B, C, D, E (264 residues)</li> <li>- PRKCA-binding protein: chain(s) F (86 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- NMR data, Not available</li> <li>- NMR data, Not available</li> <li>- Experimental model, PDB: <a href="#">7RPM</a></li> <li>- Experimental model, PDB: <a href="#">2LUI</a></li> <li>- NMR data, Not available</li> <li>- NMR data, BMRB: <a href="#">52246</a></li> <li>- NMR data, BMRB: <a href="#">52247</a></li> <li>- NMR data, BMRB: <a href="#">52248</a></li> <li>- NMR data, BMRB: <a href="#">52249</a></li> </ul>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Atomic
Number of <a href="#">rigid</a> and <a href="#">flexible</a> segments	0, 6
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	<ul style="list-style-type: none"> <li>- 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.0-24.0</li> <li>- 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 3.0-9.0</li> </ul>
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	0
<a href="#">Number of models in ensembles</a>	Not applicable
<a href="#">Number of deposited models</a>	1
<a href="#">Model precision (uncertainty of models)</a>	Not available
<a href="#">Data quality</a>	Data quality has not been assessed
<a href="#">Model quality: assessment of atomic segments</a>	<ul style="list-style-type: none"> <li>- Clashscore: 1.80</li> <li>- Ramachandran outliers: 0</li> <li>- Sidechain outliers: 1</li> </ul>

<a href="#"><i>Fit to data used for modeling</i></a>	Fit of model to information used to compute it has not been determined
<a href="#"><i>Fit to data used for validation</i></a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#"><i>Name</i></a>	docking
<a href="#"><i>Description</i></a>	docking using distance restraints between two proteins
2. <a href="#"><i>Name</i></a>	docking
<a href="#"><i>Description</i></a>	docking using alpha7nAChR E222, V226, E229, W230 as interface residues between two proteins (obtained from alpha7nAChR CSP NMR data)
3. <a href="#"><i>Name</i></a>	docking
<a href="#"><i>Description</i></a>	docking using PICK1 I15, I17, I19 as interface residues between two proteins (obtained from PICK1 CSP NMR data)
4. <a href="#"><i>Name</i></a>	refinement
5. <a href="#"><i>Name</i></a>	refinement
6. <a href="#"><i>Name</i></a>	refinement
7. <a href="#"><i>Name</i></a>	refinement
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"> <li>- <a href="#">HADDOCK</a> (version 2.4)</li> <li>- <a href="#">PHENIX</a> (version Not available)</li> <li>- <a href="#">Chiron</a> (version Not available)</li> <li>- <a href="#">MolProbity</a> (version Not available)</li> </ul>