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)

1. Model Composition	
Entry composition	- CHRNA7-FAM7A fusion protein: Chain D (264 residues) - CHRNA7-FAM7A fusion protein: Chain C (264 residues) - CHRNA7-FAM7A fusion protein: Chain A (264 residues) - CHRNA7-FAM7A fusion protein: Chain E (264 residues) - PRKCA-binding protein: Chain F (86 residues) - CHRNA7-FAM7A fusion protein: Chain B (264 residues)
Datasets used for modeling	- NMR data, Not available - NMR data, Not available - Experimental model, PDB ID: 7RPM - Experimental model, PDB ID: 2LUI - NMR data, Not available - NMR data, BMRB: 52246 - NMR data, BMRB: 52247 - NMR data, BMRB: 52248 - NMR data, BMRB: 52249
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 6
Flexible units	- A: 1-264 - F: 1-86 - B: 1-264 - C: 1-264 - D: 1-264 - E: 1-264
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 16.0-24.0 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 3.0-9.0
4. Validation	
Number of ensembles	0

Number of models in ensembles	Not applicable
Number of deposited models	1
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 = 1.8, Number of Ramachandran outliers = 0, Number of sidechain outliers = 1
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	None
Description	docking using distance restraints between two proteins
2. Method	docking
Name	None
Description	docking using alpha7nAChR E222, V226, E229, W230 as interface residues between two proteins (obtained from alpha7nAChR CSP NMR data)
3. Method	docking
Name	None
Description	docking using PICK1 I15, I17, I19 as interface residues between two proteins (obtained from PICK1 CSP NMR data)
4. Method	refinement
Name	None
5. Method	refinement
Name	None
6. Method	refinement

Name	None
7. Method	refinement
Name	None
Software	- HADDOCK (version 2.4) - PHENIX (version Not available) - Chiron (version Not available) - MolProbity (version Not available)