

Summary of integrative structure determination of Integrative structural model of alpha-synuclein compact states bound to membrane mimics (PDB ID: 9A1H, PDB-Dev ID: PDBDEV_00000089)

1. Model Composition	
Entry composition	alpha-synuclein: chain(s) A, B (110 residues)
Datasets used for modeling	- Crosslinking-MS data, PRIDE: PXD027349 - NMR data, BMRB: 50996
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 2
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: EDC, 3 crosslinks
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	5
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	- Clashscore: 4.97-20.54 - Ramachandran outliers: 0-6 - Sidechain outliers: 0-2
Fit to data used for modeling	Satisfaction of crosslinks: 0.00-0.00%
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. Name	Simulated annealing of the monomer
Method	Simulated Annealing

<i>Number of computed models</i>	2700
2. <i>Name</i>	Simulated annealing of the dimer
<i>Method</i>	Simulated Annealing
<i>Number of computed models</i>	1500
<i>Software</i>	XPLOR-NIH (version 1.49)