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 B (110 residues) - alpha-synuclein: Chain A (110 residues)
Datasets used for modeling	- Crosslinking-MS data, Linker name and number of cross-links: EDC, 3 cross-links - NMR data, BMRB: 50996
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 2
Flexible units	- A: 1-110 - B: 1-110
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: EDC, 3 cross-links
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	5
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 = 9.63, Number of Ramachandran outliers = 5, Number of sidechain outliers = 0 - Model-2: Clashscore = 18.98, Number of Ramachandran outliers = 2, Number of sidechain outliers = 1 - Model-3: Clashscore = 20.54, Number of Ramachandran outliers = 3, Number of sidechain outliers = 0 - Model-4: Clashscore = 18.67, Number of Ramachandran outliers = 2, Number of sidechain outliers = 1 - Model-5: Clashscore = 4.97, Number of Ramachandran outliers = 3, Number of sidechain outliers = 3
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	Simulated annealing of the monomer
Name	Simulated Annealing
Number of computed models	2700
2. Method	Simulated annealing of the dimer
Name	Simulated Annealing
Number of computed models	1500
Software	XPLOR-NIH (version 1.49)