

Summary of integrative structure determination of The structural models of alpha-synuclein dimer (PDB ID: 9A1Q, PDB-Dev ID: PDBDEV_00000098)

1. Model Composition	
Entry composition	alpha-synuclein: chain(s) A, B (140 residues)
Datasets used for modeling	- Crosslinking-MS data, PRIDE: PXD030299 - De Novo model, Not available
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: BS3, 1 crosslinks - 1 unique CrossLinkRestraint: Other, 0 crosslinks
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	8
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	- Clashscore: 0.00-0.00 - Ramachandran outliers: 51-71 - Sidechain outliers: 45-62
Fit to data used for modeling	Satisfaction of crosslinks: 75.80-88.54%
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	Design square-well functions based on cross-linking constraints

<i>Description</i>	At this step, cross-linking constraints are collected from experiments and used to design square-well functions for DMD simulations.
2. <i>Name</i>	Perform DMD simulations
<i>Description</i>	At this step, the designed square-well functions are incorporated into the force field. Start DMD simulations.
<i>Software</i>	DMD software (version Not available)