

Summary of integrative structure determination of The ensemble structure of alpha-synuclein monomer (PDB ID: 9A1A, PDB-Dev ID: PDBDEV_00000082)

1. Model Composition	
Entry composition	alpha-synuclein: chain(s) A (140 residues)
Datasets used for modeling	- Other, Not available: 10.1016/j.jmb.2010.11.011
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 1
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	
4. Validation	
Number of ensembles	8
Number of models in ensembles	None, None, None, None, None, None, None, None
Number of deposited models	8
Model precision (uncertainty of models)	<ul style="list-style-type: none"> - Not available - Not available - Not available - Not available - Not available - Not available - Not available - Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 7.94-17.37 - Ramachandran outliers: 22-33 - Sidechain outliers: 20-27
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. <i>Name</i>	Discrete molecular dynamics simulations
<i>Method</i>	None
<i>Number of computed models</i>	30303
<i>Software</i>	<ul style="list-style-type: none">- piDMD (version Not available)- TTClust (version Not available)