

**Summary of integrative structure determination of The structural models of alpha-synuclein dimer (PDB ID: 9A1Q, PDB-Dev ID: PDBDEV\_0000098)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	- alpha-synuclein: Chain A (140 residues) - alpha-synuclein: Chain B (140 residues)
<a href="#">Datasets used for modeling</a>	- Crosslinking-MS data, Linker name and number of cross-links: BS3, 1 cross-links - De Novo model, Not available
<b>2. Representation</b>	
<a href="#">Resolution</a>	Atomic
<a href="#">Number of rigid bodies, flexible units</a>	0, 2
<a href="#">Flexible units</a>	- A: 1-140 - B: 1-140
<a href="#">Structural coverage (rigid bodies)</a>	100%
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	- 1 unique CrossLinkRestraint: BS3, 1 cross-links - 1 unique CrossLinkRestraint: Other, 0 cross-links
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	0
<a href="#">Number of models in ensembles</a>	Not applicable
<a href="#">Number of deposited models</a>	8
<a href="#">Model precision (uncertainty of models)</a>	Model precision can not be calculated with one structure
<a href="#">Data quality</a>	Data quality has not been assessed

<a href="#">Model quality: assessment of atomic segments</a>	<ul style="list-style-type: none"> <li>- Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 59, Number of sidechain outliers = 52</li> <li>- Model-2: Clashscore = 0.0, Number of Ramachandran outliers = 63, Number of sidechain outliers = 52</li> <li>- Model-3: Clashscore = 0.0, Number of Ramachandran outliers = 71, Number of sidechain outliers = 51</li> <li>- Model-4: Clashscore = 0.0, Number of Ramachandran outliers = 65, Number of sidechain outliers = 52</li> <li>- Model-5: Clashscore = 0.0, Number of Ramachandran outliers = 67, Number of sidechain outliers = 54</li> <li>- Model-6: Clashscore = 0.0, Number of Ramachandran outliers = 56, Number of sidechain outliers = 47</li> <li>- Model-7: Clashscore = 0.0, Number of Ramachandran outliers = 65, Number of sidechain outliers = 49</li> <li>- Model-8: Clashscore = 0.0, Number of Ramachandran outliers = 51, Number of sidechain outliers = 55</li> </ul>
<a href="#">Model quality: assessment of excluded volume</a>	Not applicable
<a href="#">Fit to data used for modeling</a>	Fit of model to information used to compute it has not been determined
<a href="#">Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#">Method</a>	Design square-well functions based on cross-linking constraints
<a href="#">Name</a>	None
<a href="#">Description</a>	At this step, cross-linking constraints are collected from experiments and used to design square-well functions for DMD simulations.
2. <a href="#">Method</a>	Perform DMD simulations
<a href="#">Name</a>	None
<a href="#">Description</a>	At this step, the designed square-well functions are incorporated into the force field. Start DMD simulations.
<a href="#">Software</a>	<a href="#">DMD software</a> (version Not available)