

Summary of integrative structure determination of Structure of SH3 domain from chicken alpha spectrin determined using restraints from solid-state NMR (PDB ID: 9A3E, PDB-Dev ID: PDBDEV_00000199)

1. Model Composition	
Entry composition	spectrin alpha chain: chain(s) A (62 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 2NUZ - Experimental model, PDB: 6SCW - NMR data, BMRB: 34785 - Experimental model, PDB: 8CF4
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 3
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 2 unique DerivedDistanceRestraint: Upper Bound Distance: 4.882
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	16
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 0.00-1.96 - Ramachandran outliers: 0-3 - Sidechain outliers: 0-6
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. Name	modeling

<i>Method</i>	Restrained Molecular Dynamics Simulation
<i>Number of computed models</i>	256000
<i>Software</i>	GROMACS (version 2019.2)