

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 A (62 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB ID: 2NUZ - Experimental model, PDB ID: 6SCW - NMR data, BMRB: 34785 - Experimental model, PDB ID: 8CF4
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 3
Flexible units	A: 1-6, 7-61, 62-62
Structural coverage (rigid bodies)	100%
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)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed

<p><i>Model quality: assessment of atomic segments</i></p>	<ul style="list-style-type: none"> - Model-1: Clashscore = 0.98, Number of Ramachandran outliers = 1, Number of sidechain outliers = 1 - Model-2: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 6 - Model-3: Clashscore = 0.0, Number of Ramachandran outliers = 2, Number of sidechain outliers = 1 - Model-4: Clashscore = 0.98, Number of Ramachandran outliers = 2, Number of sidechain outliers = 0 - Model-5: Clashscore = 1.96, Number of Ramachandran outliers = 1, Number of sidechain outliers = 1 - Model-6: Clashscore = 0.0, Number of Ramachandran outliers = 2, Number of sidechain outliers = 3 - Model-7: Clashscore = 1.96, Number of Ramachandran outliers = 3, Number of sidechain outliers = 0 - Model-8: Clashscore = 0.98, Number of Ramachandran outliers = 1, Number of sidechain outliers = 2 - Model-9: Clashscore = 1.96, Number of Ramachandran outliers = 2, Number of sidechain outliers = 3 - Model-10: Clashscore = 0.98, Number of Ramachandran outliers = 2, Number of sidechain outliers = 0 - Model-11: Clashscore = 1.96, Number of Ramachandran outliers = 1, Number of sidechain outliers = 1 - Model-12: Clashscore = 0.98, Number of Ramachandran outliers = 1, Number of sidechain outliers = 0 - Model-13: Clashscore = 0.98, Number of Ramachandran outliers = 1, Number of sidechain outliers = 1 - Model-14: Clashscore = 1.96, Number of Ramachandran outliers = 0, Number of sidechain outliers = 1 - Model-15: Clashscore = 1.96, Number of Ramachandran outliers = 0, Number of sidechain outliers = 2 - Model-16: Clashscore = 0.0, Number of Ramachandran outliers = 1, Number of sidechain outliers = 2
<p><i>Model quality: assessment of excluded volume</i></p>	<p>Not applicable</p>
<p><i>Fit to data used for modeling</i></p>	<p>Fit of model to information used to compute it has not been determined</p>
<p><i>Fit to data used for validation</i></p>	<p>Fit of model to information not used to compute it has not been determined</p>
<p>5. Methodology and Software</p>	
<p><i>1. Method</i></p>	<p>modeling</p>

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