

Summary of integrative structure determination of Driving Integrative Structural Modeling with Serial Capture Affinity Purification (PDB ID: 9A0P, PDB-Dev ID: PDBDEV_00000061)

1. Model Composition	
<u>Entry composition</u>	<ul style="list-style-type: none"> - SPINDOC: Chain C (381 residues) - SPINDOC: Chain B (381 residues) - SPIN1: Chain A (203 residues)
<u>Datasets used for modeling</u>	<ul style="list-style-type: none"> - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 21 cross-links - Experimental model, PDB ID: 4MZF - De Novo model, Not available
2. Representation	
<u>Resolution</u>	Atomic
<u>Number of rigid bodies, flexible units</u>	0, 3
<u>Flexible units</u>	<ul style="list-style-type: none"> - A: 1-203 - B: 1-381 - C: 1-381
<u>Structural coverage (rigid bodies)</u>	100%
3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSSO, 21 cross-links
4. Validation	
<u>Number of ensembles</u>	0
<u>Number of models in ensembles</u>	Not applicable
<u>Number of deposited models</u>	1
<u>Model precision (uncertainty of models)</u>	Model precision can not be calculated with one structure
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of atomic segments</u>	Model-1: Clashscore = 20.06, Number of Ramachandran outliers = 92, Number of sidechain outliers = 196
<u>Model quality: assessment of excluded volume</u>	Not applicable

<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <u>Method</u>	ab initio modeling of SPINDOC
<u>Name</u>	None
2. <u>Method</u>	integrative modeling of SPIN1-SPINDOC complex
<u>Name</u>	None
<u>Software</u>	<ul style="list-style-type: none"> - HADDOCK (version Not available) - I-TASSER (version Not available)