

Summary of integrative structure determination of Integrative model of ROCA-ROCA2 by crosslinking MS and deep learning (PDB ID: 9A6G, PDB-Dev ID: PDBDEV_00000309)

1. Model Composition	
Entry composition	- ROCA_BACSU: Chain A (515 residues) - ROCA2_BACSU: Chain B (515 residues)
Datasets used for modeling	Crosslinking-MS data, Linker name and number of cross-links: SDA, 2 cross-links
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 2
Flexible units	- A: 1-515 - B: 1-515
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: SDA, 2 cross-links
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	Model-1: Clashscore = 0.63, Number of Ramachandran outliers = 2, Number of sidechain outliers = 2
Model quality: assessment of excluded volume	Not applicable
Fit to data used for modeling	Fit of model to information used to compute it has not been determined

<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Method</i>	AlphaLink2
<i>Name</i>	AlphaLink2
<i>Number of computed models</i>	1
<i>Software</i>	AlphaLink2 (version 1.0)