

**Summary of integrative structure determination of Integrative model of RPOA-RPOC by crosslinking MS and deep learning (PDB ID: 9A4W, PDB-Dev ID: PDBDEV\_00000253)**

<b>1. Model Composition</b>	
<a href="#"><u>Entry composition</u></a>	- RPOC_BACSU: Chain B (1199 residues) - RPOA_BACSU: Chain A (314 residues)
<a href="#"><u>Datasets used for modeling</u></a>	Crosslinking-MS data, Linker name and number of cross-links: SDA, 4 cross-links
<b>2. Representation</b>	
<a href="#"><u>Resolution</u></a>	Atomic
<a href="#"><u>Number of rigid bodies, flexible units</u></a>	0, 2
<a href="#"><u>Flexible units</u></a>	- A: 1-314 - B: 1-1199
<a href="#"><u>Structural coverage (rigid bodies)</u></a>	100%
<b>3. Restraints</b>	
<a href="#"><u>Physical principles</u></a>	Information about physical principles was not provided
<a href="#"><u>Experimental data</u></a>	- 1 unique CrossLinkRestraint: SDA, 4 cross-links
<b>4. Validation</b>	
<a href="#"><u>Number of ensembles</u></a>	0
<a href="#"><u>Number of models in ensembles</u></a>	Not applicable
<a href="#"><u>Number of deposited models</u></a>	1
<a href="#"><u>Model precision (uncertainty of models)</u></a>	Model precision can not be calculated with one structure
<a href="#"><u>Data quality</u></a>	Data quality has not been assessed
<a href="#"><u>Model quality: assessment of atomic segments</u></a>	Model-1: Clashscore = 1.83, Number of Ramachandran outliers = 1, Number of sidechain outliers = 58
<a href="#"><u>Model quality: assessment of excluded volume</u></a>	Not applicable
<a href="#"><u>Fit to data used for modeling</u></a>	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
<b>5. Methodology and Software</b>	
1. <u>Method</u>	AlphaLink2
<u>Name</u>	AlphaLink2
<u>Number of computed models</u>	1
<u>Software</u>	<a href="#">AlphaLink2</a> (version 1.0)