

**Summary of integrative structure determination of Integrative model of ATPA-ATPG by crosslinking MS and deep learning (PDB ID: 9A4F, PDB-Dev ID: PDBDEV\_00000236)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	- ATPA_BACSU: chain(s) A (502 residues) - ATPG_BACSU: chain(s) B (287 residues)
<a href="#">Datasets used for modeling</a>	- Crosslinking-MS data, PRIDE: <a href="#">PXD035508</a>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Atomic
Number of <a href="#">rigid</a> and <a href="#">flexible</a> segments	0, 2
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	- 1 unique CrossLinkRestraint: SDA, 1 crosslinks
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	0
<a href="#">Number of models in ensembles</a>	Not applicable
<a href="#">Number of deposited models</a>	1
<a href="#">Model precision (uncertainty of models)</a>	Not available
<a href="#">Data quality</a>	Data quality has not been assessed
<a href="#">Model quality: assessment of atomic segments</a>	- Clashscore: 1.15 - Ramachandran outliers: 7 - Sidechain outliers: 16
<a href="#">Fit to data used for modeling</a>	Satisfaction of crosslinks: 100.00%
<a href="#">Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#">Name</a>	AlphaLink2
<a href="#">Method</a>	AlphaLink2

---

<a href="#"><i>Number of computed models</i></a>	1
<a href="#"><i>Software</i></a>	<a href="#">AlphaLink2</a> (version 1.0)