

**Summary of integrative structure determination of Integrative model of ATPA-ATPG by crosslinking MS and deep learning (PDB ID: 9A4F, PDB-Dev ID: PDBDEV\_0000236)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	- ATPA_BACSU: Chain A (502 residues) - ATPG_BACSU: Chain B (287 residues)
<a href="#">Datasets used for modeling</a>	Crosslinking-MS data, Linker name and number of cross-links: SDA, 1 cross-links
<b>2. Representation</b>	
<a href="#">Resolution</a>	Atomic
<a href="#">Number of rigid bodies, flexible units</a>	0, 2
<a href="#">Flexible units</a>	- A: 1-502 - B: 1-287
<a href="#">Structural coverage (rigid bodies)</a>	100%
<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 cross-links
<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>	Model precision can not be calculated with one structure
<a href="#">Data quality</a>	Data quality has not been assessed
<a href="#">Model quality: assessment of atomic segments</a>	Model-1: Clashscore = 1.15, Number of Ramachandran outliers = 7, Number of sidechain outliers = 16
<a href="#">Model quality: assessment of excluded volume</a>	Not applicable
<a href="#">Fit to data used for modeling</a>	Fit of model to information used to compute it has not been determined

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<a href="#"><i>Fit to data used for validation</i></a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#"><i>Method</i></a>	AlphaLink2
<a href="#"><i>Name</i></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)