

**Summary of integrative structure determination of Model of E. coli btuB by in-cell photo-crosslinking MS and deep learning (PDB ID: 9A30, PDB-Dev ID: PDBDEV\_00000185)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	P06129: chain(s) A (614 residues)
<a href="#">Datasets used for modeling</a>	- Crosslinking-MS data, jPOSTrepo: JPST001851
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Atomic
<a href="#">Number of <i>rigid</i> and <i>flexible</i> segments</a>	0, 1
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	- 1 unique CrossLinkRestrict: L-Photo-Leucine, 7 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>	10
<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: 1.91-6.16 - Ramachandran outliers: 7-25 - Sidechain outliers: 6-15
<a href="#">Fit to data used for modeling</a>	Satisfaction of crosslinks: 42.86-71.43%
<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>	
<a href="#">1. Name</a>	AlphaLink
<a href="#">Method</a>	AlphaLink with 10 msa subsamples

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<a href="#"><i>Number of computed models</i></a>	10
<a href="#"><i>Software</i></a>	<a href="#">AlphaLink</a> (version 1.0)