

Summary of integrative structure determination of Model of E. coli TolB by in-cell photo-crosslinking MS and deep learning (PDB ID: 9A2L, PDB-Dev ID: PDBDEV_00000170)

1. Model Composition	
Entry composition	P0A855: Chain A (430 residues)
Datasets used for modeling	Crosslinking-MS data, Linker name and number of cross-links: L-Photo-Leucine, 6 cross-links
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 1
Flexible units	A: 1-430
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: L-Photo-Leucine, 6 cross-links
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	10
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed

<p><i>Model quality: assessment of atomic segments</i></p>	<ul style="list-style-type: none"> - Model-1: Clashscore = 2.49, Number of Ramachandran outliers = 5, Number of sidechain outliers = 4 - Model-2: Clashscore = 2.03, Number of Ramachandran outliers = 7, Number of sidechain outliers = 6 - Model-3: Clashscore = 2.34, Number of Ramachandran outliers = 3, Number of sidechain outliers = 7 - Model-4: Clashscore = 2.03, Number of Ramachandran outliers = 8, Number of sidechain outliers = 7 - Model-5: Clashscore = 1.71, Number of Ramachandran outliers = 8, Number of sidechain outliers = 4 - Model-6: Clashscore = 2.96, Number of Ramachandran outliers = 3, Number of sidechain outliers = 5 - Model-7: Clashscore = 2.96, Number of Ramachandran outliers = 1, Number of sidechain outliers = 5 - Model-8: Clashscore = 1.25, Number of Ramachandran outliers = 7, Number of sidechain outliers = 4 - Model-9: Clashscore = 1.4, Number of Ramachandran outliers = 4, Number of sidechain outliers = 4 - Model-10: Clashscore = 2.34, Number of Ramachandran outliers = 6, Number of sidechain outliers = 6
<p><i>Model quality: assessment of excluded volume</i></p>	<p>Not applicable</p>
<p><i>Fit to data used for modeling</i></p>	<p>Fit of model to information used to compute it has not been determined</p>
<p><i>Fit to data used for validation</i></p>	<p>Fit of model to information not used to compute it has not been determined</p>
<p>5. Methodology and Software</p>	
<p>1. <i>Method</i></p>	<p>AlphaLink</p>
<p><i>Name</i></p>	<p>AlphaLink with 10 msa subsamples</p>
<p><i>Number of computed models</i></p>	<p>10</p>
<p><i>Software</i></p>	<p>AlphaLink (version 1.0)</p>