

**Summary of integrative structure determination of Model of E. coli fhuA by in-cell photo-crosslinking MS and deep learning (PDB ID: 9A31, PDB-Dev ID: PDBDEV\_00000186)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	P06971: Chain A (747 residues)
<a href="#">Datasets used for modeling</a>	Crosslinking-MS data, Linker name and number of cross-links: L-Photo-Leucine, 28 cross-links
<b>2. Representation</b>	
<a href="#">Resolution</a>	Atomic
Number of <a href="#">rigid bodies</a> , <a href="#">flexible units</a>	0, 1
<a href="#">Flexible units</a>	A: 1-747
<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: L-Photo-Leucine, 28 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>	10
<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

<p><a href="#"><i>Model quality: assessment of atomic segments</i></a></p>	<ul style="list-style-type: none"> <li>- Model-1: Clashscore = 8.19, Number of Ramachandran outliers = 42, Number of sidechain outliers = 17</li> <li>- Model-2: Clashscore = 2.73, Number of Ramachandran outliers = 15, Number of sidechain outliers = 16</li> <li>- Model-3: Clashscore = 7.31, Number of Ramachandran outliers = 21, Number of sidechain outliers = 11</li> <li>- Model-4: Clashscore = 4.67, Number of Ramachandran outliers = 24, Number of sidechain outliers = 5</li> <li>- Model-5: Clashscore = 6.17, Number of Ramachandran outliers = 15, Number of sidechain outliers = 17</li> <li>- Model-6: Clashscore = 4.76, Number of Ramachandran outliers = 28, Number of sidechain outliers = 6</li> <li>- Model-7: Clashscore = 11.89, Number of Ramachandran outliers = 12, Number of sidechain outliers = 21</li> <li>- Model-8: Clashscore = 8.72, Number of Ramachandran outliers = 41, Number of sidechain outliers = 11</li> <li>- Model-9: Clashscore = 4.76, Number of Ramachandran outliers = 16, Number of sidechain outliers = 7</li> <li>- Model-10: Clashscore = 5.46, Number of Ramachandran outliers = 13, Number of sidechain outliers = 11</li> </ul>
<p><a href="#"><i>Model quality: assessment of excluded volume</i></a></p>	<p>Not applicable</p>
<p><a href="#"><i>Fit to data used for modeling</i></a></p>	<p>Fit of model to information used to compute it has not been determined</p>
<p><a href="#"><i>Fit to data used for validation</i></a></p>	<p>Fit of model to information not used to compute it has not been determined</p>
<p><b>5. Methodology and Software</b></p>	
<p>1. <a href="#"><i>Method</i></a></p>	<p>AlphaLink</p>
<p><a href="#"><i>Name</i></a></p>	<p>AlphaLink with 10 msa subsamples</p>
<p><a href="#"><i>Number of computed models</i></a></p>	<p>10</p>
<p><a href="#"><i>Software</i></a></p>	<p><a href="#">AlphaLink</a> (version 1.0)</p>