

**Summary of integrative structure determination of Model of E. coli MlaD by in-cell photo-crosslinking MS and deep learning (PDB ID: 9A3A, PDB-Dev ID: PDBDEV\_00000195)**

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|---|---|
| <b>1. Model Composition</b>   |   |
| <a href="#">Entry composition</a>                                   | P64604: chain(s) A (183 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 CrossLinkRestraint: L-Photo-Leucine, 2 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: 0.36-2.53<br>- Ramachandran outliers: 4-13<br>- Sidechain outliers: 2-6 |
| <a href="#">Fit to data used for modeling</a>                       | Satisfaction of crosslinks: 0.00-50.00%   |
| <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>                                  |   |
| <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) |