

Summary of integrative structure determination of Model of E. coli TolC by in-cell photo-crosslinking MS and deep learning (PDB ID: 9A2X, PDB-Dev ID: PDBDEV_00000182)

1. Model Composition	
Entry composition	P02930: chain(s) A (493 residues)
Datasets used for modeling	- Crosslinking-MS data, jPOSTrepo: JPST001851
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 1
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: L-Photo-Leucine, 5 crosslinks
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	10
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	- Clashscore: 0.13-4.66 - Ramachandran outliers: 3-17 - Sidechain outliers: 4-11
Fit to data used for modeling	Satisfaction of crosslinks: 0.00-20.00%
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Name	AlphaLink
Method	AlphaLink with 10 msa subsamples
Number of computed models	10

[Software](#)

[AlphaLink](#) (version 1.0)