Summary of integrative structure determination of Model of E. coli OmpA by in-cell photo-crosslinking MS and deep learning (PDB ID: 9A2M, PDB-Dev ID: PDBDEV_00000171)

1. Model Composition	
Entry composition	P0A910: chain(s) A (346 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, 151 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: 0.77-9.26 - Ramachandran outliers: 13-47 - Sidechain outliers: 4-13
Fit to data used for modeling	Satisfaction of crosslinks: 15.23-26.49%
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)

IM Summary Table