

Summary of integrative structure determination of Integrative model of YXKC-DACA by crosslinking MS and deep learning (PDB ID: 9A4Z, PDB-Dev ID: PDBDEV_00000256)

1. Model Composition	
Entry composition	- YXKC_BACSU: chain(s) A (180 residues) - DACA_BACSU: chain(s) B (443 residues)
Datasets used for modeling	- Crosslinking-MS data, PRIDE: PXD035508
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 2
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: SDA, 1 crosslinks
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	- Clashscore: 0.52 - Ramachandran outliers: 10 - Sidechain outliers: 9
Fit to data used for modeling	Satisfaction of crosslinks: 0.00%
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	AlphaLink2
Method	AlphaLink2

<i>Number of computed models</i>	1
<i>Software</i>	AlphaLink2 (version 1.0)