

Summary of integrative structure determination of Integrative model of CLPQ-CLPY by crosslinking MS and deep learning (PDB ID: 9A4T | pdb_00009a4t, PDB-Dev ID: PDBDEV_00000250)

1. Model Composition	
1.1. Entry composition	- CLPQ_BACSU: chain(s) A (181 residues) - CLPY_BACSU: chain(s) B (467 residues)
1.2. Datasets used for modeling	- Crosslinking-MS data, PRIDE: PXD035508
2. Representation	
2.1. Number of representations	1
2.2. Scale	Atomic
2.3. Number of rigid and flexible segments	0, 2
3. Restraints	
3.1. Physical principles	Information about physical principles was not provided
3.2. Experimental data	- 1 unique CrossLinkRestraint: SDA, 2 crosslinks
4. Validation	
4.2. Number of ensembles	0
4.3. Number of models in ensembles	Not applicable
4.4. Number of deposited models	1
4.5. Model precision	Not available
4.6. Data quality	- PXD035508: 50.00% of crosslinks found in the data. - PXD035508: 0.25% of crosslinks from the data were used for modeling.
4.7. Model quality: assessment of atomic segments	- Clashscore: 1.37 - Ramachandran outliers: 4 - Sidechain outliers: 9
4.8. Fit to data used for modeling	Satisfaction of crosslinks: 100.00%
4.9. 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. 5.1. Method name	AlphaLink2
5.2. Method type	AlphaLink2

<i>5.4. Number of computed models</i>	1
<i>5.5. Software</i>	AlphaLink2 (version 1.0)