

Summary of integrative structure determination of Integrative model of GATB-SUCD by crosslinking MS and deep learning (PDB ID: 9A6E, PDB-Dev ID: PDBDEV_00000307)

1. Model Composition	
<u>Entry composition</u>	- GATB_BACSU: chain(s) A (476 residues) - SUCD_BACSU: chain(s) B (300 residues)
<u>Datasets used for modeling</u>	- Crosslinking-MS data, PRIDE: PXD035508
2. Representation	
<u>Number of representations</u>	1
<u>Scale</u>	Atomic
<u>Number of rigid and flexible segments</u>	0, 2
3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	- 1 unique CrossLinkRestraint: SDA, 1 crosslinks
4. Validation	
<u>Number of ensembles</u>	0
<u>Number of models in ensembles</u>	Not applicable
<u>Number of deposited models</u>	1
<u>Model precision (uncertainty of models)</u>	Not available
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of atomic segments</u>	- Clashscore: 0.33 - Ramachandran outliers: 1 - Sidechain outliers: 4
<u>Fit to data used for modeling</u>	Satisfaction of crosslinks: 0.00%
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<u>1. Name</u>	AlphaLink2
<u>Method</u>	AlphaLink2
<u>Number of computed models</u>	1

[Software](#)

[AlphaLink2](#) (version 1.0)