

Summary of integrative structure determination of Integrative model of PDXS-YPBS by crosslinking MS and deep learning (PDB ID: 9A6V, PDB-Dev ID: PDBDEV_00000324)

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|---|---|
| 1. Model Composition | |
| Entry composition | - PDXS_BACSU: chain(s) A (294 residues) - YPBS_BACSU: chain(s) B (85 residues) |
| Datasets used for modeling | - Crosslinking-MS data, PRIDE: PXD035508 |
| 2. Representation | |
| Number of representations | 1 |
| Scale | Atomic |
| Number of <i>rigid</i> and <i>flexible</i> segments | 0, 2 |
| 3. Restraints | |
| Physical principles | Information about physical principles was not provided |
| Experimental data | - 1 unique CrossLinkRestraint: SDA, 4 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: 1.20 - Ramachandran outliers: 0 - Sidechain outliers: 3 |
| 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 |
| Number of computed models | 1 |

[Software](#)

[AlphaLink2](#) (version 1.0)