

Summary of integrative structure determination of Model of YLAN-FUR by crosslinking MS and deep learning (PDB ID: 9A4A, PDB-Dev ID: PDBDEV_00000231)

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| 1. Model Composition | |
| Entry composition | - YLAN_BACSU: chain(s) A (93 residues) - FUR_BACSU: chain(s) B (149 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, 2 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: 1.52 - Ramachandran outliers: 2 - Sidechain outliers: 5 |
| Fit to data used for modeling | Satisfaction of crosslinks: 100.00% |
| 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 |

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