

Summary of integrative structure determination of Integrative model of BUK-SYGB by crosslinking MS and deep learning (PDB ID: 9A71, PDB-Dev ID: PDBDEV_00000330)

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| 1. Model Composition | |
| Entry composition | - SYGB_BACSU: Chain B (679 residues) - BUK_BACSU: Chain A (363 residues) |
| Datasets used for modeling | Crosslinking-MS data, Linker name and number of cross-links: SDA, 1 cross-links |
| 2. Representation | |
| Resolution | Atomic |
| Number of rigid bodies, flexible units | 0, 2 |
| Flexible units | - A: 1-363 - B: 1-679 |
| Structural coverage (rigid bodies) | 100% |
| 3. Restraints | |
| Physical principles | Information about physical principles was not provided |
| Experimental data | - 1 unique CrossLinkRestraint: SDA, 1 cross-links |
| 4. Validation | |
| Number of ensembles | 0 |
| Number of models in ensembles | Not applicable |
| Number of deposited models | 1 |
| Model precision (uncertainty of models) | Model precision can not be calculated with one structure |
| Data quality | Data quality has not been assessed |
| Model quality: assessment of atomic segments | Model-1: Clashscore = 0.86, Number of Ramachandran outliers = 0, Number of sidechain outliers = 13 |
| Model quality: assessment of excluded volume | Not applicable |
| Fit to data used for modeling | Fit of model to information used to compute it has not been determined |

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| <i>Fit to data used for validation</i> | Fit of model to information not used to compute it has not been determined |
| 5. Methodology and Software | |
| 1. <i>Method</i> | AlphaLink2 |
| <i>Name</i> | AlphaLink2 |
| <i>Number of computed models</i> | 1 |
| <i>Software</i> | AlphaLink2 (version 1.0) |