

**Summary of integrative structure determination of Integrative model of MURA2-MURA1 by crosslinking MS and deep learning (PDB ID: 9A7B, PDB-Dev ID: PDBDEV\_00000340)**

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|---|--|
| <b>1. Model Composition</b>   |  |
| <a href="#">Entry composition</a>                                     | - MURA2_BACSU: chain(s) A (429 residues)<br>- MURA1_BACSU: chain(s) B (436 residues) |
| <a href="#">Datasets used for modeling</a>                            | - Crosslinking-MS data, PRIDE: <a href="#">PXD035508</a>                             |
| <b>2. Representation</b>  |  |
| <a href="#">Number of representations</a>                             | 1  |
| <a href="#">Scale</a>   | Atomic   |
| Number of <a href="#">rigid</a> and <a href="#">flexible</a> segments | 0, 2   |
| <b>3. Restraints</b>  |  |
| <a href="#">Physical principles</a>                                   | Information about physical principles was not provided                               |
| <a href="#">Experimental data</a>                                     | - 1 unique CrossLinkRestraint: SDA, 1 crosslinks                                     |
| <b>4. Validation</b>  |  |
| <a href="#">Number of ensembles</a>                                   | 0  |
| <a href="#">Number of models in ensembles</a>                         | Not applicable   |
| <a href="#">Number of deposited models</a>                            | 1  |
| <a href="#">Model precision (uncertainty of models)</a>               | Not available  |
| <a href="#">Data quality</a>  | Data quality has not been assessed   |
| <a href="#">Model quality: assessment of atomic segments</a>          | - Clashscore: 1.22<br>- Ramachandran outliers: 1<br>- Sidechain outliers: 3          |
| <a href="#">Fit to data used for modeling</a>                         | Satisfaction of crosslinks: 0.00%  |
| <a href="#">Fit to data used for validation</a>                       | Fit of model to information not used to compute it has not been determined           |
| <b>5. Methodology and Software</b>                                    |  |
| 1. <a href="#">Name</a>   | AlphaLink2   |
| <a href="#">Method</a>  | AlphaLink2   |

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| <a href="#"><i>Number of computed models</i></a> | 1  |
| <a href="#"><i>Software</i></a>                  | <a href="#">AlphaLink2</a> (version 1.0) |