

**Summary of integrative structure determination of Integrative model of ODPB-ODPA by crosslinking MS and deep learning (PDB ID: 9A70, PDB-Dev ID: PDBDEV\_00000329)**

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| <b>1. Model Composition</b>                                  |   |
| <a href="#">Entry composition</a>                            | - ODPB_BACSU: Chain B (325 residues)<br>- ODPB_BACSU: Chain A (371 residues)                      |
| <a href="#">Datasets used for modeling</a>                   | Crosslinking-MS data, Linker name and number of cross-links: SDA, 9 cross-links                   |
| <b>2. Representation</b>                                     |   |
| <a href="#">Resolution</a>                                   | Atomic  |
| <a href="#">Number of rigid bodies, flexible units</a>       | 0, 2  |
| <a href="#">Flexible units</a>                               | - A: 1-371<br>- B: 1-325  |
| <a href="#">Structural coverage (rigid bodies)</a>           | 100%  |
| <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, 9 cross-links   |
| <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>      | Model precision can not be calculated with one structure  |
| <a href="#">Data quality</a>                                 | Data quality has not been assessed  |
| <a href="#">Model quality: assessment of atomic segments</a> | Model-1: Clashscore = 0.46, Number of Ramachandran outliers = 3, Number of sidechain outliers = 1 |
| <a href="#">Model quality: assessment of excluded volume</a> | Not applicable  |
| <a href="#">Fit to data used for modeling</a>                | Fit of model to information used to compute it has not been determined                            |

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