# Summary of integrative structure determination of Integrative model of ATPA-ATPB by crosslinking MS and deep learning (PDB ID: 9A4G, PDB-Dev ID: PDBDEV_00000237)

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| ***1. Model Composition*** | |
| *Entry composition* | - ATPA_BACSU: Chain A (502 residues)<br>- ATPB_BACSU: Chain B (473 residues) |
| *Datasets used for modeling* | Crosslinking-MS data, Linker name and number of cross-links: SDA, 4 cross-links |
| ***2. Representation*** | |
| *Resolution* | Atomic |
| *Number of rigid bodies, flexible units* | 0, 2 |
| *Flexible units* | - A: 1-502<br>- B: 1-473 |
| *Structural coverage (rigid bodies)* | 100% |
| ***3. Restraints*** | |
| *Physical principles* | Information about physical principles was not provided |
| *Experimental data* | - 1 unique CrossLinkRestraint: SDA, 4 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 = 1.07, Number of Ramachandran outliers = 5, Number of sidechain outliers = 17 |
| *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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| *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. Method* | AlphaLink2 |
| *Name* | AlphaLink2 |
| *Number of computed models* | 1 |
| *Software* | AlphaLink2 (version 1.0) |