**Summary of integrative structure determination of Integrative structure of the XcpHIJK quaternary complex of a type II secretion system pseudopilin (PDB ID: 9A1E, PDB-Dev ID: PDBDEV_00000086)**

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| ***1. Model Composition*** | |
| *Entry composition* | - XcpH: chain(s) A (131 residues)<br>- XcpI: chain(s) B (89 residues)<br>- XcpJ: chain(s) C (162 residues)<br>- XcpK: chain(s) D (273 residues) |
| *Datasets used for modeling* | - Experimental model, PDB: 5VTM<br>- NMR data, BMRB: 50449<br>- Crosslinking-MS data, MASSIVE: MSV000086915<br>- Comparative model, Not available<br>- Experimental model, PDB: 2QV8 |
| ***2. Representation*** | |
| *Number of representations* | 1 |
| *Scale* | Atomic |
| *Number of rigid and flexible segments* | 4, 0 |
| ***3. Restraints*** | |
| *Physical principles* | Information about physical principles was not provided |
| *Experimental data* | - 1 unique CrossLinkRestraint: ADH, 14 crosslinks<br>- 25 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 6.0-18.0 |
| ***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: 0.00<br>- Ramachandran outliers: 4<br>- Sidechain outliers: 46 |
| *Fit to data used for modeling* | Satisfaction of crosslinks: 28.57% |
| *Fit to data used for validation* | Fit of model to information not used to compute it has not been determined |

| ***5. Methodology and Software*** | |
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| *1. Name* | XcpH modeling |
| *2. Name* | Docking |
| *Method* | HADDOCK |
| *Number of computed models* | 1000 |
| *Software* | - Pymol (version Not available)<br>- Haddock (version Not available)<br>- Phyre2 (version Not available) |