Summary of integrative structure determination of Integrative structure of the XcpGHIJK pseudo pilus filament model of a type II secretion system (PDB ID: 9A1F, PDB-Dev ID: PDBDEV_00000087)

1. Model Composition	
Entry composition	- XcpG: Chain L (134 residues) - XcpJ: Chain S (199 residues) - XcpG: Chain H (134 residues) - XcpG: Chain K (134 residues) - XcpI: Chain R (120 residues) - XcpK: Chain T (309 residues) - XcpG: Chain C (134 residues) - XcpG: Chain G (134 residues) - XcpG: Chain P (134 residues) - XcpG: Chain A (134 residues) - XcpG: Chain N (134 residues) - XcpG: Chain E (134 residues) - XcpG: Chain J (134 residues) - XcpG: Chain I (134 residues) - XcpG: Chain O (134 residues) - XcpG: Chain M (134 residues) - XcpH: Chain Q (161 residues) - XcpG: Chain D (134 residues) - XcpG: Chain B (134 residues) - XcpG: Chain F (134 residues)
Datasets used for modeling	- Experimental model, PDB ID: 5VTM - NMR data, BMRB: 50449 - Crosslinking-MS data, Linker name and number of cross-links: ADH, 14 cross-links - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 2QV8 - Experimental model, PDB ID: 2KEP - Integrative model, PDB-Dev: PDBDEV_00000086
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	40, 0

Rigid bodies	- A: 1-24:None, 25-134 - B: 1-24:None, 25-134 - C: 1-24:None, 25-134 - D: 1-24:None, 25-134 - E: 1-24:None, 25-134 - F: 1-24:None, 25-134 - G: 1-24:None, 25-134 - H: 1-24:None, 25-134 - I: 1-24:None, 25-134 - J: 1-24:None, 25-134 - K: 1-24:None, 25-134 - L: 1-24:None, 25-134 - M: 1-24:None, 25-134 - N: 1-24:None, 25-134 - O: 1-24:None, 25-134 - P: 1-24:None, 25-134 - Q: 1-30:None, 31-161 - R: 1-31:None, 32-120 - S: 1-37:None, 38-199 - T: 1-36:None, 37-309
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: ADH, 14 cross-links - 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)	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 = 0.0, Number of Ramachandran outliers = 19, 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
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	Docking
Name	HADDOCK
Number of computed models	1000
2. Method	Helix models
Name	Homology modeling
3. Method	Add helices
Name	Manual modeling
4. Method	Modeling Helices
Name	Semi-Manual modeling
Number of computed models	300
5. Method	Create XcpG filament
Name	Manual modeling
6. Method	Minimize filament
Name	Minimization
Number of computed models	10
Software	- Pymol (version Not available) - Haddock (version Not available) - Python (version Not available) - pyRosetta (version Not available) - Phyre2 (version Not available)