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(s) A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P (134 residues) - XcpH: chain(s) Q (161 residues) - XcpI: chain(s) R (120 residues) - XcpJ: chain(s) S (199 residues) - XcpK: chain(s) T (309 residues)
Datasets used for modeling	- Experimental model, PDB: 5VTM - NMR data, BMRB: 50449 - Crosslinking-MS data, MASSIVE: MSV000086915 - Comparative model, Not available - Experimental model, PDB: 2QV8 - Experimental model, PDB: 2KEP - Integrative model, PDB: 9A1E
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	40, 0
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: ADH, 14 crosslinks - 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 - Ramachandran outliers: 19 - Sidechain outliers: 13
Fit to data used for modeling	Satisfaction of crosslinks: 7.14%
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. Name	Docking
Method	HADDOCK
Number of computed models	1000
2. Name	Helix models
3. Name	Add helices
4. Name	Modeling Helices
Method	Semi-Manual modeling
Number of computed models	300
5. Name	Create XcpG filament
6. Name	Minimize filament
Method	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)