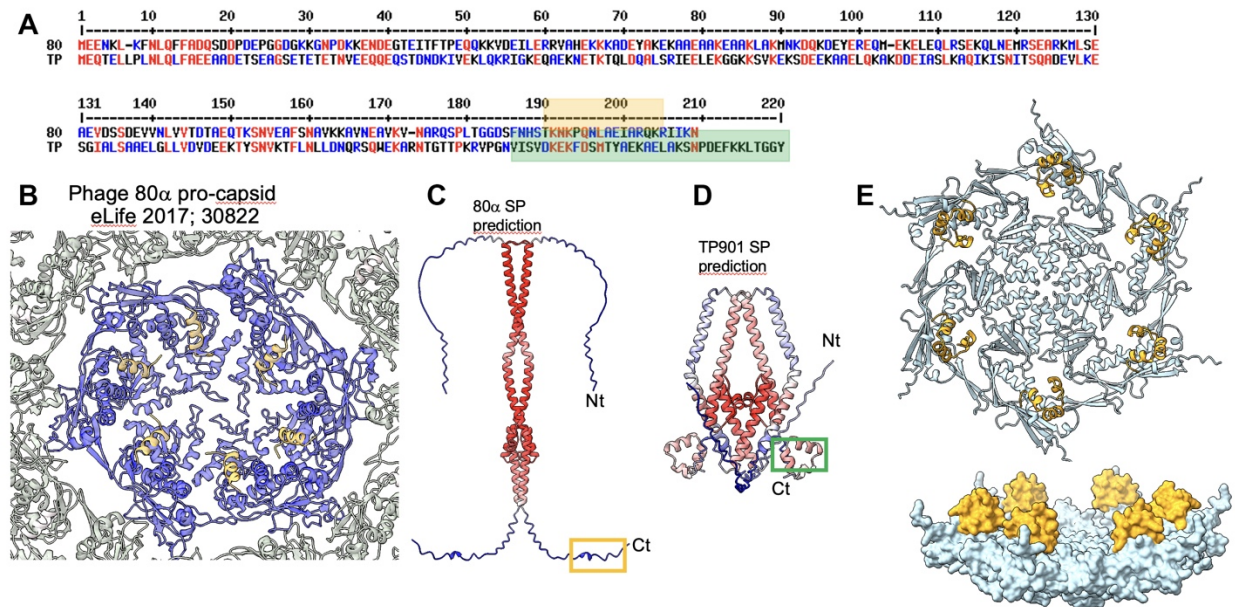
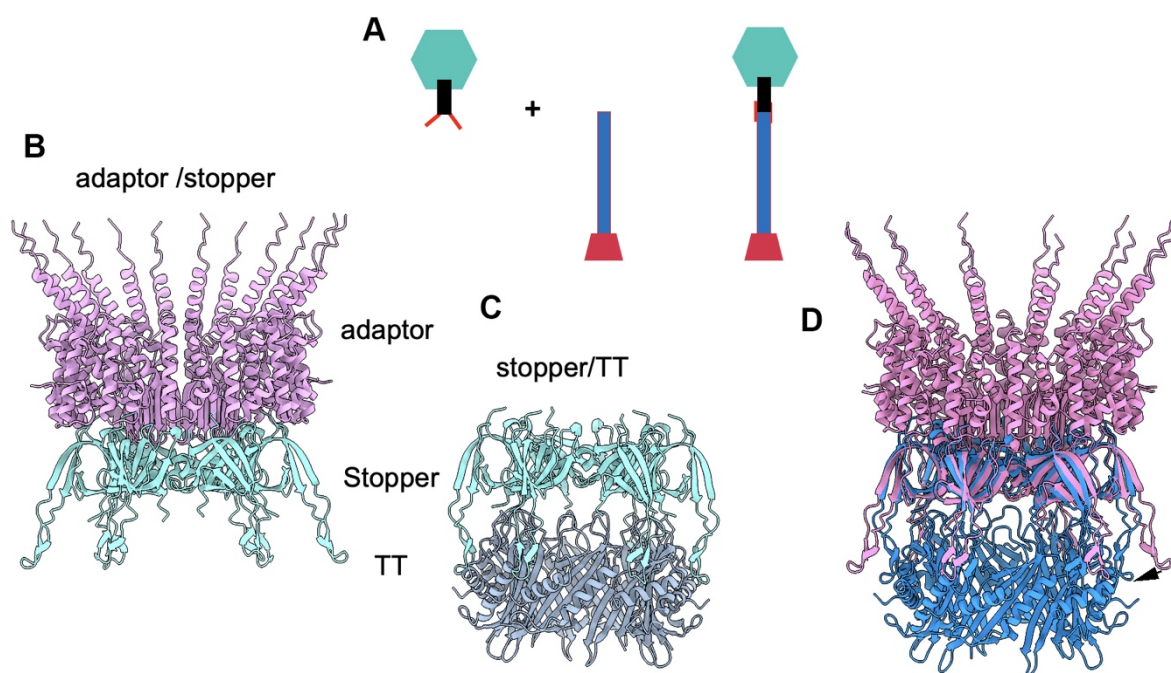


Supplementary Figure S1: AlphaFold predicted local distance difference test (pLDDT) and predicted aligned errors (PAE) of the complexes between TP901-1 components.



Supplementary Figure S2: The procapsid's scaffolding proteins (SP). (A) Amino-acids alignment between the scaffolding proteins of staphylococcal phage 80 α and lactococcal phage TP901-1. (B) Ribbon representation of the cryoEM structure of phage 80 α MCP hexamer (blue) in complex with the C-terminus of the scaffolding protein [1] (orange; see also the orange box in (A)). (C) AlphaFold prediction of the full-length phage 80 α scaffolding protein. The orange box corresponds to the orange helix in (B). (D) AlphaFold prediction of the full-length phage TP901-1 scaffolding protein. The green boxed helices correspond to the green box in (A). (E, **top**) Ribbon representation of phage TP901- MCP hexamer (light blue) in complex with the C-terminus of the scaffolding protein (orange; see also the green box in (A)). (E, **bottom**) Surface view of the same structure rotated 90°.



Supplementary Figure S3: The capsid-neck assembly with the tail-baseplate. (A) Schematic representation of the last step of a siphophage assembly. The capsid-neck and the tail-baseplate ensembles are assembled separately and joined together in a last step through a stopper/tail-terminator contact. (B) Ribbon view of the dodecameric adaptor (pink) and the hexameric stopper (blue) complex. (C) Ribbon view of the hexameric stopper (blue) and the hexameric tail-terminator (TT; grey) complex. (D) Superposition of the ribbon view of the dodecameric adaptor and the hexameric stopper complex (blue) on the hexameric stopper and the hexameric tail-terminator (TT) complex (blue). Note how the b-hairpins of the stopper rotate (by 20°) to contact the TT (black arrow on the left side).

Supplementary Movie 1: ChimeraX [2] morphing of the stopper (top) / tail-terminator (bottom) docking. Representation of atoms as spheres.

- [1] Dearborn, A. D., E. A. Wall, J. L. Kizziah, L. Klenow, L. K. Parker, K. A. Manning, M. S. Spilman, J. M. Spear, G. E. Christie, and T. Dokland. "Competing Scaffolding Proteins Determine Capsid Size During Mobilization of *Staphylococcus Aureus* Pathogenicity Islands." *Elife* 6 (2017).
- [2] Pettersen, E. F., T. D. Goddard, C. C. Huang, G. S. Couch, D. M. Greenblatt, E. C. Meng, and T. E. Ferrin. "Ucsf Chimera--a Visualization System for Exploratory Research and Analysis." *J Comput Chem* 25, no. 13 (2004): 1605-12.