

# **2025 SEA Faculty Meeting**

## **Sunday, June 8, Working Session**

### **AlphaFold**

#### **Pre-work:**

To ensure ample folding time during the Sunday working session, please make sure to complete the following steps prior to the session. Happy folding!

#### **1. Download an updated version of ChimeraX:**

<https://www.cgl.ucsf.edu/chimerax/download.html>

#### **2. Access the AlphaFold3 Server and sign in with a Google account:**

<https://alphafoldserver.com/>

#### **3. Download Bxb1 PDB files to your computer:**

<https://www.dropbox.com/scl/fo/sg8c1ih813a28lva6qyt6/AJqOWETANYrc1sV76-JiW2U?rlkey=czm1harb1db7bjlul3djilsfz&dl=0>

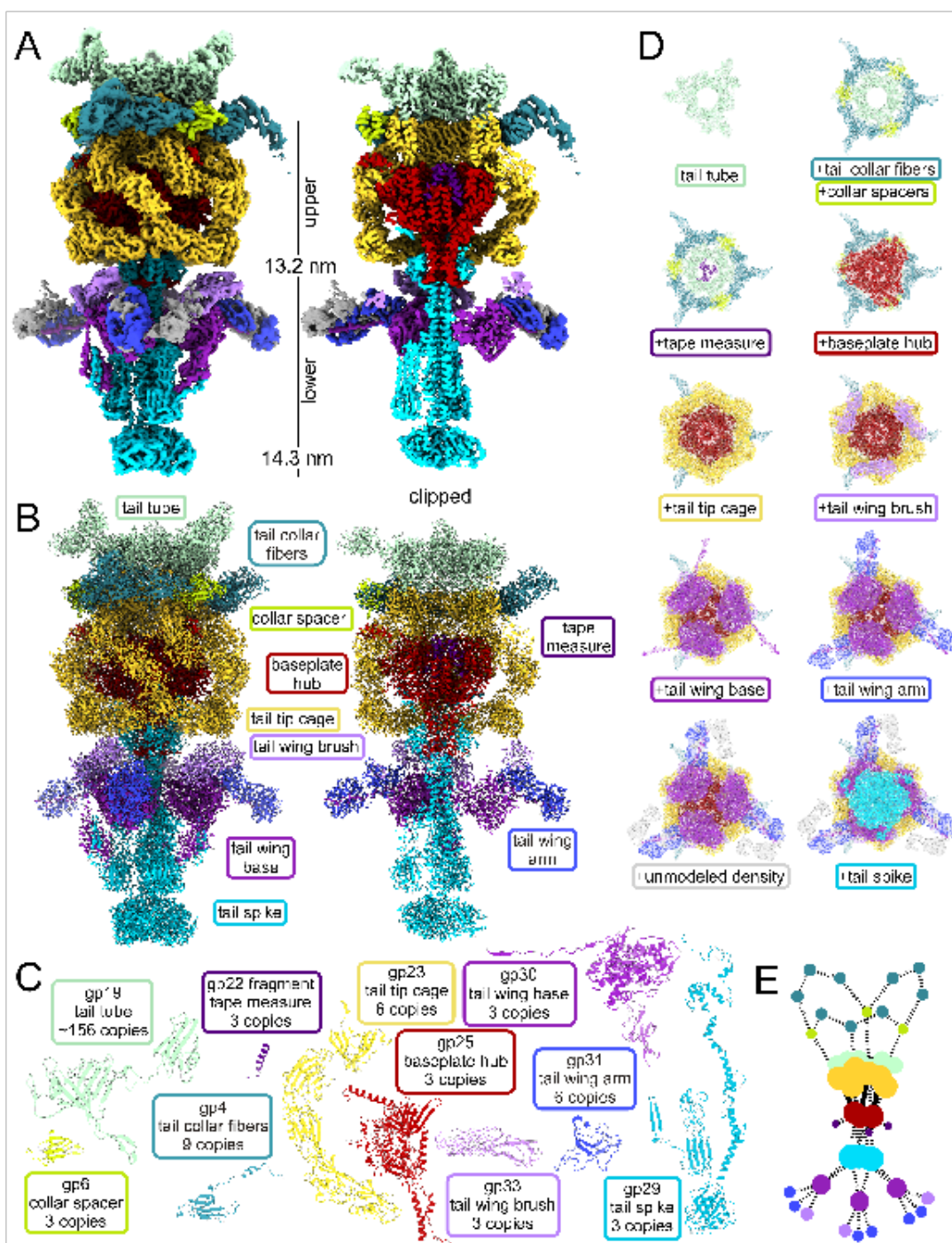
#### **4. Download the Violac Alphafold3 predictions and Word document analysis to your computer:**

[https://www.dropbox.com/scl/fo/dbordul49m1e0inv1slzv/AA19QZAvG\\_Ds11Gwv7Kv7F0?rlkey=54359sl4ejc8sdpnvryvubcrw&dl=0](https://www.dropbox.com/scl/fo/dbordul49m1e0inv1slzv/AA19QZAvG_Ds11Gwv7Kv7F0?rlkey=54359sl4ejc8sdpnvryvubcrw&dl=0)

## Extra Tools & Learning Resources:

- **FoldSeek:** <https://search.foldseek.com/search>
- **AlphaFold3 Paper:** <https://www.nature.com/articles/s41586-024-07487-w>
- **Full Bxb1 Paper:** [https://www.cell.com/cell/fulltext/S0092-8674\(25\)00345-9](https://www.cell.com/cell/fulltext/S0092-8674(25)00345-9)
- **EMBL-EBI AlphaFold Practical Guide:**  
<https://www.ebi.ac.uk/training/online/courses/alphafold/inputs-and-outputs/evaluating-alphafolds-predicted-structures-using-confidence-scores/>

**Figure 5, Freeman et al., 2025**



**Figure 5. Bxb1 tail-tip complex structure**

(A) A composite cryo-EM map of the entire Bxb1 tail tip, with density segments colored as in Figure 1 (unmodeled density is shown in gray). Full density map on the left, clipped map on the right to show the interior organization.

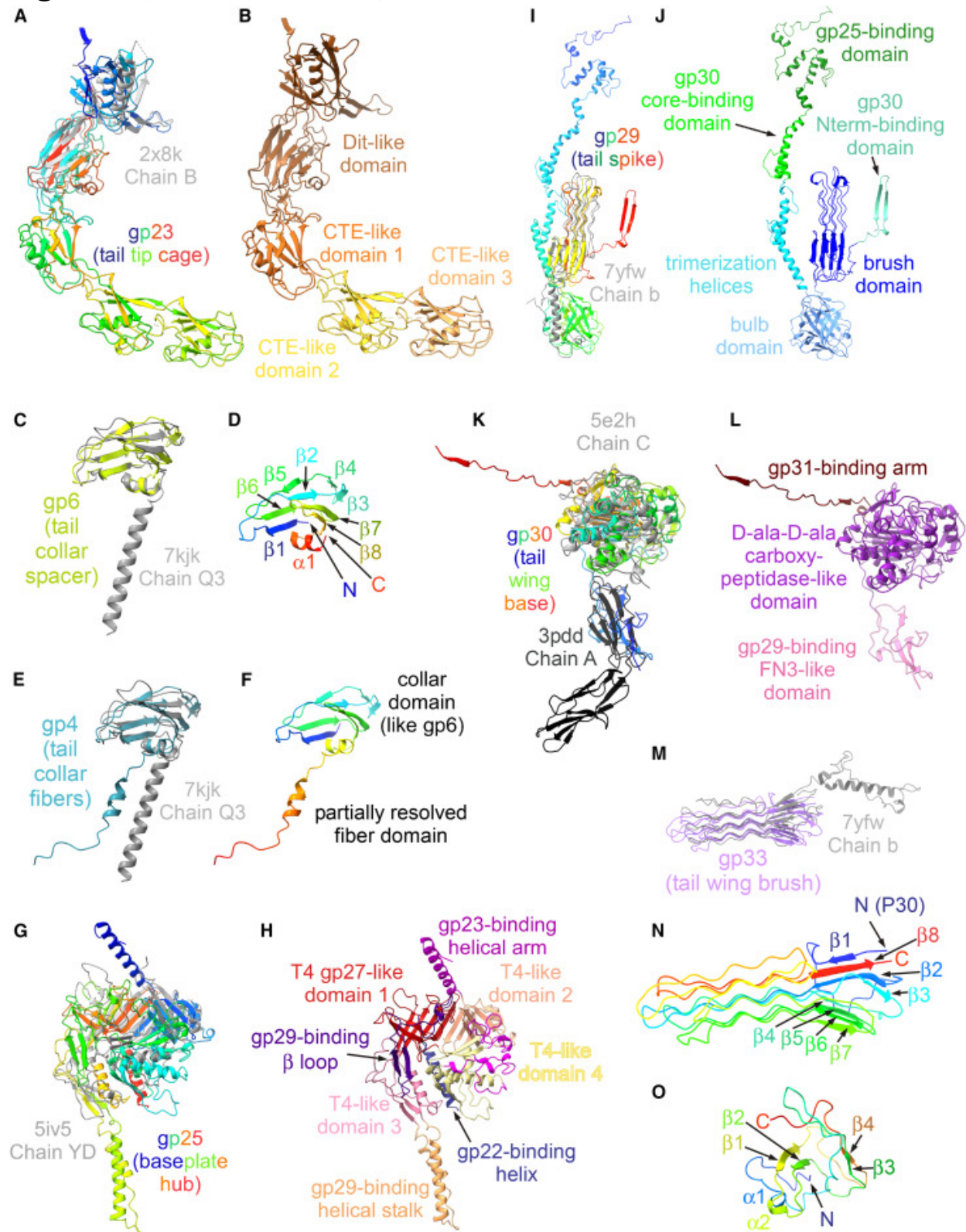
(B) The complete protein model built into the density map is displayed as cartoons with atoms shown as sticks and balls. The model is in the same pose as in (A), and ten distinct proteins are labeled and color-coded to (A). Full model on the left, clipped view on the right to show the interior organization.

(C) Gene products present in the tail-tip complex are shown as monomers. Each subunit is labeled, and its copy number per phage particle is indicated.

(D) The tail-tip complex is viewed from the bottom and displayed piece by piece, starting from the tail tube and moving toward the tail spike, as labeled. Segmented cryo-EM densities are shown as transparent surfaces, and protein models are shown as cartoons for each component.

(E) A color-coded interface map of the tail-tip complex. The circles represent individual protein subunits, and the lines connect subunits with interface areas  $\geq 300 \text{ \AA}^2$ .

**Figure S6, Freeman et al., 2025**



- (A) The tail-tip cage protein, gp23, is shown in rainbow from N to C termini and aligned with its Foldseek hit 2x8k in gray.
- (B) The gp23 model is colored and labeled according to domains.
- (C) The tail collar spacer, gp6, is shown in yellow-green and aligned with its Foldseek hit 7kjk in gray.
- (D) The gp6 model is colored in rainbow from N to C termini with all secondary structure features labeled.
- (E) The tail collar fiber, gp4, is shown in yellow-green and aligned with its Foldseek hit 7kjk in gray.
- (F) The gp4 model is colored in rainbow from N to C termini with all secondary structure features labeled.
- (G) The base plate hub protein, gp25, is shown in rainbow from N to C termini and aligned with its Foldseek hit 5iv5 in gray.
- (H) The gp25 model is colored and labeled according to domains.
- (I) The tail spike protein, gp29, is shown in rainbow from N to C termini and aligned with its Foldseek hit 7yfw in gray.
- (J) The gp29 model is colored and labeled according to domains.
- (K) The tail wing base protein, gp30, is shown in rainbow from N to C termini and aligned with its Foldseek hit 3pdd in gray.
- (L) The gp30 model is colored and labeled according to domains.
- (M) The tail wing brush, gp33, is shown in lavender and aligned with its Foldseek hit 7yfw in gray.
- (N) The gp33 model is colored in rainbow from N to C termini with all secondary structure features labeled.
- (O) The tail wing arm protein, gp33, model is colored in rainbow from N to C termini with all secondary structure features labeled.