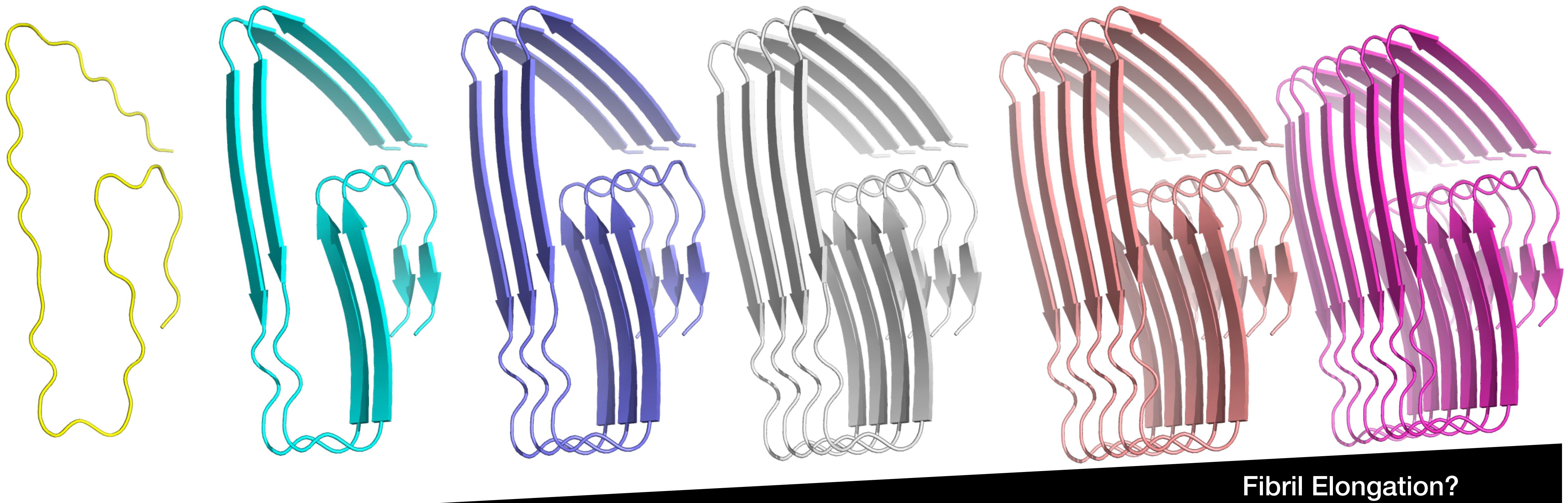


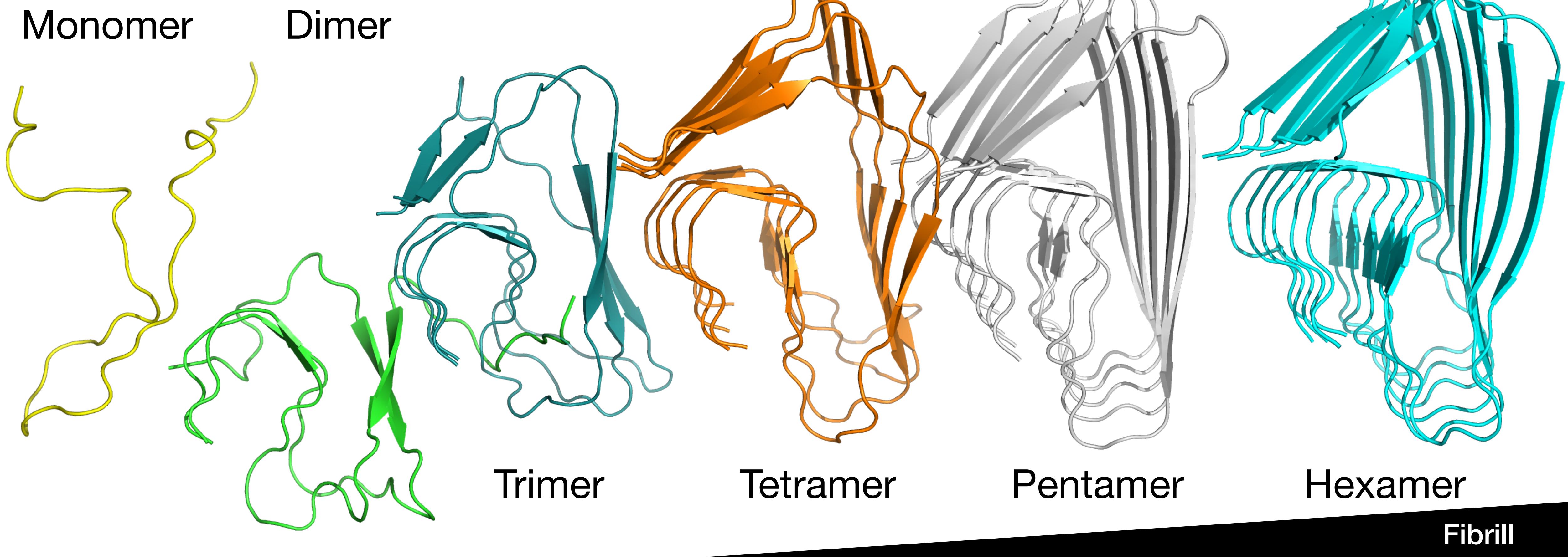
# Which conformer marks as the pivot point for A $\beta$ 42 fibril elongation?

- **Hypothesis:** Trimer is the initial fibril construct for elongation due to stabilization of the beta sheet, trimer is the first step of elongation
- **Calculation:** construct monomer - hexamer system to investigate the beta-sheet stability and energetic of the system (for both S-shape (RCSB: 8EZE) and L-shape (RCSB: 5OQV) initial structures)



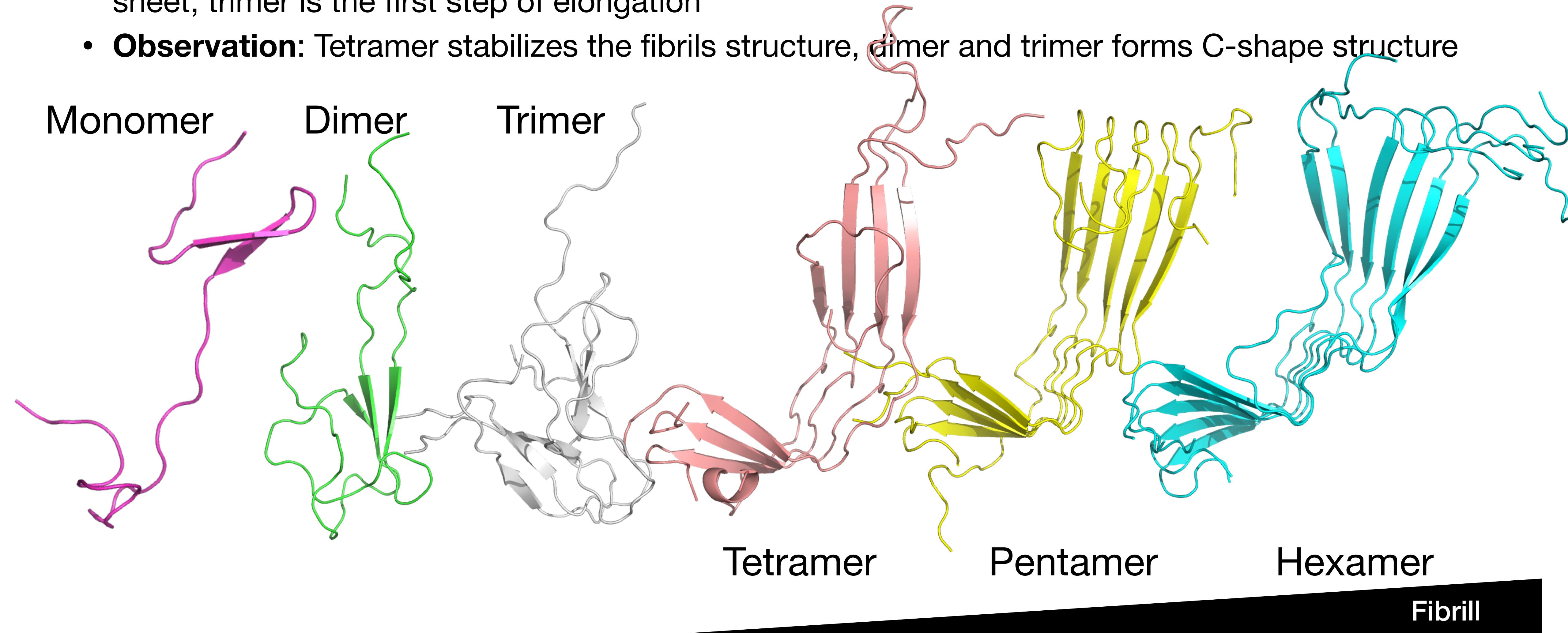
# L-Shape 5OQV initial prediction

- **Hypothesis:** Trimer is the initial fibril construct for elongation due to stabilization of the beta sheet, trimer is the first step of elongation
- **Observation:** Under 400ns dynamics, tetramer stabilizes the fibrils structure, L-shape is more stable than the S-shape confirmation

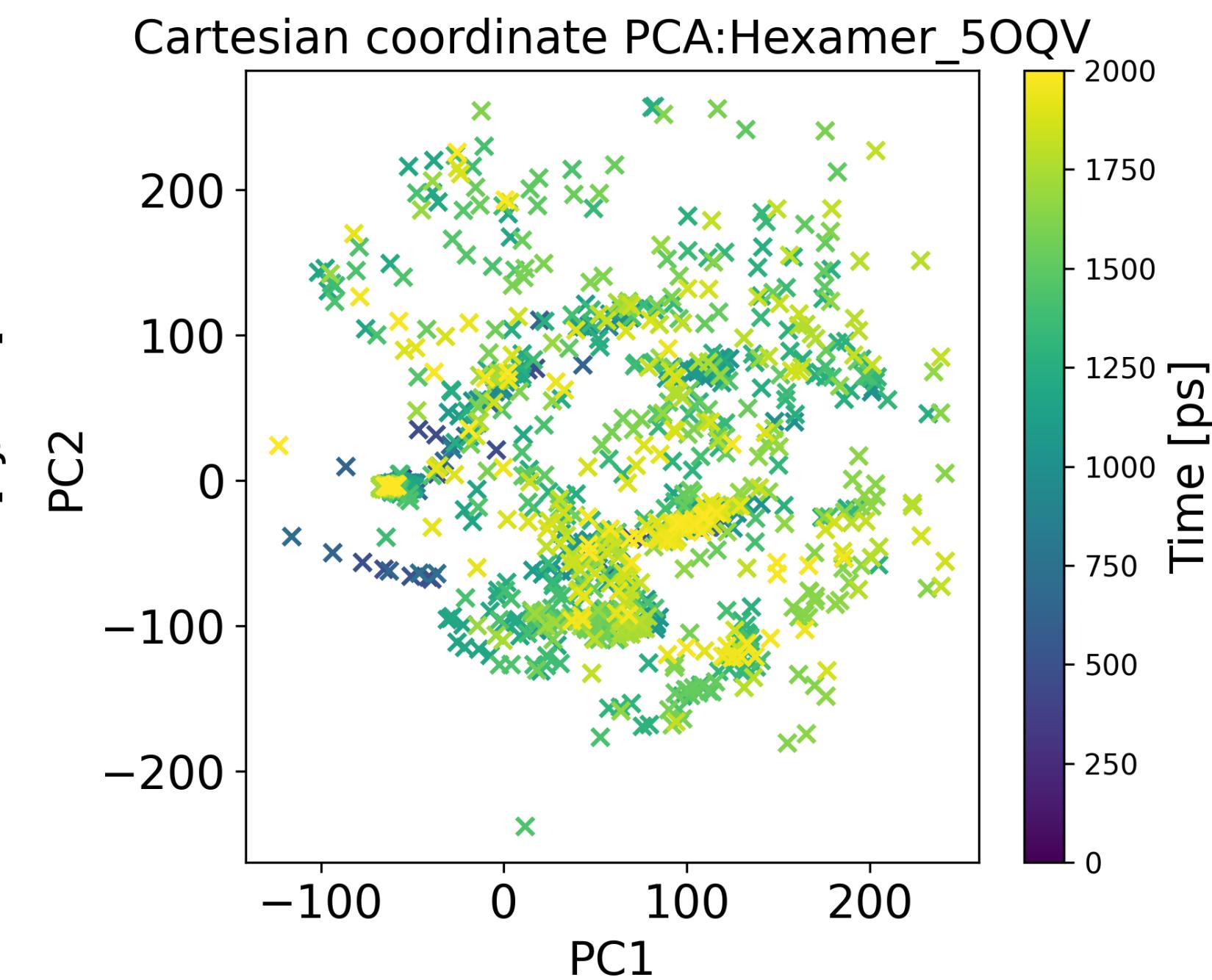
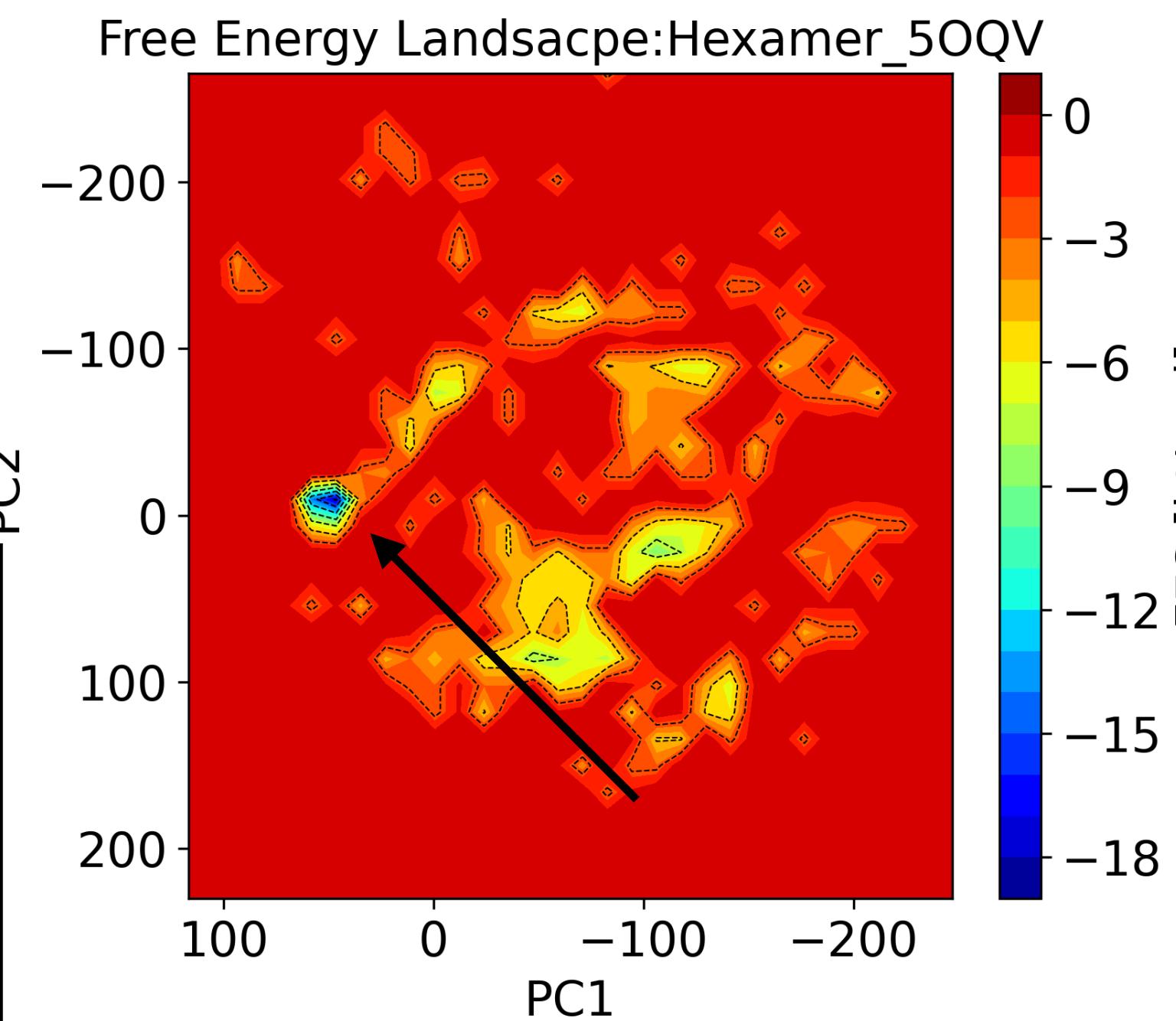
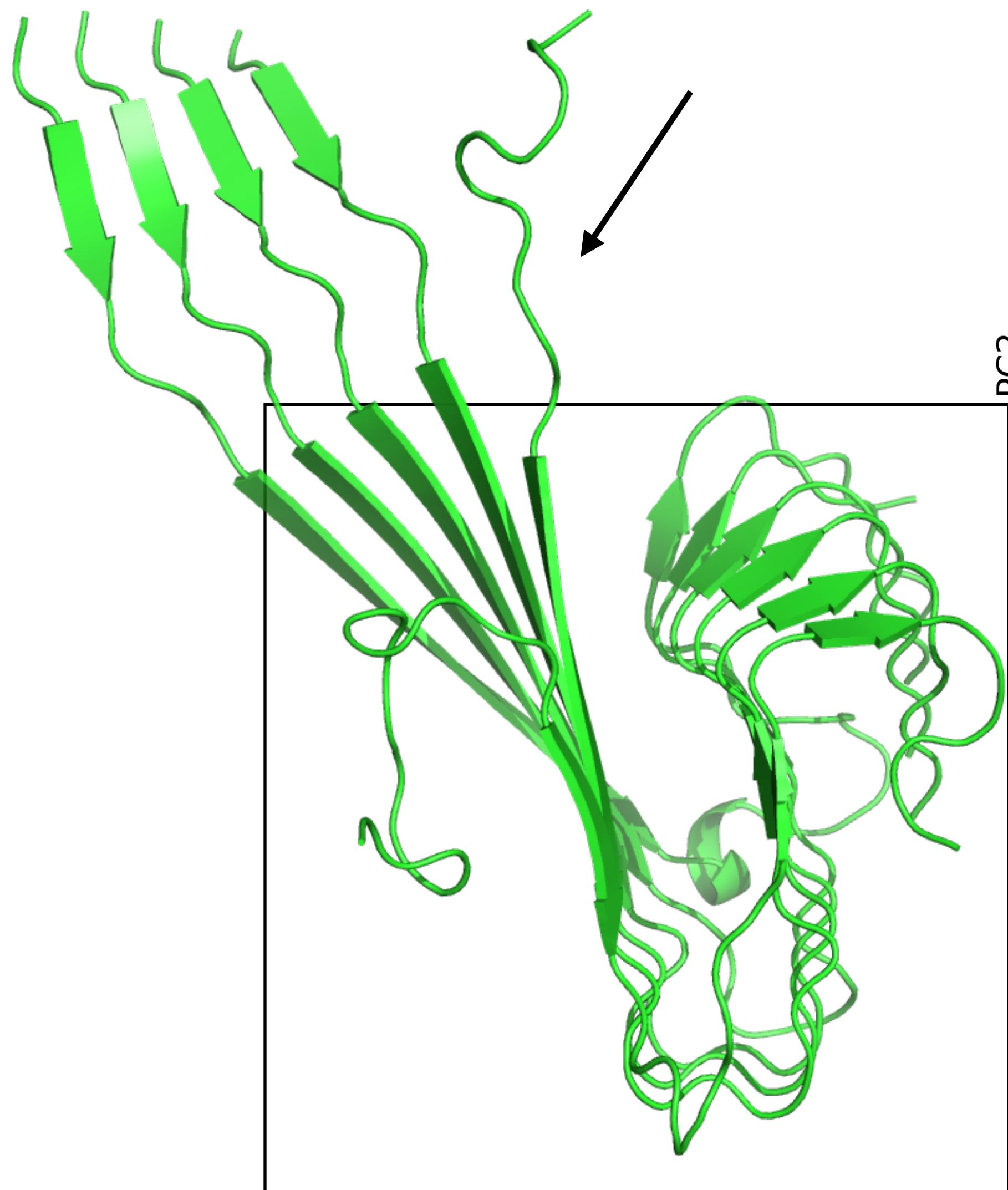


# S-Shape 8EZE initial prediction

- **Hypothesis:** Trimer is the initial fibril construct for elongation due to stabilization of the beta sheet, trimer is the first step of elongation
- **Observation:** Tetramer stabilizes the fibrils structure, dimer and trimer forms C-shape structure



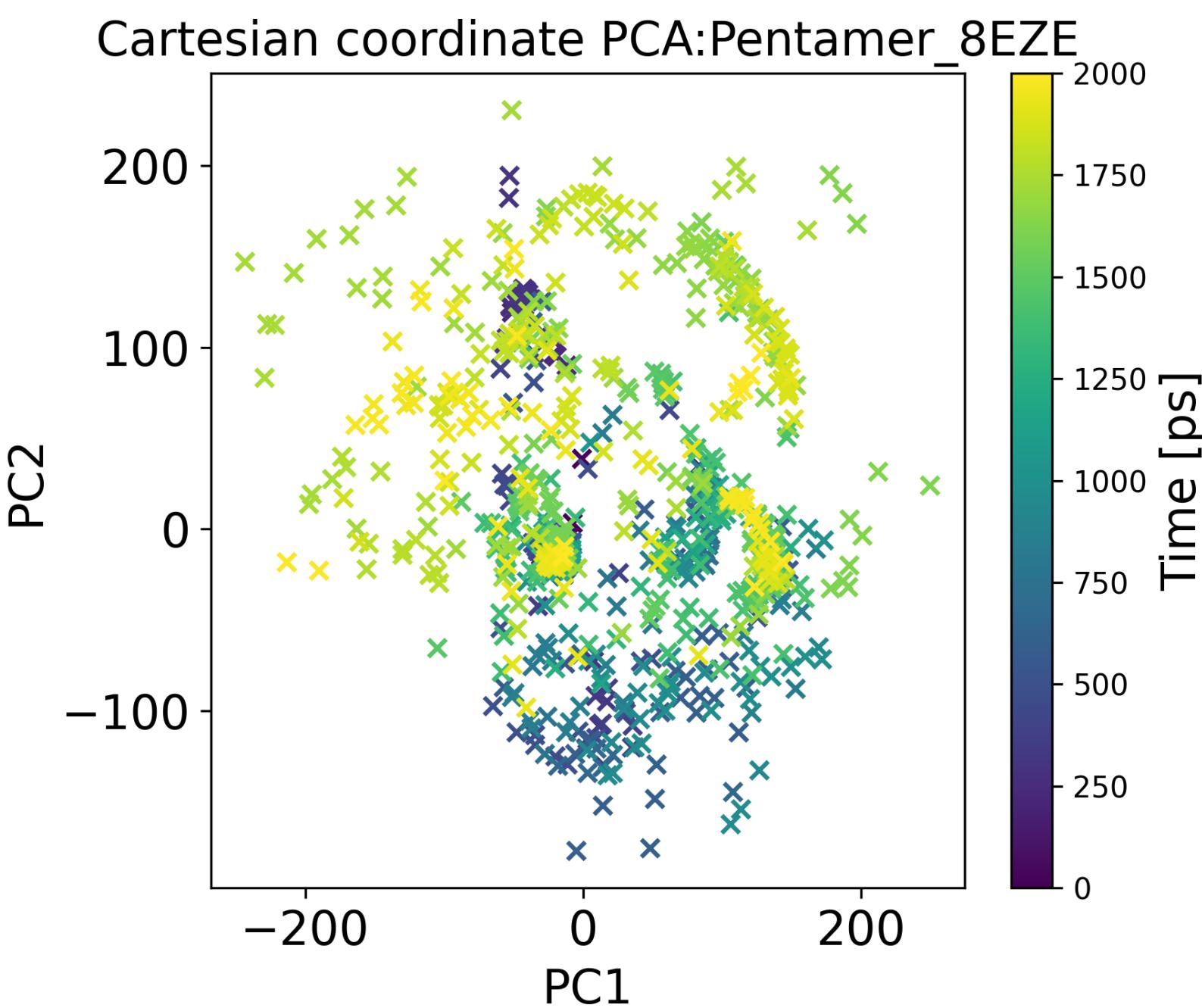
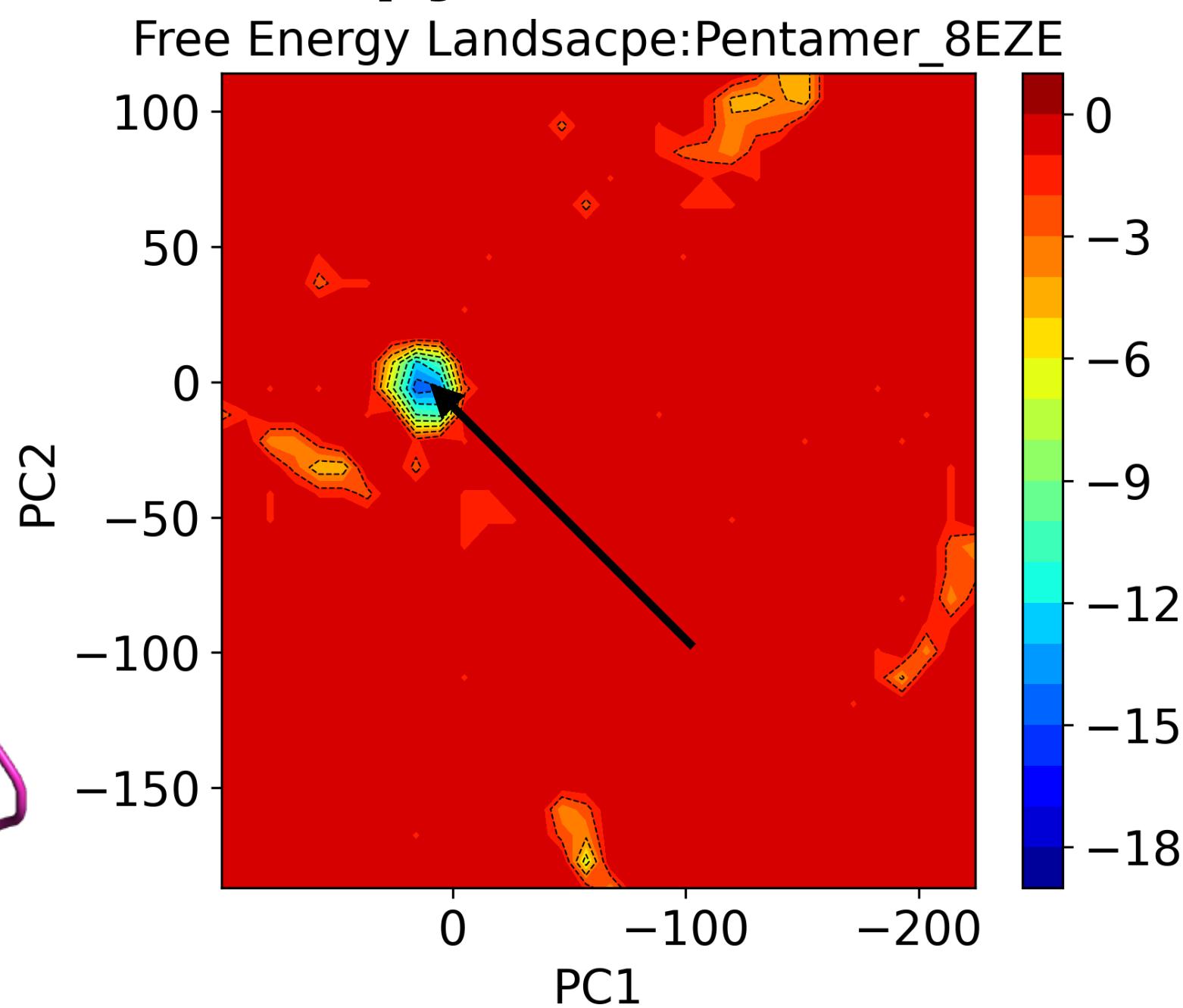
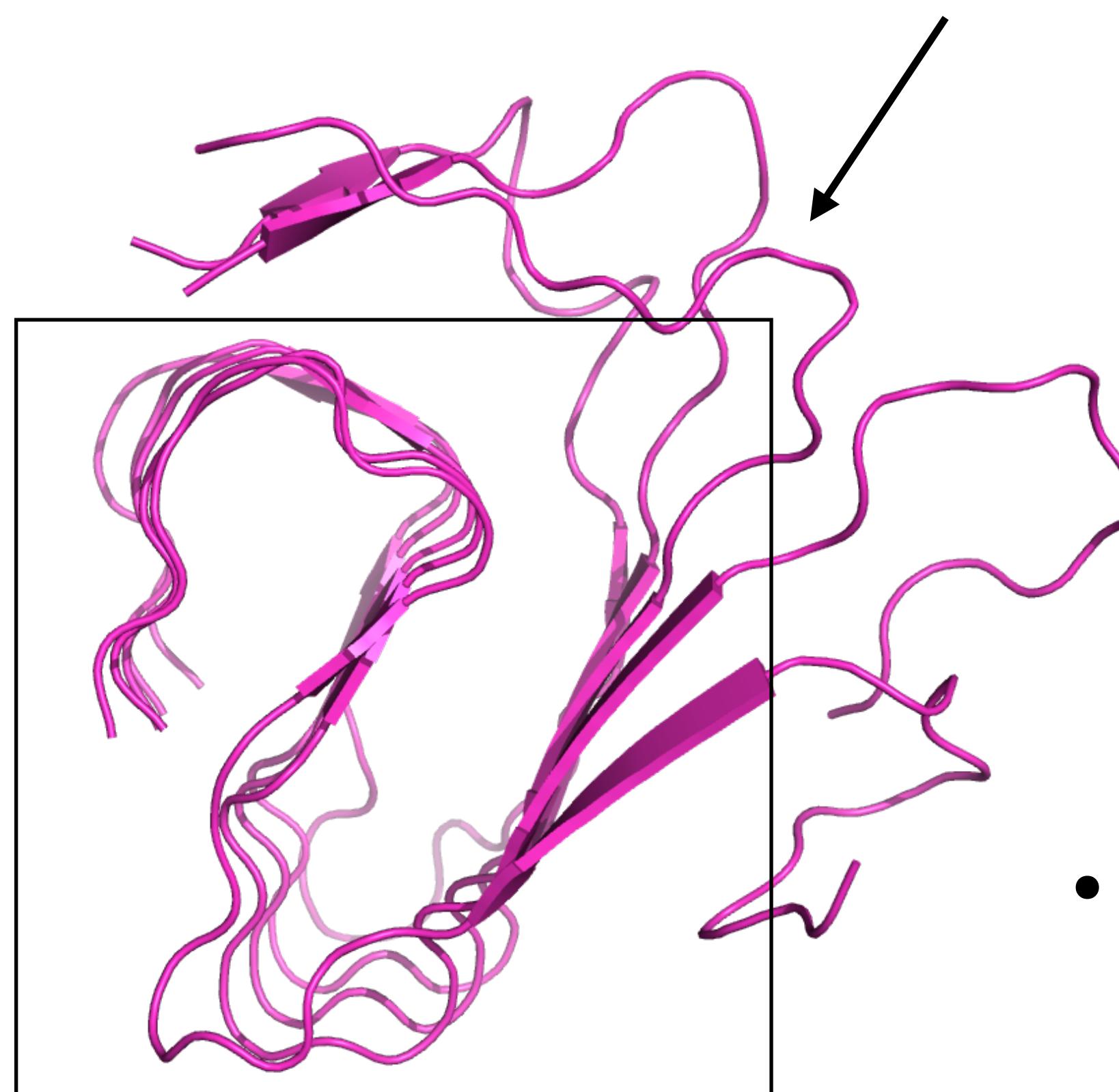
# Hexamer 5OQV (L-shape) Exhibits 1 Conformers



- **Hypothesis:** Trimer is the initial fibril construct for elongation due to stabilization of the beta sheet, trimer is the first step of elongation
- **Observation:** Tetramer stabilizes the fibrils structure, dimer and trimer forms C-shape structure

# Pentamer 5OQV (L-shape) Exhibits 1 Conformers

## Translational PCA with Shannon Entropy Calculation



- **Hypothesis:** Trimer is the initial fibril construct for elongation due to stabilization of the beta sheet, trimer is the first step of elongation
- **Observation:** Tetramer stabilizes the fibrils structure, dimer and trimer forms C-shape structure

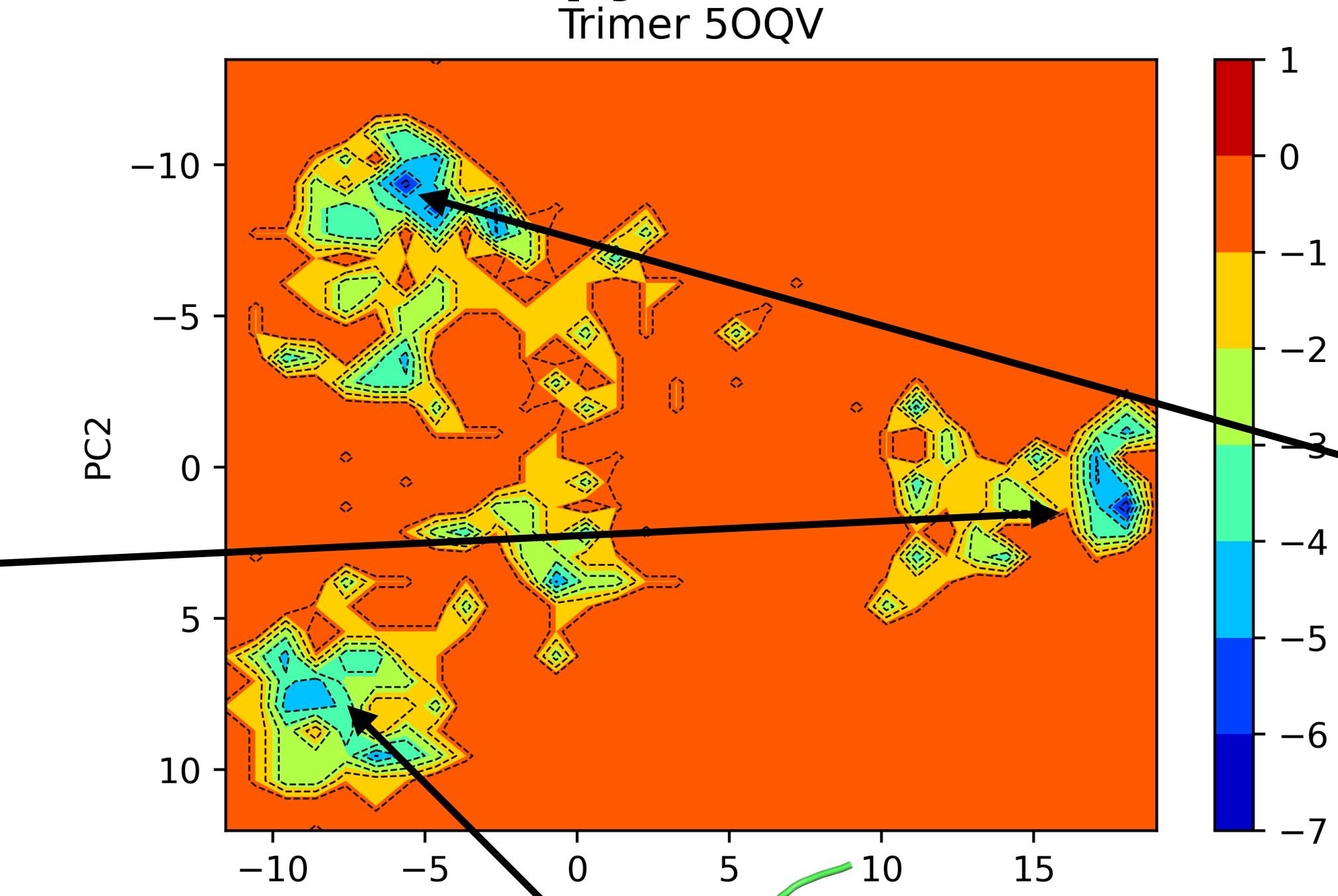
# Trimer 5OQV (L-shape) Exhibits Three Conformers

Translational PCA with Shannon Entropy Calculation



Conformer #1

Original L-shape Conformation  
is preserved

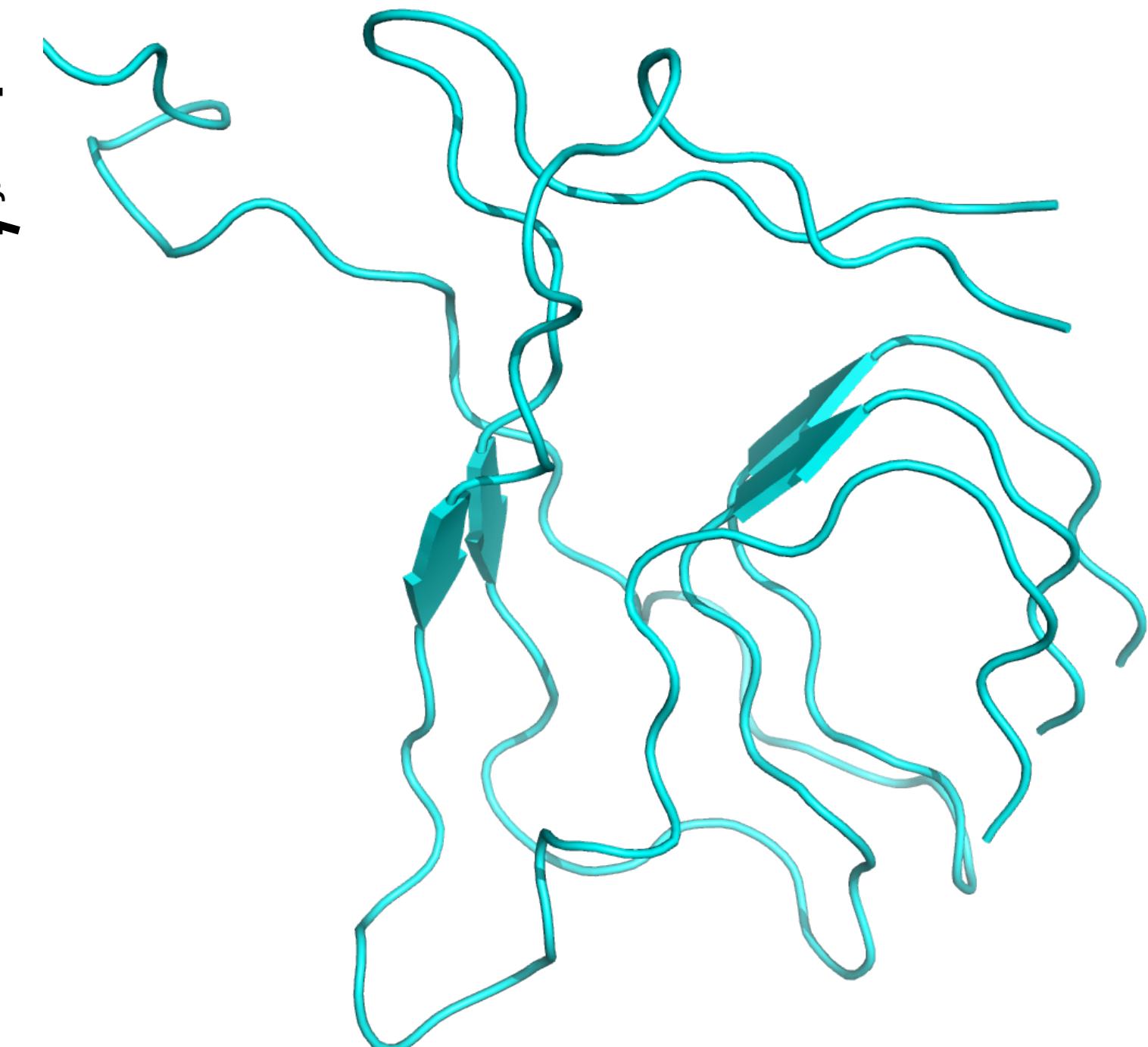


Conformer #2



Random coils extended

Conformer #3



Random coils extended further

# Trimer 8EZE (S-shape) Exhibits Three Conformers

## Translational PCA with Shannon Entropy Calculation

