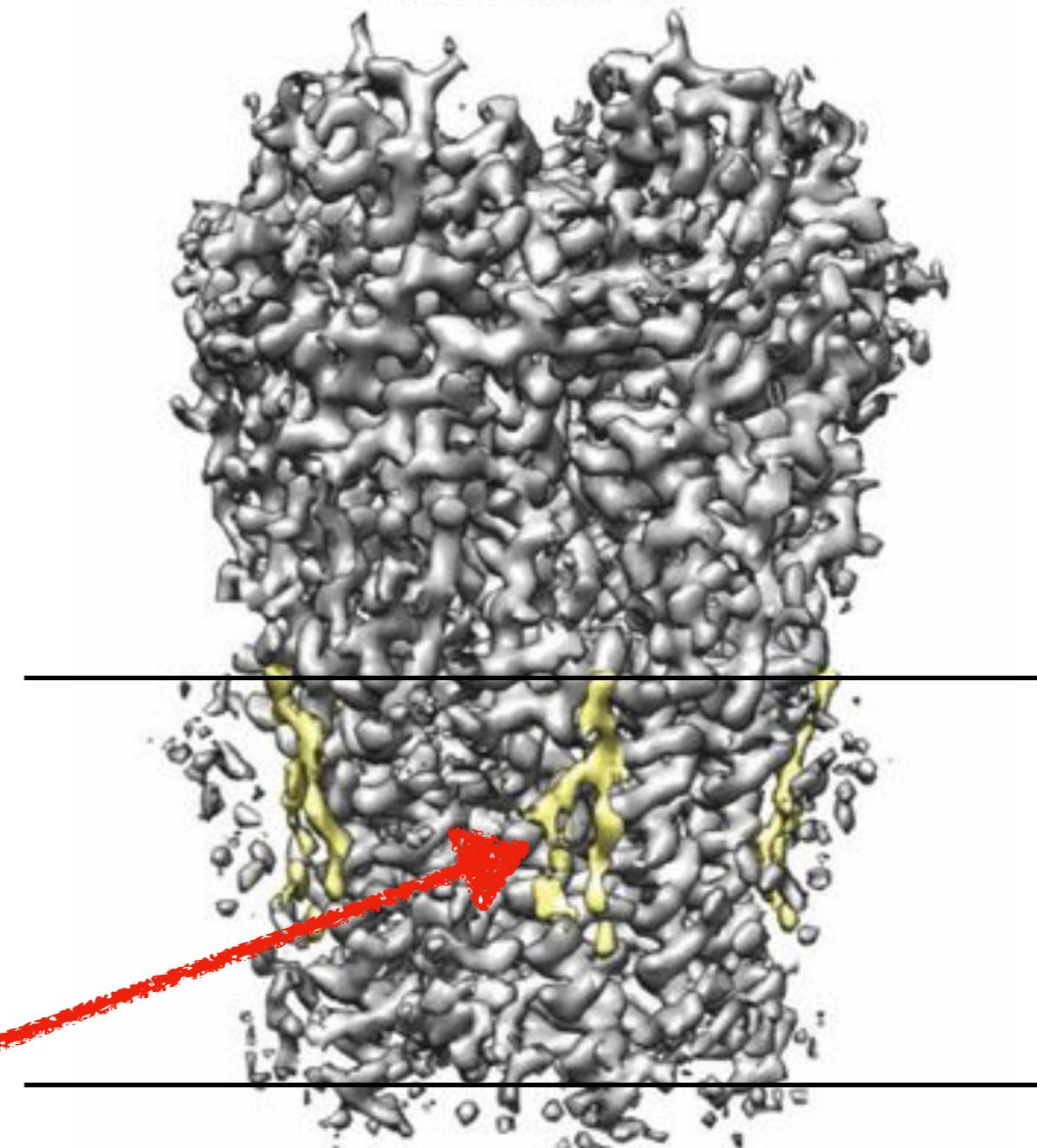
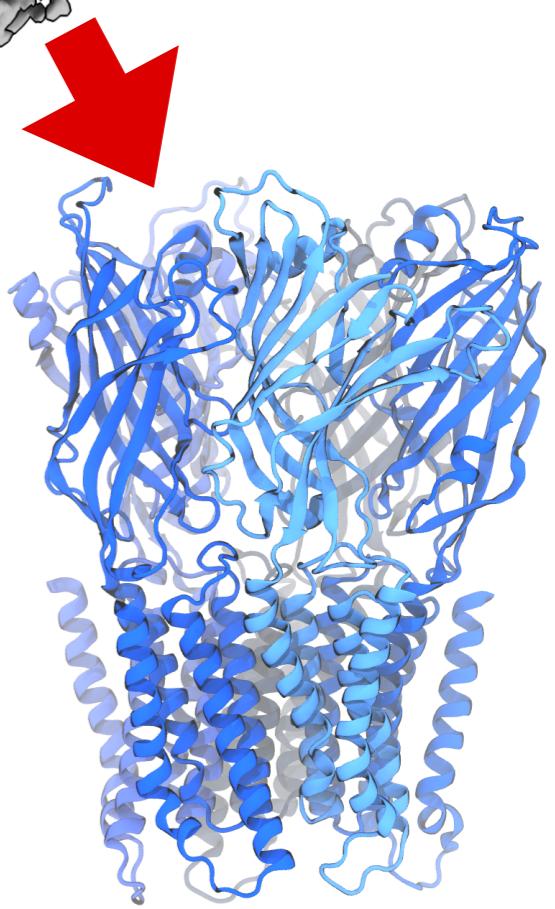
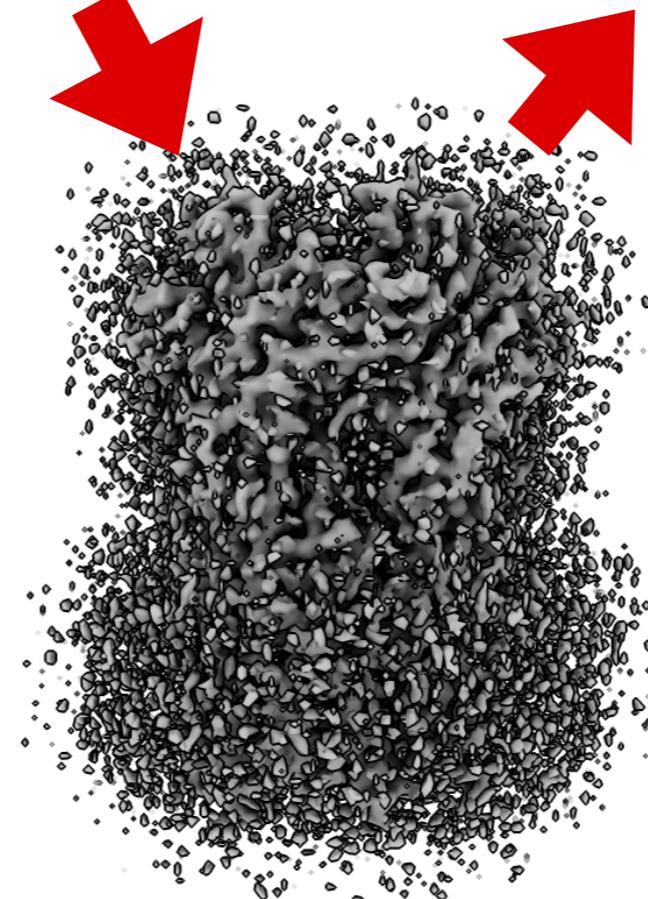
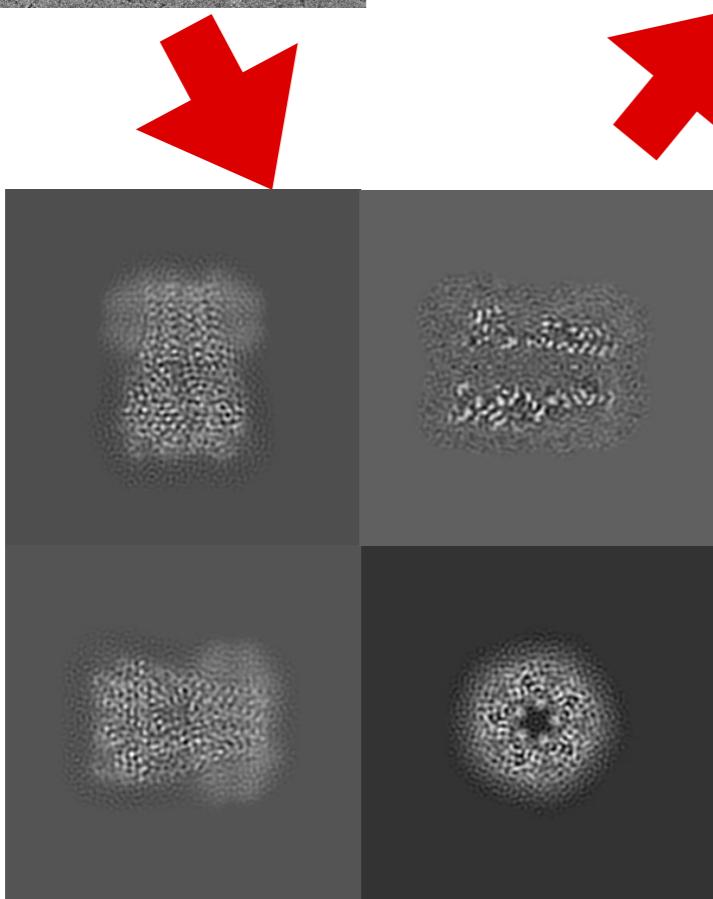
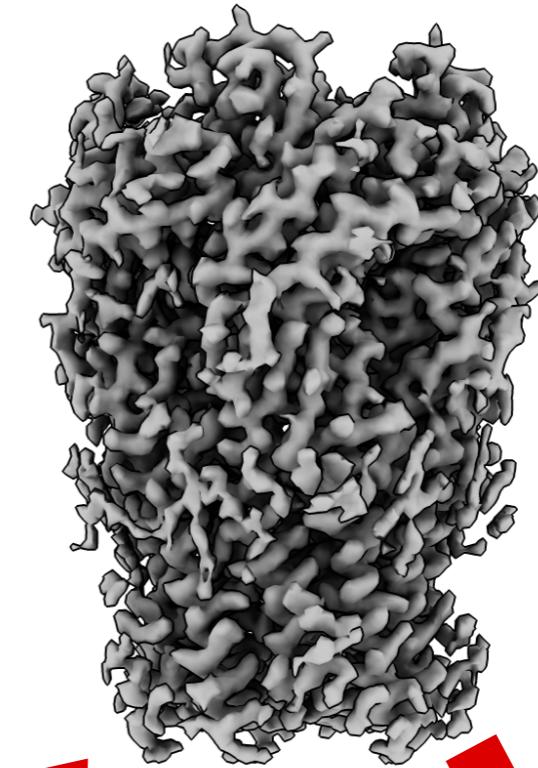
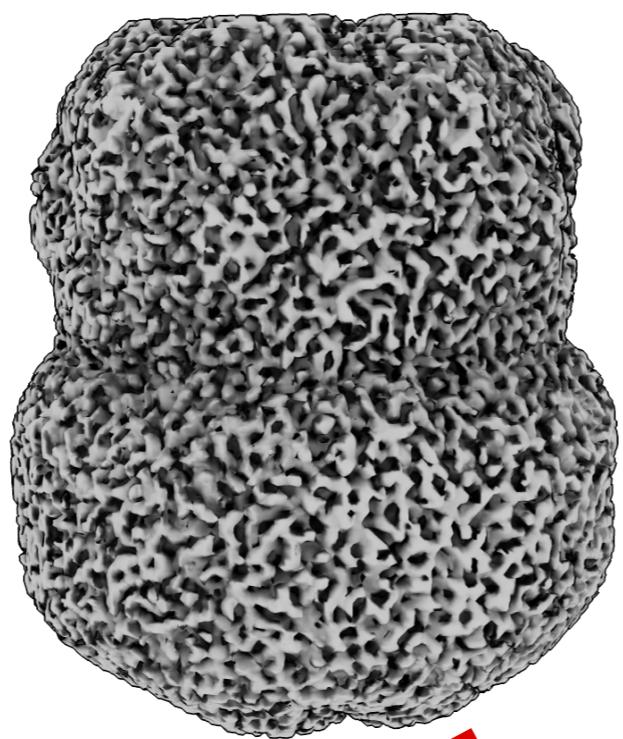
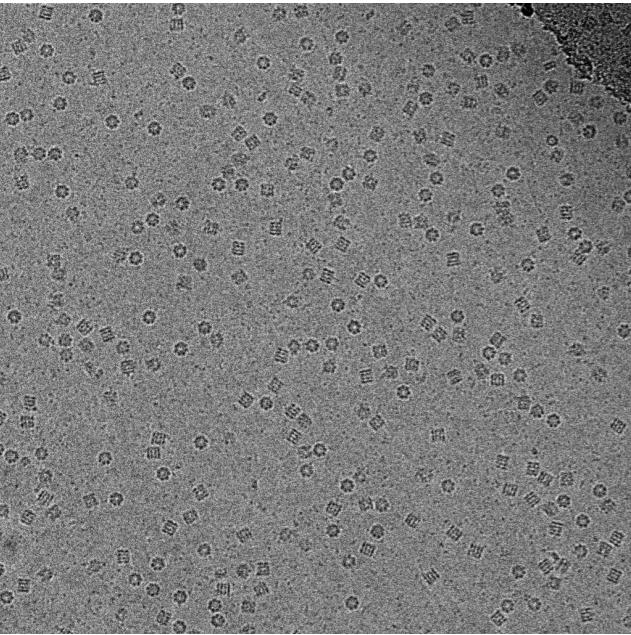


# Streamlined Alchemical Free Energy Perturbation

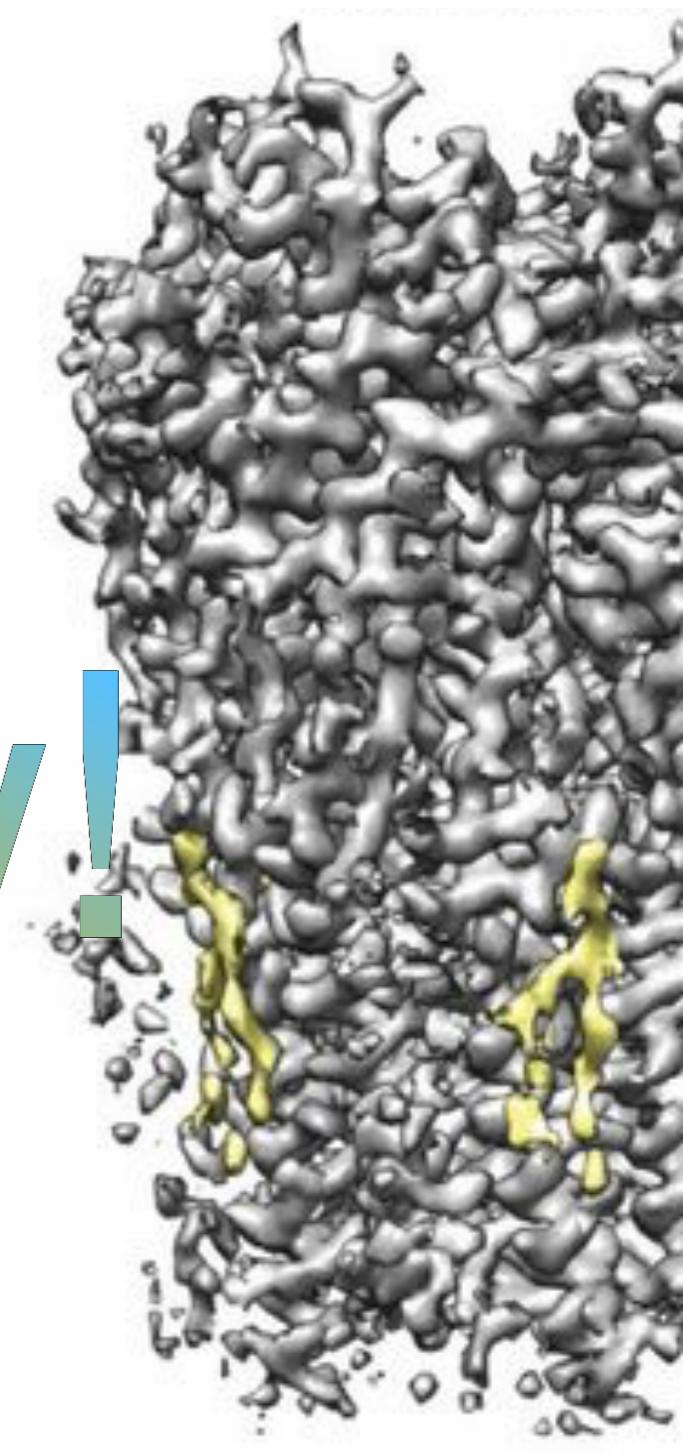
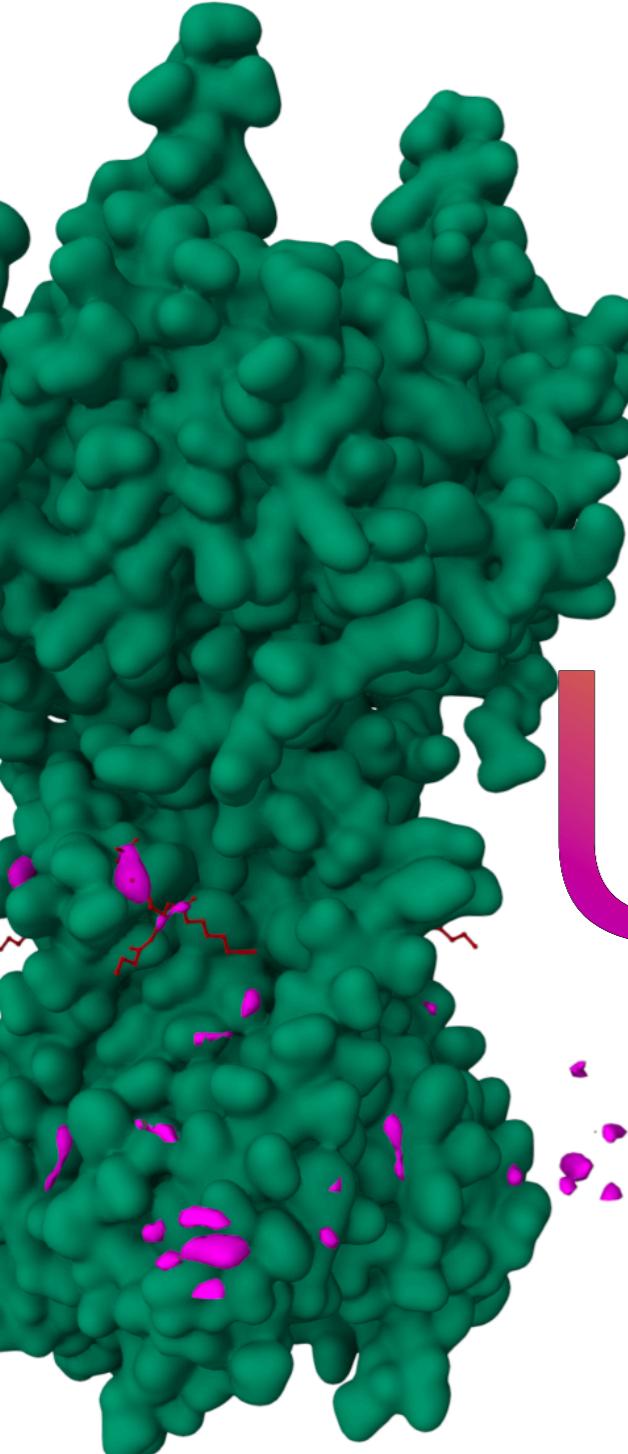
What are those?!



# We infer protein structures from densities



# But Densities are Often Ambiguous



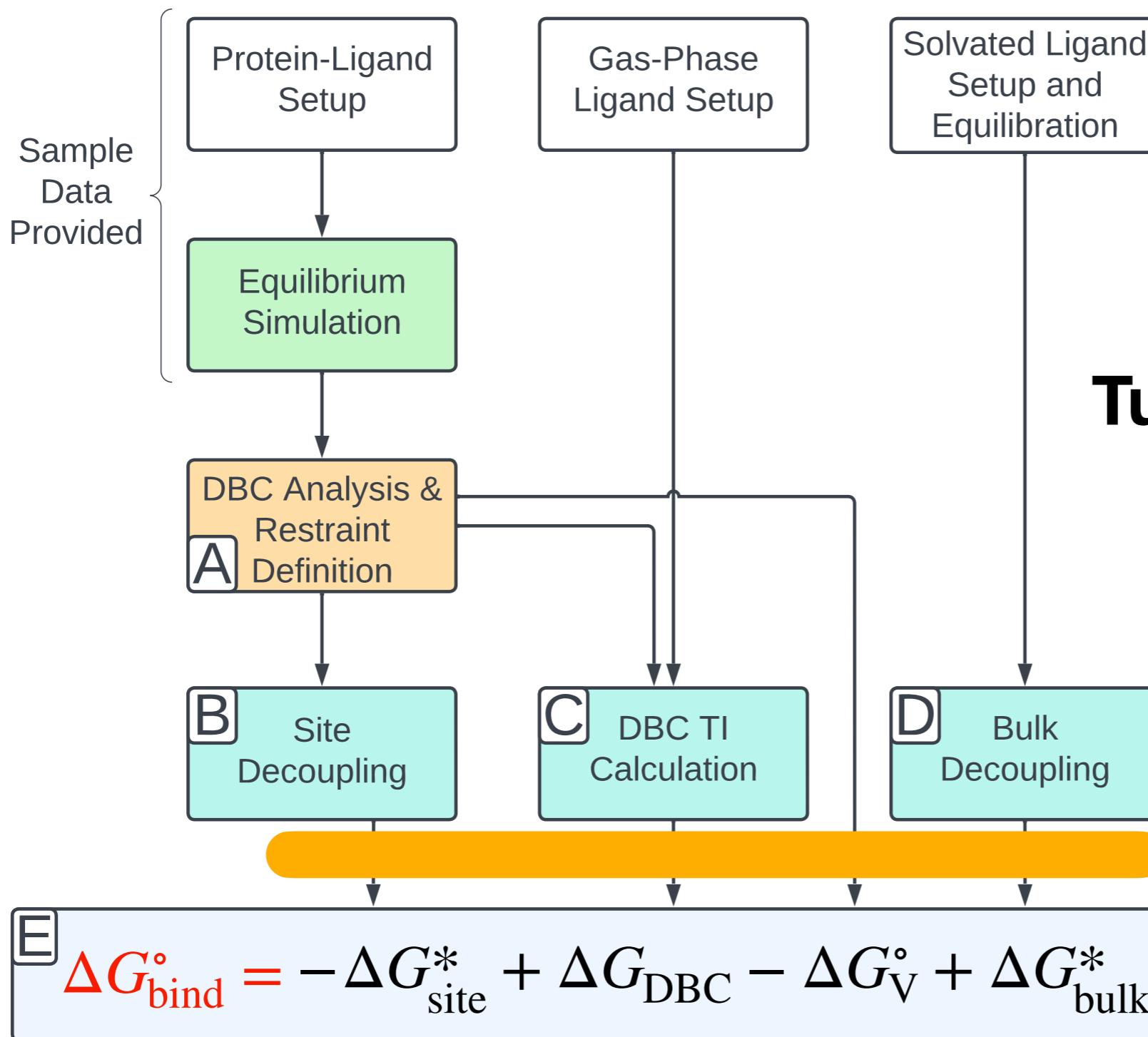
Probability is a  
function of  $\Delta G$

No experimental method

Until now!

No high-precision  
computational methods  
work for flexible molecules

# SAFEP Overview



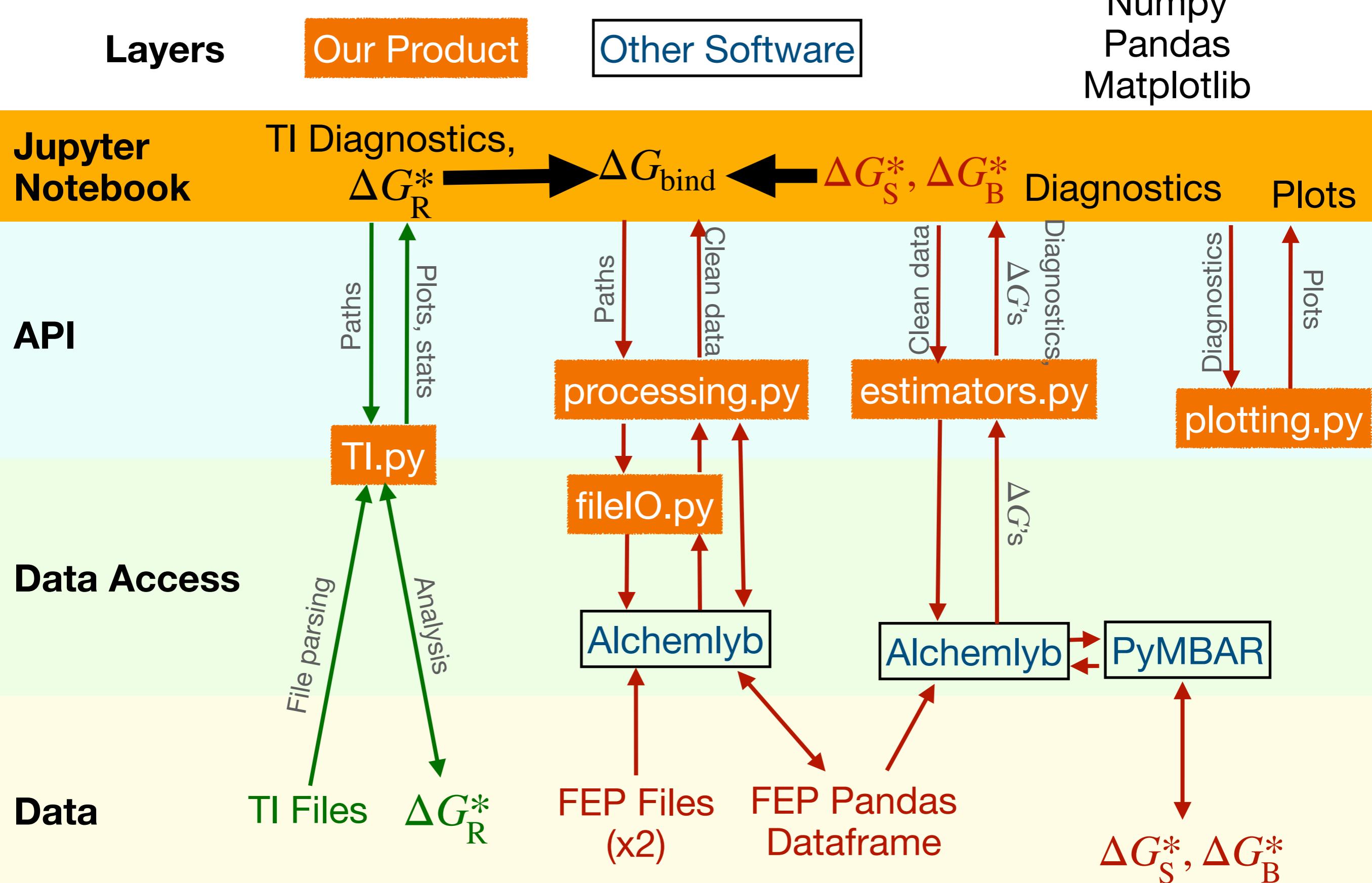
Tutorial:



SAFEP package

# SAFEP Package Architecture

Main dependencies:  
Numpy  
Pandas  
Matplotlib



# Development and Testing



Visual Studio Code



End-to-End  
Testing

New (conda)  
environment  
Clean installation  
Run test data

Unmoderated  
Remote  
Assessment

Unit  
Testing

Pytest



Usability  
Testing

Real data  
(alchemtest)

Synthetic data  
(planned)

Functional  
Testing



# Current Challenges

- Efficiency: key data are stored in large, sparse dataframes
- Documentation: Currently limited to docstrings
- Diagnostics:
  - Problems are not detected automatically
  - Some problems can only be detected by considering the trajectory

# Conclusion & Next Steps

- Successfully applied to two protein structures
- Wide interest in the membrane structural biology community
- Performance
- Testing
- Documentation
- Protocols
  - Part 1 in-press:

