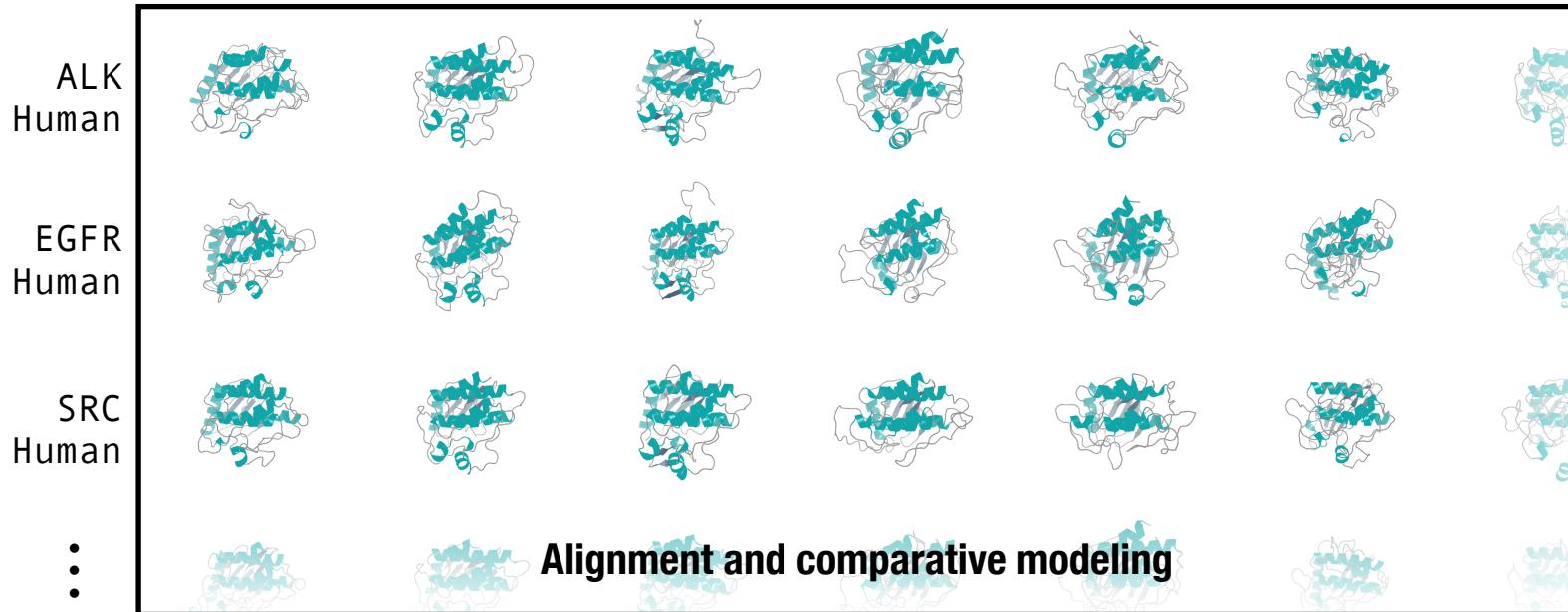




## TEMPLATE STRUCTURES

|                       |                      |                      |                        |                         |                          |     |
|-----------------------|----------------------|----------------------|------------------------|-------------------------|--------------------------|-----|
| AAK1<br>Human<br>4WSQ | ABL<br>Human<br>1OPL | ABL<br>Mouse<br>1FPU | ACVR1<br>Human<br>3H9R | ACVRL1<br>Human<br>3MY0 | ADRBK1<br>Bovine<br>10MW | ... |
|-----------------------|----------------------|----------------------|------------------------|-------------------------|--------------------------|-----|



Alignment and comparative modeling

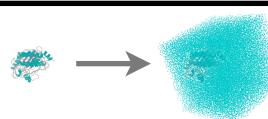


RMSD-based clustering to filter out non-unique models

Energy minimization & implicit solvent MD simulation



Solvation with explicit water



Explicit solvent MD simulation

