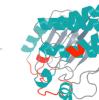




Reconstruction of missing loops



TEMPLATE STRUCTURES

4433 kinase structures (any species)

AAK1
Human
4WSQ

ABL
Human
10PL

ABL
Mouse
1FPU

ACVR1
Human
3H9R

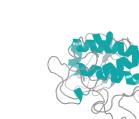
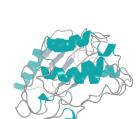
ACVRL1
Human
3MY0

ADRBK1
Bovine
10MW

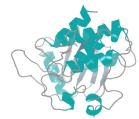
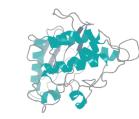
AKT1
Human
3CQU

...

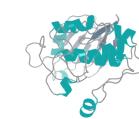
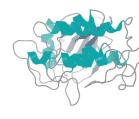
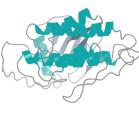
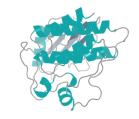
ALK
Human



EGFR
Human



SRC
Human



4250 models per target

Alignment and comparative modeling

:

90 human TK targets

4150 models

Filter out non-unique models by clustering on RMSD



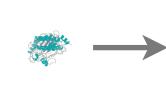
4148 models

Energy minimization & implicit solvent MD simulation



TODO models

Solvation with explicit water



TODO models

Explicit solvent MD simulation

