

B. **TEMPLATE STRUCTURES**

	AAK1 Human 4WSQ	ABL Human 1OPL	ABL Mouse 1FPU	ACVR1 Human 3H9R	ACVRL1 Human 3MY0	ADRBK1 Bovine 1OMW	...
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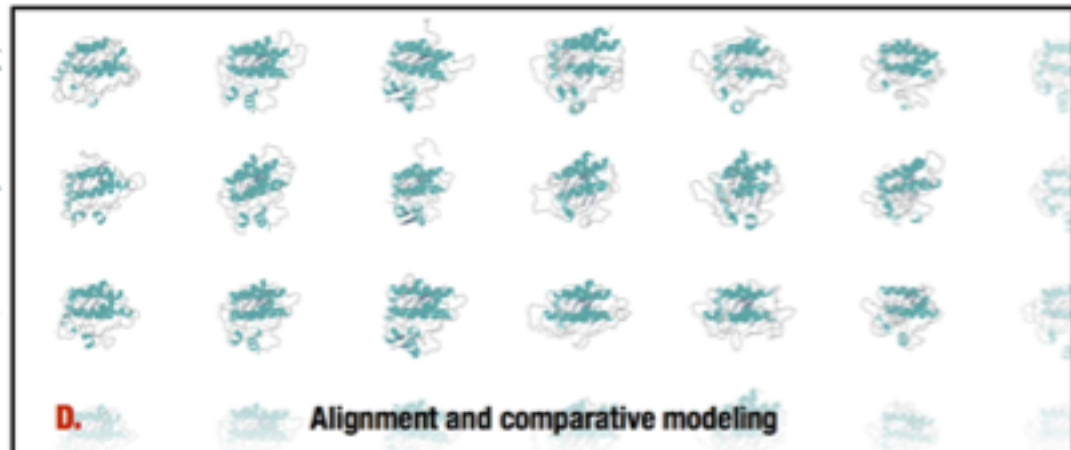
A.
TARGET
SEQUENCES

ALK
Human

EGFR
Human

SRC
Human

⋮



RMSD-based clustering to filter out non-unique models



E. Energy minimization & implicit solvent MD simulation



F. Solvation with explicit water



Explicit solvent MD simulation

