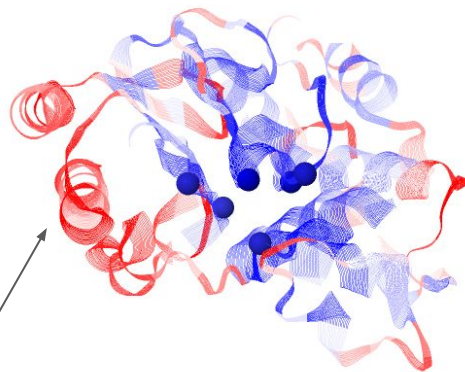


Structural divergence (RMSD)

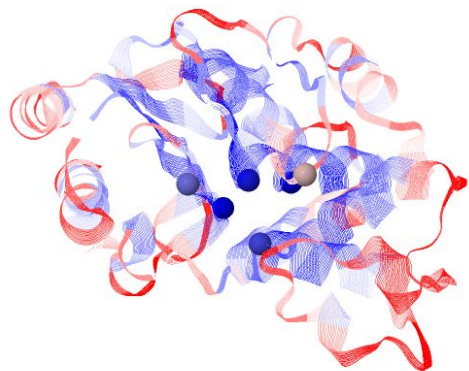
(a)



$\rho = 0.63$

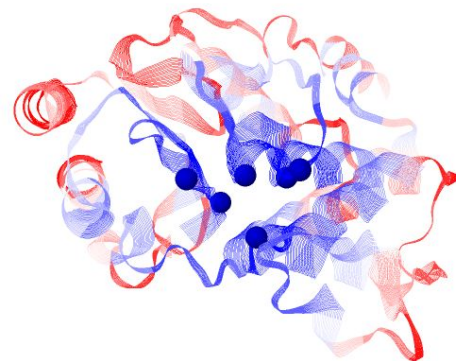
$\rho = 0.60$

(b)



Conformational flexibility (RMSF)

(c)



Distance from active site (d)

$\rho = 0.63$