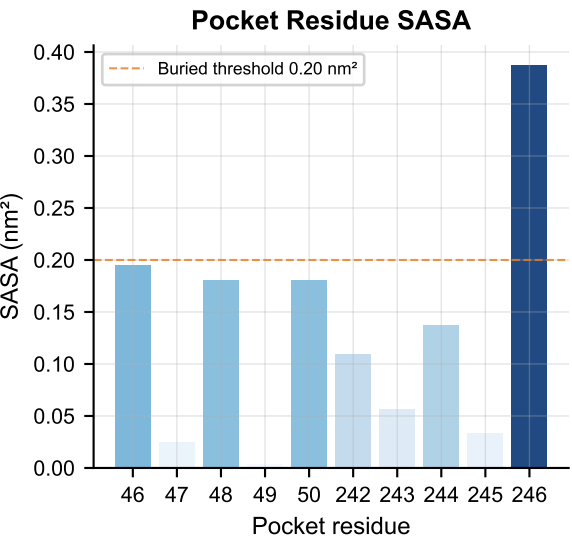
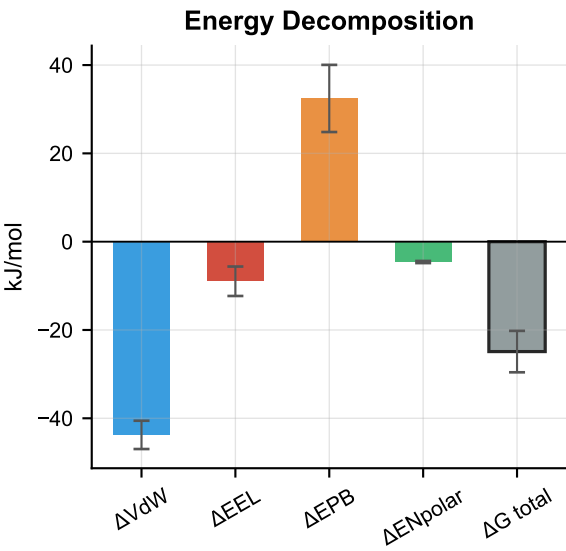
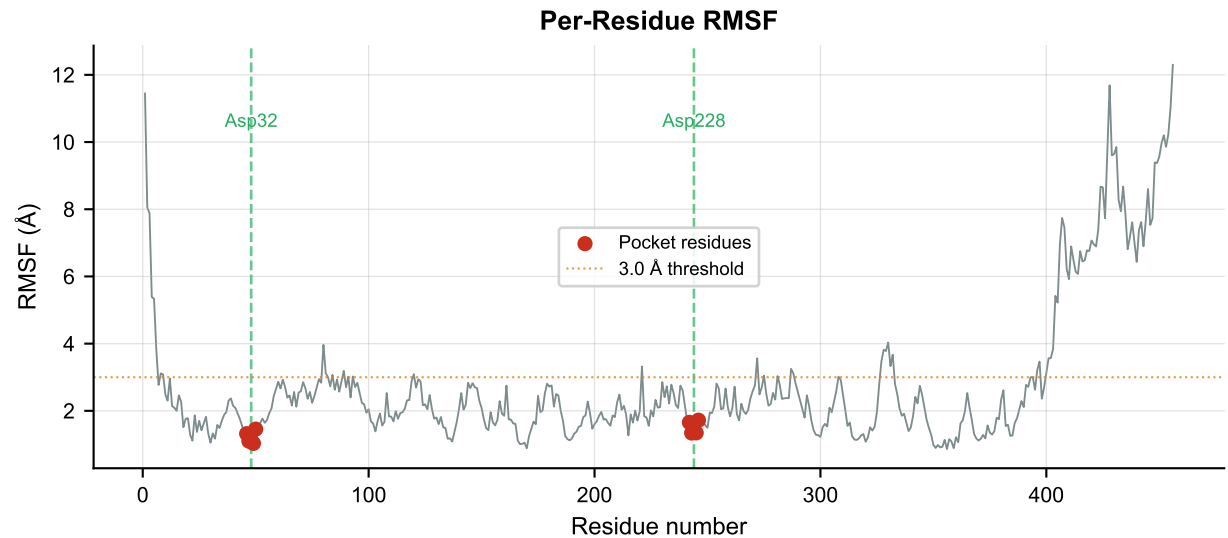




Simulation Summary

H-bonds (mean):	1.17 ± 0.66
H-bond pairs ≤3.5Å:	1.32
H-bonds unique:	19
Max H-bond occupancy:	0.837
Mean H-bond occupancy:	0.062
Min P-L distance:	2.03 Å
Rg (mean):	3.0252 ± 0.0659 nm
SASA protein (mean):	247.93 nm ²
RMSD ligand (mean):	4.06 ± 1.08 Å
RMSD protein (mean):	5.25 ± 1.31 Å
RMSF pocket (mean):	1.345 ± 0.214 Å

Classification

Marginal

$\Delta G = -24.89$ kJ/mol
RMSD lig = 4.06 Å
H-bonds = 1.17