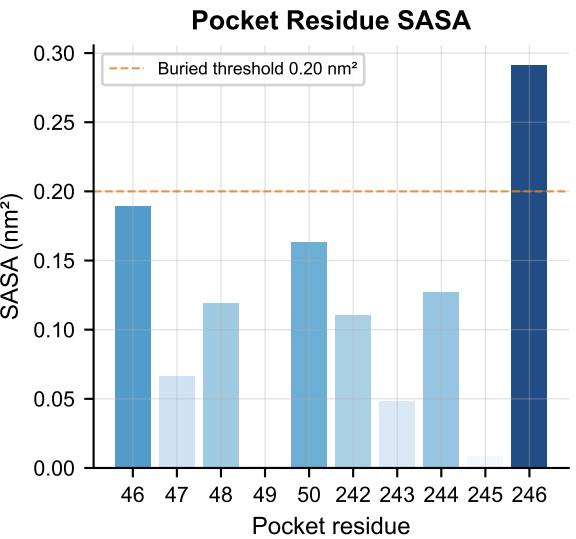
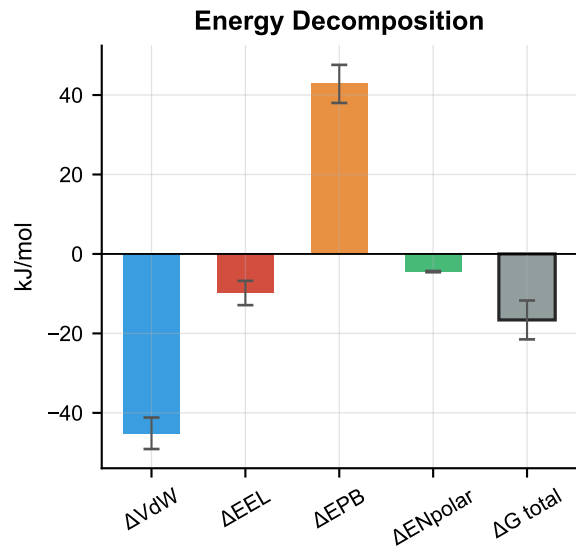
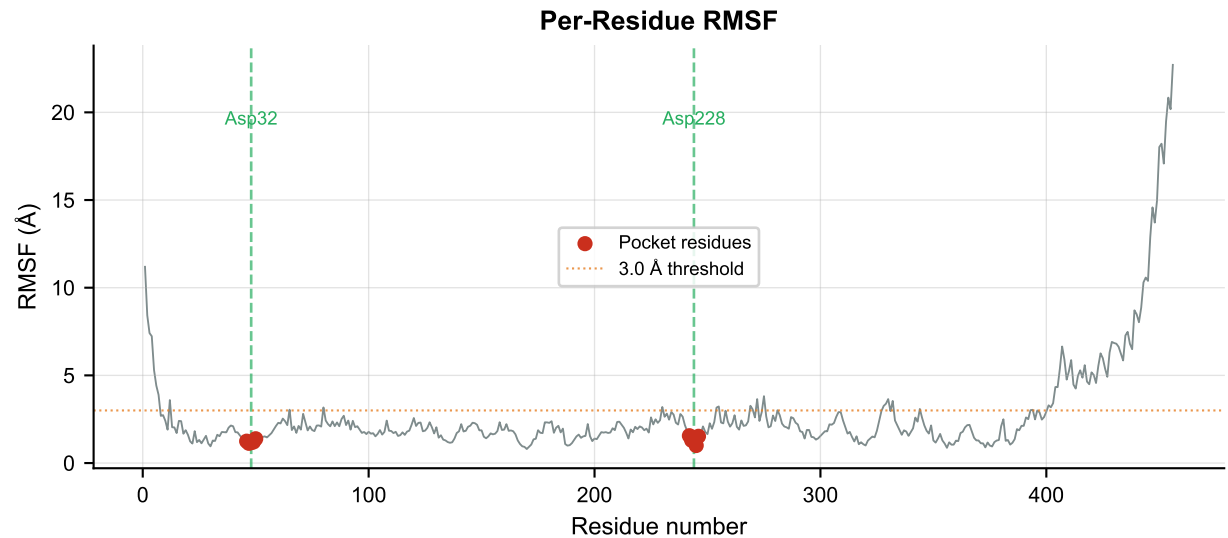




Simulation Summary

H-bonds (mean):	1.05 ± 0.94
H-bond pairs ≤3.5Å:	3.18
H-bonds unique:	20
Max H-bond occupancy:	0.315
Mean H-bond occupancy:	0.052
Min P-L distance:	1.94 Å
Rg (mean):	2.8950 ± 0.0811 nm
SASA protein (mean):	248.39 nm ²
RMSD ligand (mean):	2.41 ± 0.70 Å
RMSD protein (mean):	5.00 ± 1.77 Å
RMSF pocket (mean):	1.280 ± 0.164 Å

Classification

Marginal

$\Delta G = -16.61$ kJ/mol
RMSD lig = 2.41 Å
H-bonds = 1.05