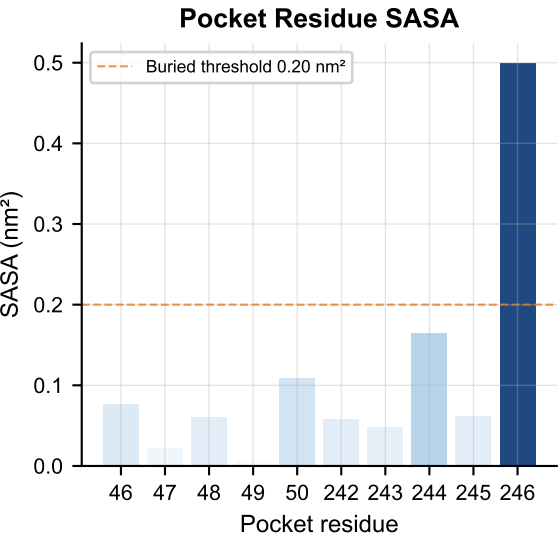
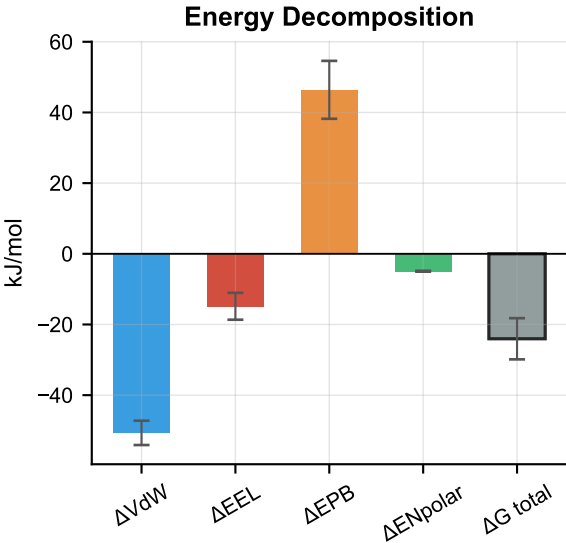
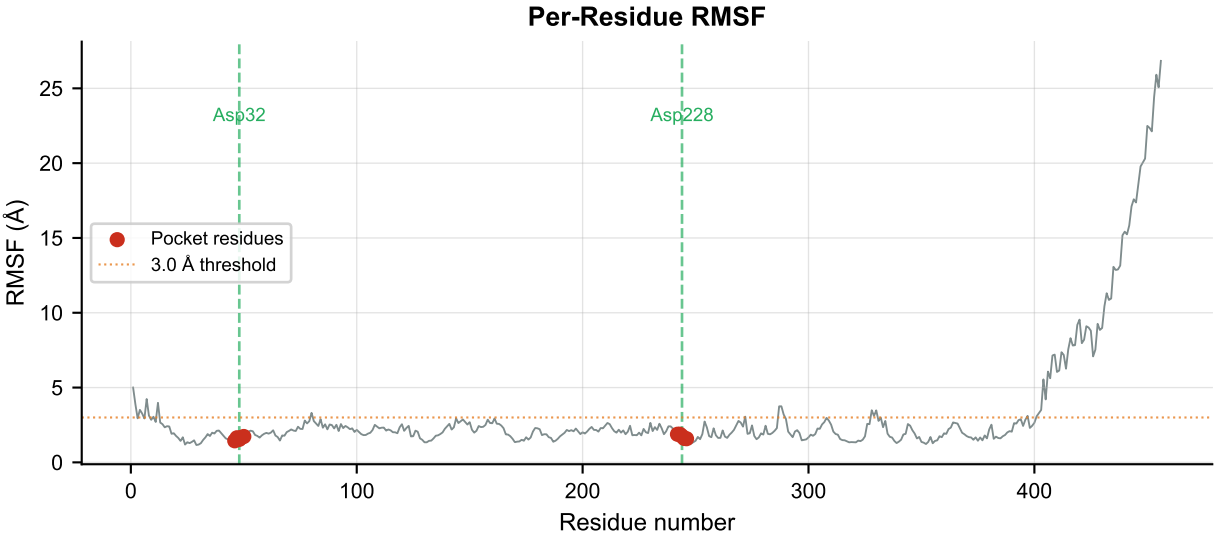




Simulation Summary

H-bonds (mean):	1.48 ± 0.87
H-bond pairs ≤3.5Å:	1.90
H-bonds unique:	10
Max H-bond occupancy:	0.667
Mean H-bond occupancy:	0.148
Min P-L distance:	2.04 Å
Rg (mean):	2.7033 ± 0.1633 nm
SASA protein (mean):	242.49 nm ²
RMSD ligand (mean):	3.24 ± 1.18 Å
RMSD protein (mean):	7.77 ± 3.47 Å
RMSF pocket (mean):	1.671 ± 0.135 Å

Classification

Marginal

$\Delta G = -24.05$ kJ/mol
RMSD lig = 3.24 Å
H-bonds = 1.48