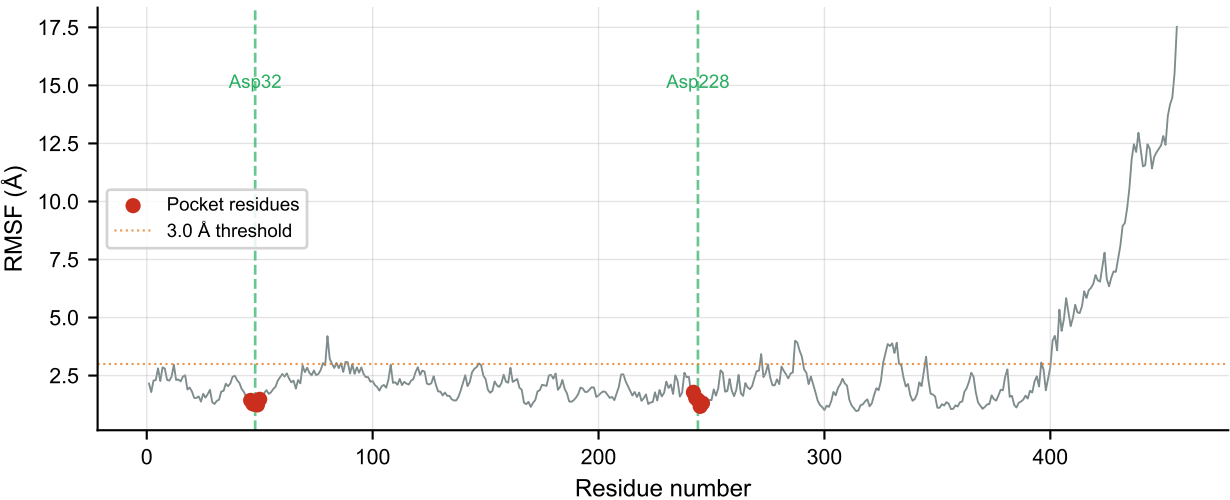
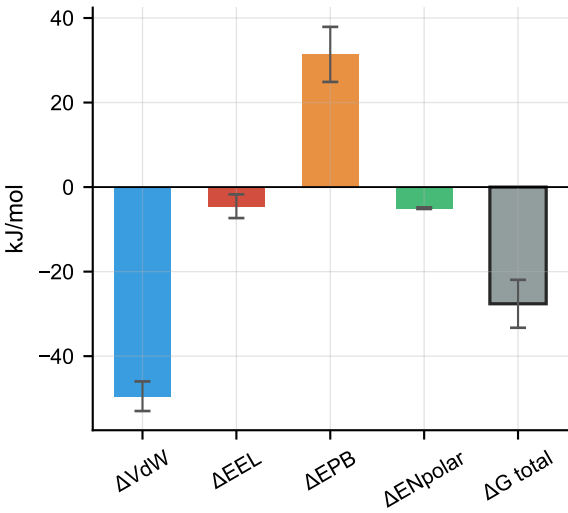


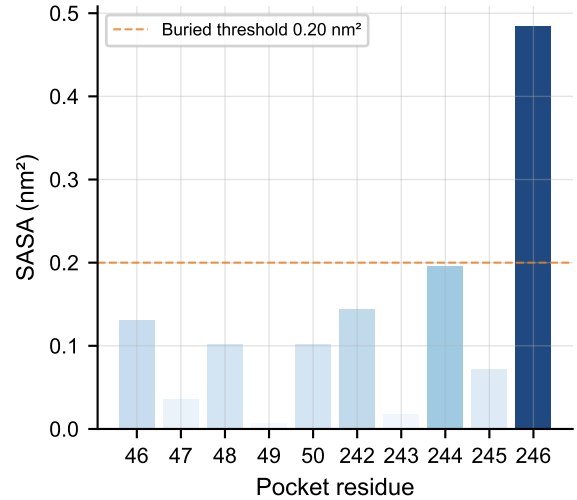
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.50 ± 0.54
H-bond pairs ≤3.5Å:	0.87
H-bonds unique:	10
Max H-bond occupancy:	0.456
Mean H-bond occupancy:	0.050
Min P-L distance:	2.03 Å
Rg (mean):	2.8911 ± 0.1650 nm
SASA protein (mean):	242.78 nm²
RMSD ligand (mean):	5.96 ± 1.35 Å
RMSD protein (mean):	5.79 ± 1.99 Å
RMSF pocket (mean):	1.393 ± 0.170 Å

Classification

Marginal

$\Delta G = -27.61$ kJ/mol
RMSD lig = 5.96 Å
H-bonds = 0.50