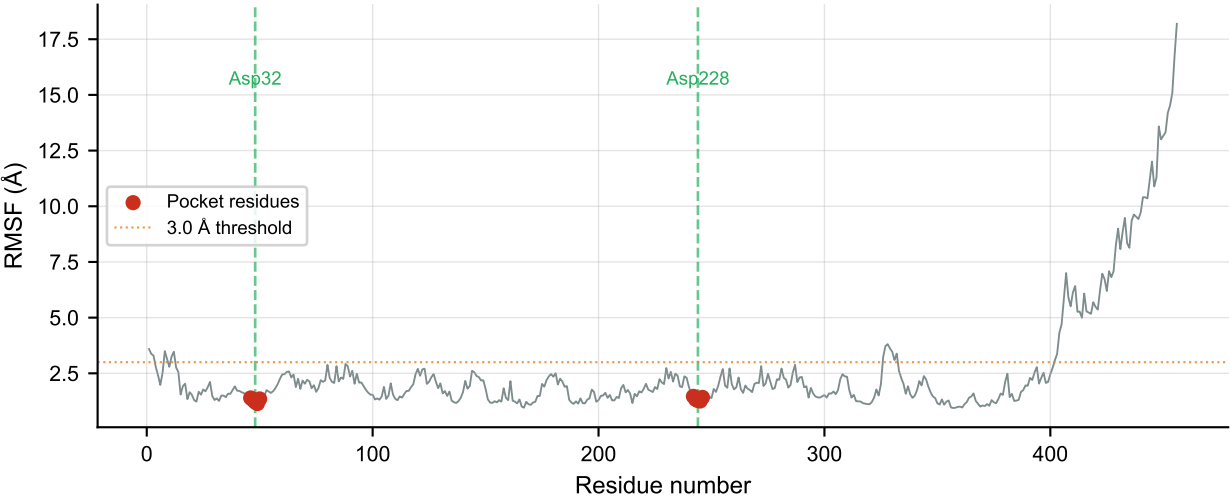
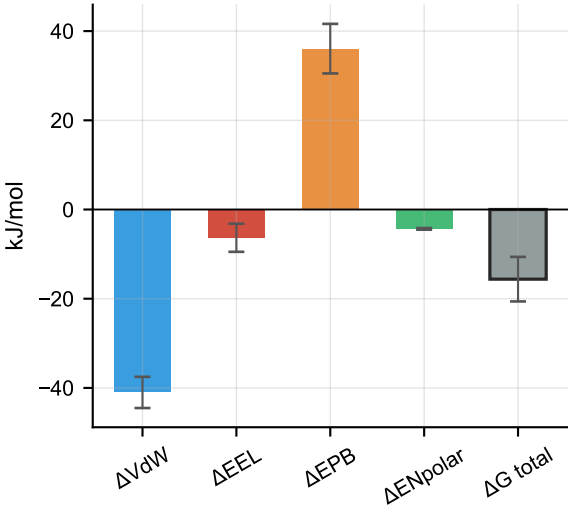


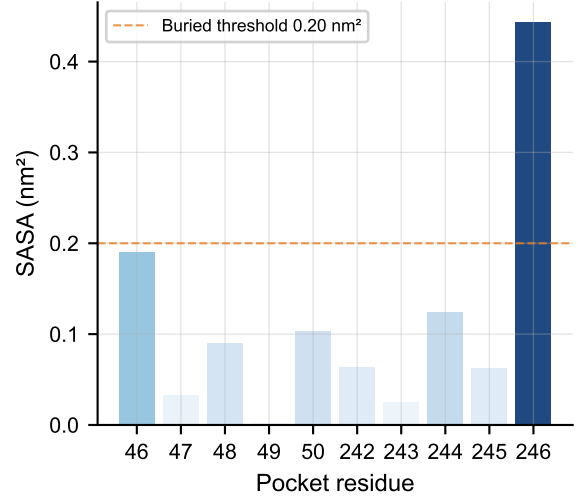
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.74 ± 0.57
H-bond pairs ≤3.5Å:	1.64
H-bonds unique:	13
Max H-bond occupancy:	0.637
Mean H-bond occupancy:	0.057
Min P-L distance:	1.87 Å
Rg (mean):	2.8608 ± 0.0470 nm
SASA protein (mean):	241.68 nm ²
RMSD ligand (mean):	3.71 ± 1.02 Å
RMSD protein (mean):	3.97 ± 1.04 Å
RMSF pocket (mean):	1.316 ± 0.093 Å

Classification

Marginal

$\Delta G = -15.62$ kJ/mol
RMSD lig = 3.71 Å
H-bonds = 0.74