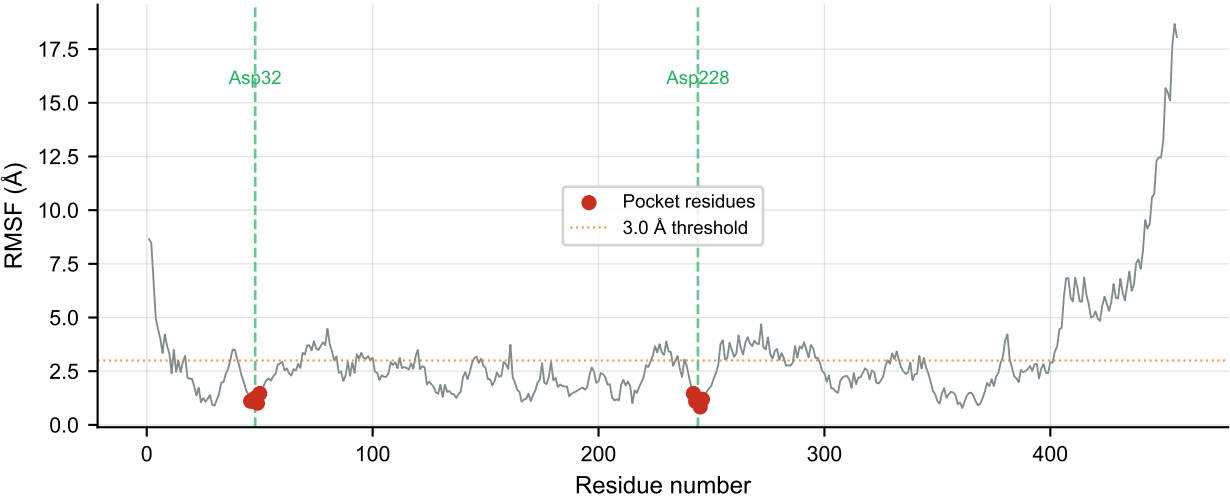
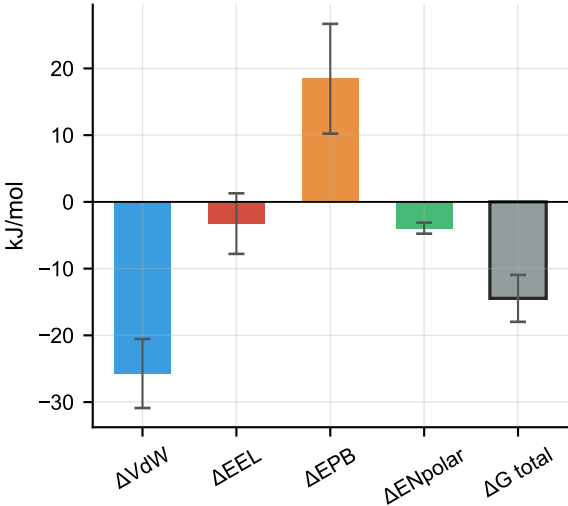


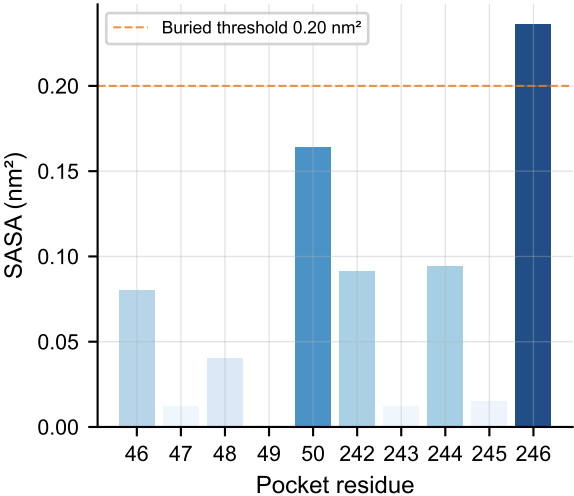
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.59 ± 0.78
H-bond pairs ≤3.5Å:	2.14
H-bonds unique:	59
Max H-bond occupancy:	0.083
Mean H-bond occupancy:	0.010
Min P-L distance:	2.04 Å
Rg (mean):	2.8125 ± 0.0971 nm
SASA protein (mean):	244.24 nm ²
RMSD ligand (mean):	10.83 ± 2.65 Å
RMSD protein (mean):	7.39 ± 2.01 Å
RMSF pocket (mean):	1.176 ± 0.180 Å

Classification

Marginal

$\Delta G = -14.46$ kJ/mol
RMSD lig = 10.83 Å
H-bonds = 0.59