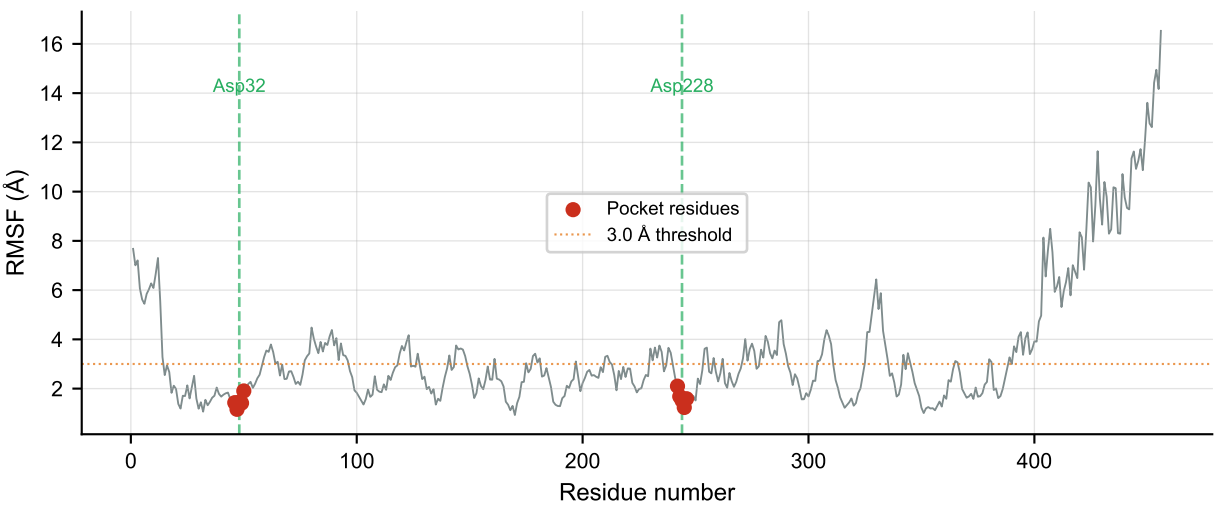
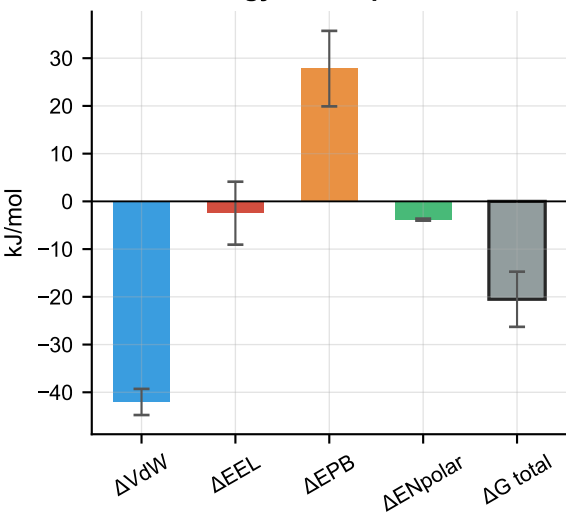


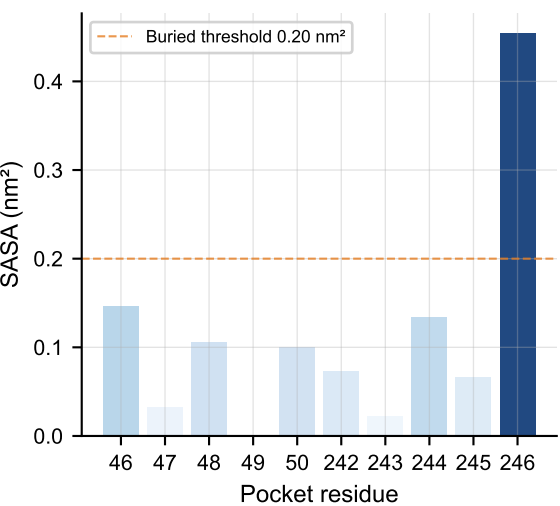
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.08 ± 0.27
H-bond pairs ≤3.5Å:	0.71
H-bonds unique:	5
Max H-bond occupancy:	0.048
Mean H-bond occupancy:	0.016
Min P-L distance:	2.49 Å
Rg (mean):	2.9848 ± 0.0641 nm
SASA protein (mean):	246.54 nm ²
RMSD ligand (mean):	4.76 ± 1.69 Å
RMSD protein (mean):	4.57 ± 1.93 Å
RMSF pocket (mean):	1.548 ± 0.273 Å

Classification

Marginal

$\Delta G = -20.51$ kJ/mol
RMSD lig = 4.76 Å
H-bonds = 0.08