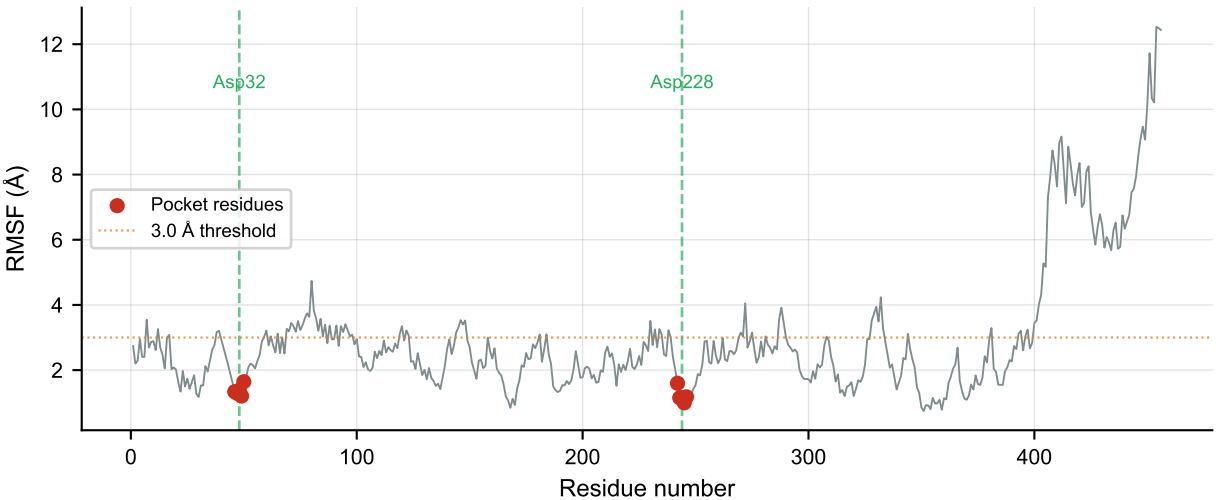
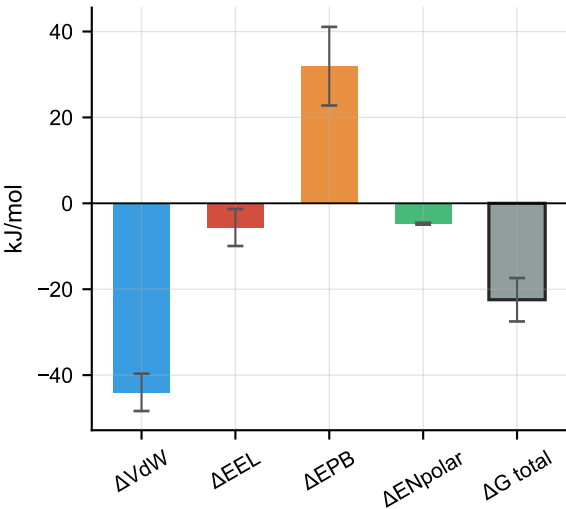


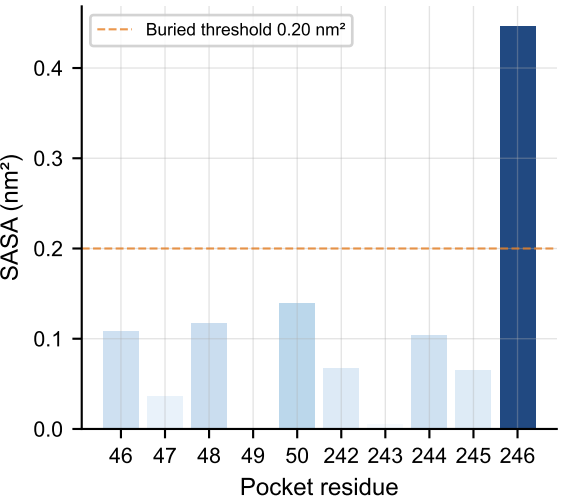
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.75 ± 0.85
H-bond pairs ≤3.5Å:	2.77
H-bonds unique:	22
Max H-bond occupancy:	0.224
Mean H-bond occupancy:	0.034
Min P-L distance:	2.04 Å
Rg (mean):	3.1292 ± 0.0701 nm
SASA protein (mean):	242.82 nm ²
RMSD ligand (mean):	5.33 ± 1.47 Å
RMSD protein (mean):	6.76 ± 1.79 Å
RMSF pocket (mean):	1.294 ± 0.194 Å

Classification

Marginal

$\Delta G = -22.45$ kJ/mol
RMSD lig = 5.33 Å
H-bonds = 0.75