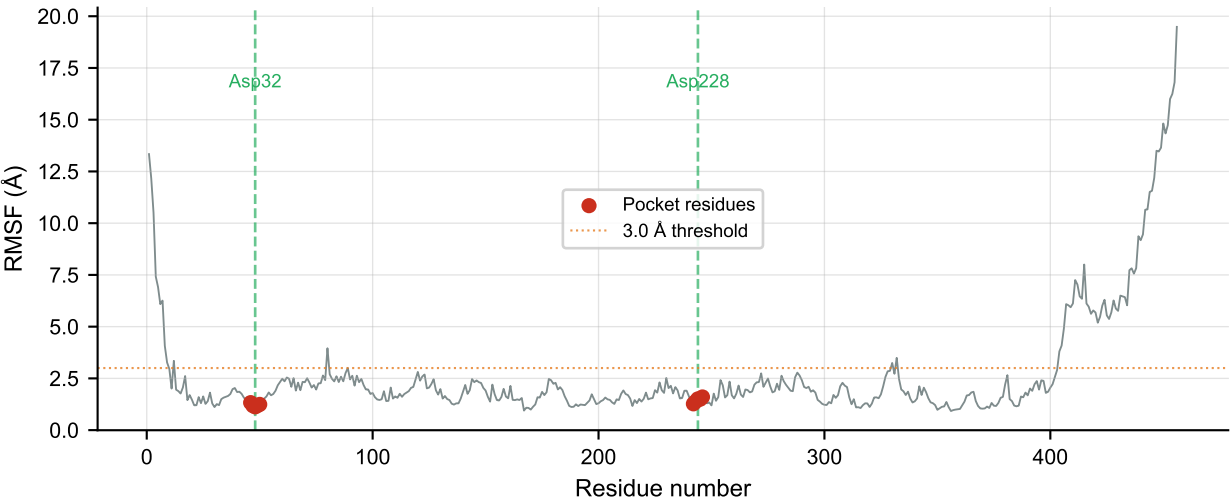
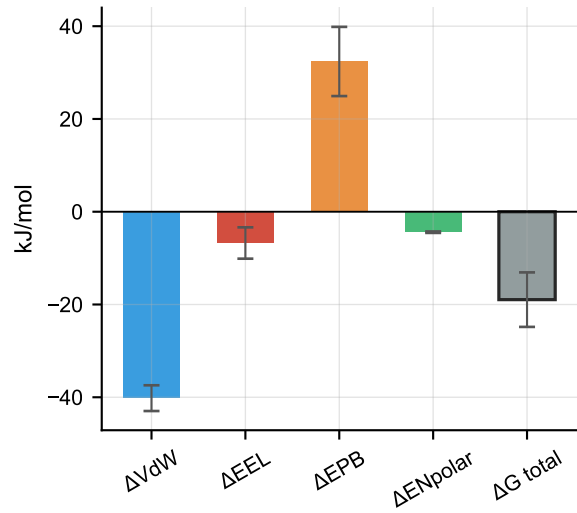


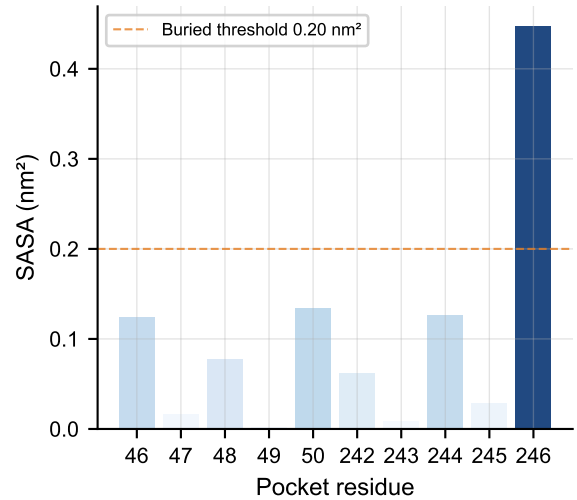
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	1.15 ± 0.72
H-bond pairs ≤3.5Å:	3.02
H-bonds unique:	15
Max H-bond occupancy:	0.718
Mean H-bond occupancy:	0.076
Min P-L distance:	2.06 Å
Rg (mean):	2.9854 ± 0.0519 nm
SASA protein (mean):	248.41 nm²
RMSD ligand (mean):	4.85 ± 1.00 Å
RMSD protein (mean):	5.81 ± 1.72 Å
RMSF pocket (mean):	1.333 ± 0.152 Å

Classification

Marginal

$\Delta G = -18.96$ kJ/mol
RMSD lig = 4.85 Å
H-bonds = 1.15