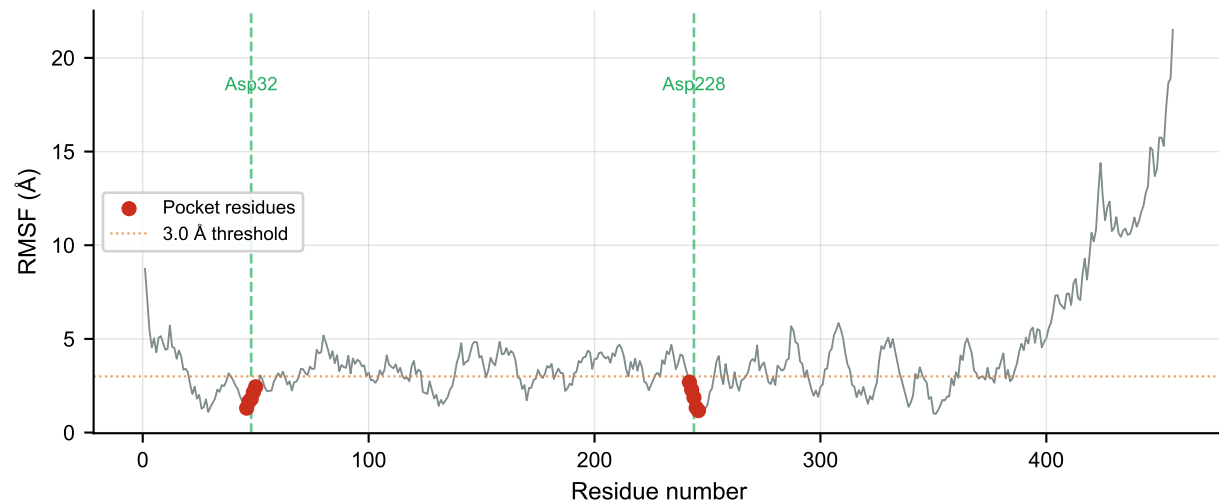
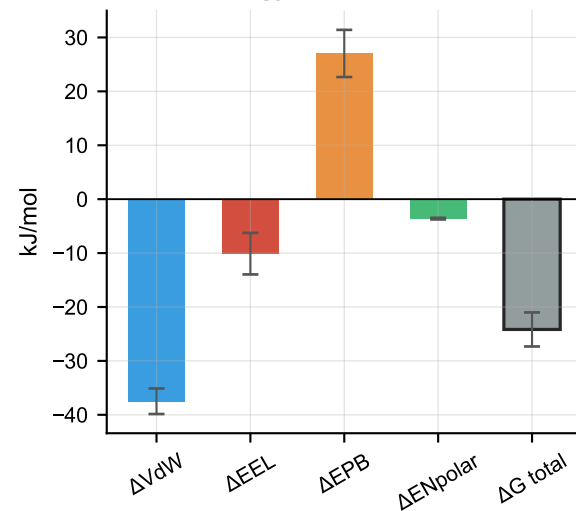


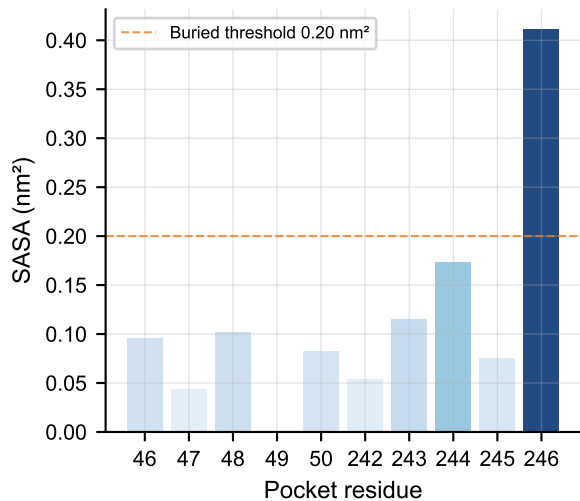
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.07 ± 0.26
H-bond pairs ≤3.5Å:	0.22
H-bonds unique:	4
Max H-bond occupancy:	0.061
Mean H-bond occupancy:	0.018
Min P-L distance:	2.42 Å
Rg (mean):	2.8172 ± 0.1924 nm
SASA protein (mean):	241.82 nm ²
RMSD ligand (mean):	5.79 ± 1.41 Å
RMSD protein (mean):	9.66 ± 3.49 Å
RMSF pocket (mean):	1.871 ± 0.492 Å

Classification

Marginal

$\Delta G = -24.17$ kJ/mol
RMSD lig = 5.79 Å
H-bonds = 0.07