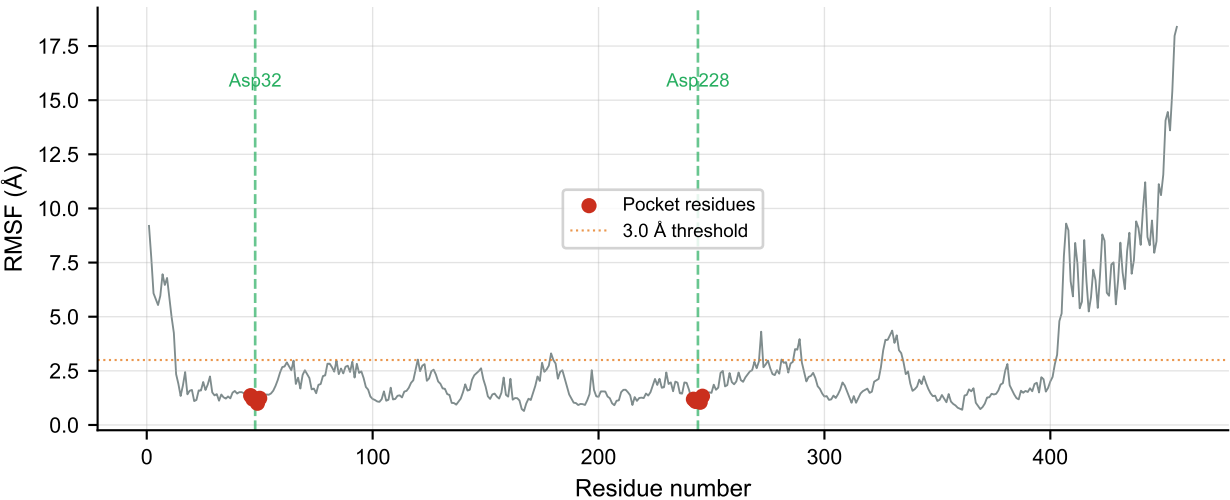
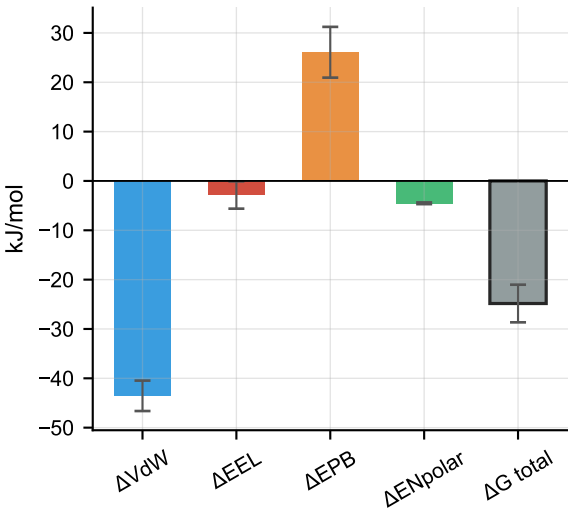


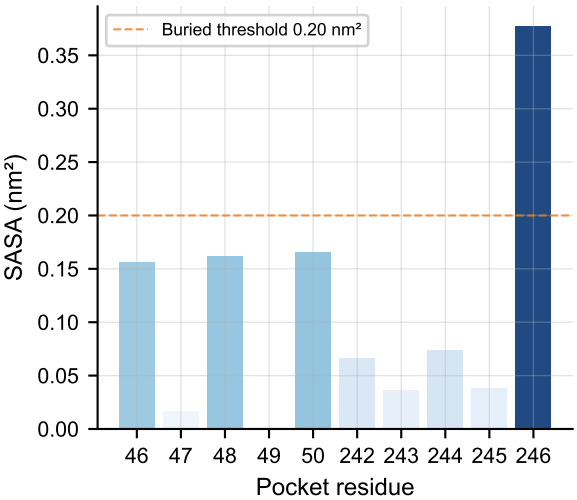
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.10 ± 0.33
H-bond pairs ≤3.5Å:	0.41
H-bonds unique:	8
Max H-bond occupancy:	0.074
Mean H-bond occupancy:	0.013
Min P-L distance:	2.05 Å
Rg (mean):	2.7783 ± 0.1171 nm
SASA protein (mean):	248.43 nm²
RMSD ligand (mean):	4.81 ± 0.92 Å
RMSD protein (mean):	5.60 ± 2.15 Å
RMSF pocket (mean):	1.181 ± 0.106 Å

Classification

Marginal

$\Delta G = -24.84$ kJ/mol
RMSD lig = 4.81 Å
H-bonds = 0.10