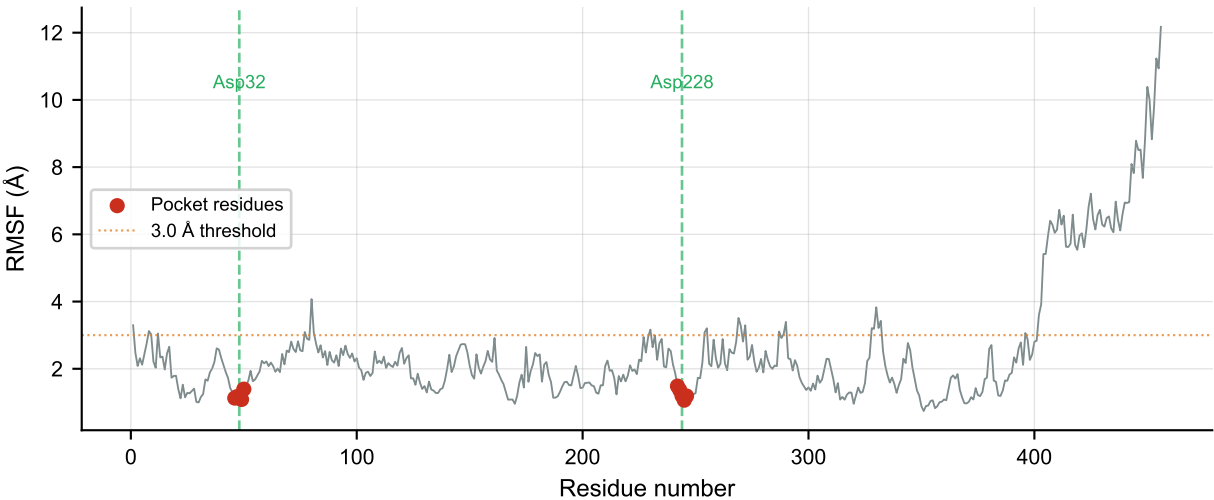
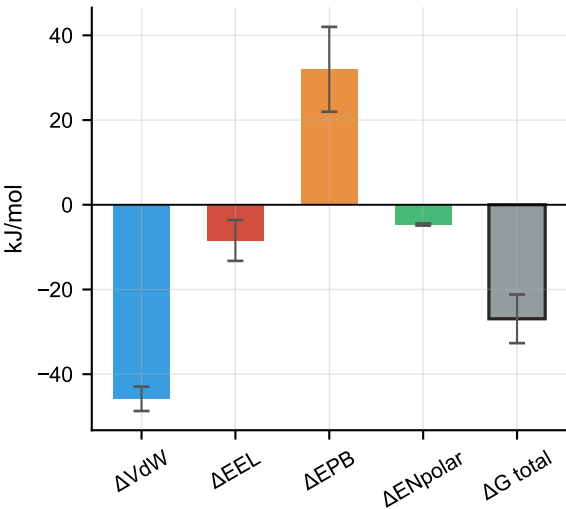


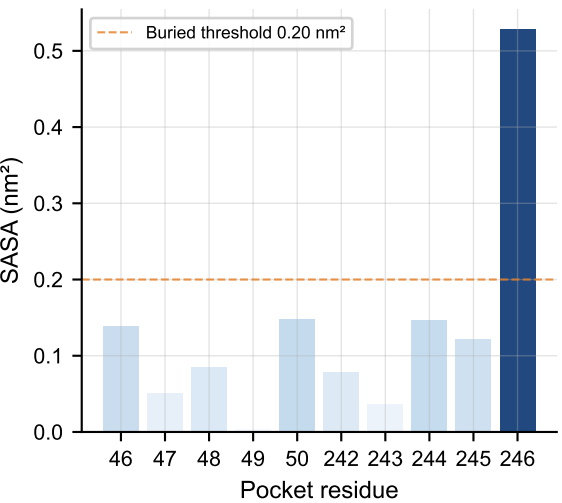
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	1.06 ± 0.83
H-bond pairs ≤3.5Å:	1.68
H-bonds unique:	26
Max H-bond occupancy:	0.361
Mean H-bond occupancy:	0.041
Min P-L distance:	2.00 Å
Rg (mean):	3.0818 ± 0.0887 nm
SASA protein (mean):	243.90 nm²
RMSD ligand (mean):	6.59 ± 1.89 Å
RMSD protein (mean):	5.05 ± 1.15 Å
RMSF pocket (mean):	1.224 ± 0.134 Å

Classification

Marginal

$\Delta G = -26.92$ kJ/mol
RMSD lig = 6.59 Å
H-bonds = 1.06