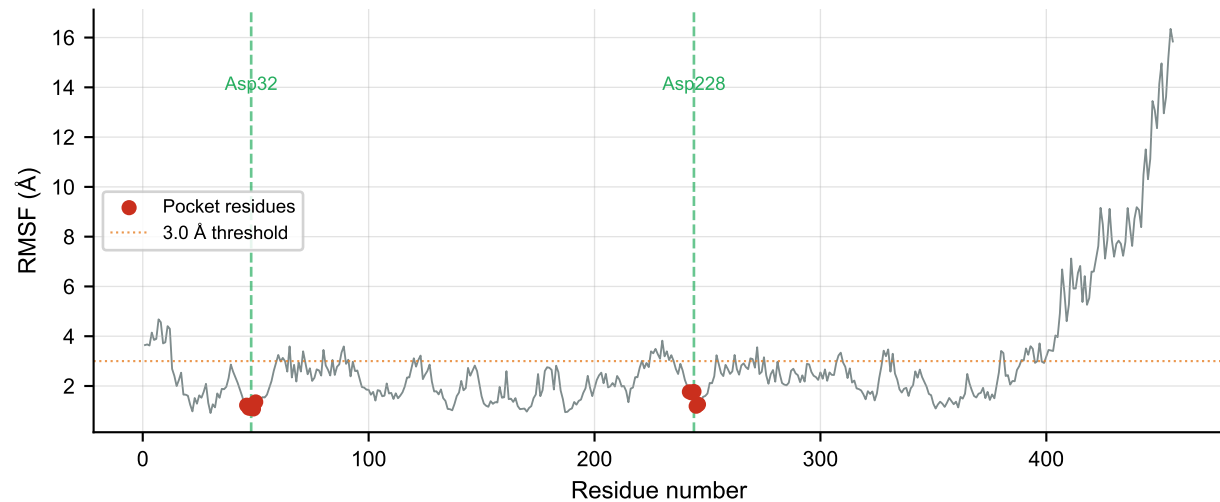
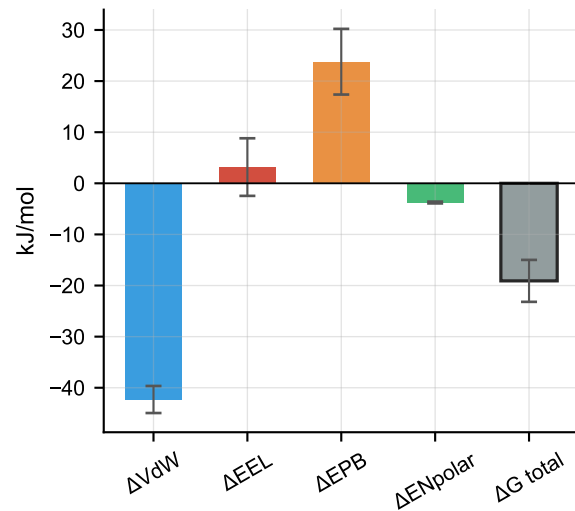


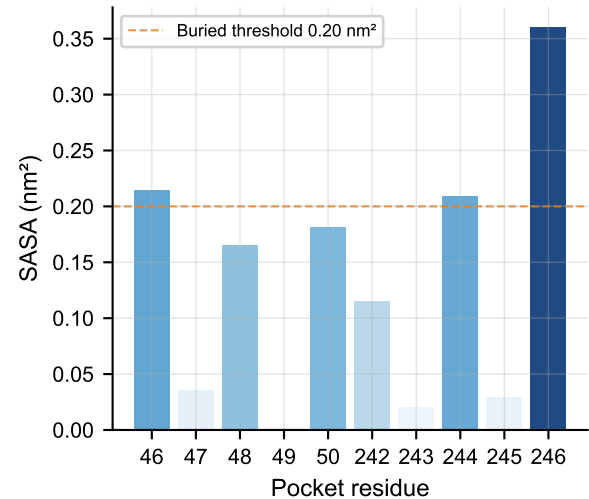
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.02 ± 0.15
H-bond pairs ≤3.5Å:	0.19
H-bonds unique:	5
Max H-bond occupancy:	0.012
Mean H-bond occupancy:	0.005
Min P-L distance:	2.41 Å
Rg (mean):	2.7513 ± 0.1042 nm
SASA protein (mean):	247.15 nm²
RMSD ligand (mean):	5.13 ± 1.51 Å
RMSD protein (mean):	6.63 ± 2.59 Å
RMSF pocket (mean):	1.360 ± 0.271 Å

Classification

Marginal

$\Delta G = -19.09$ kJ/mol
RMSD lig = 5.13 Å
H-bonds = 0.02