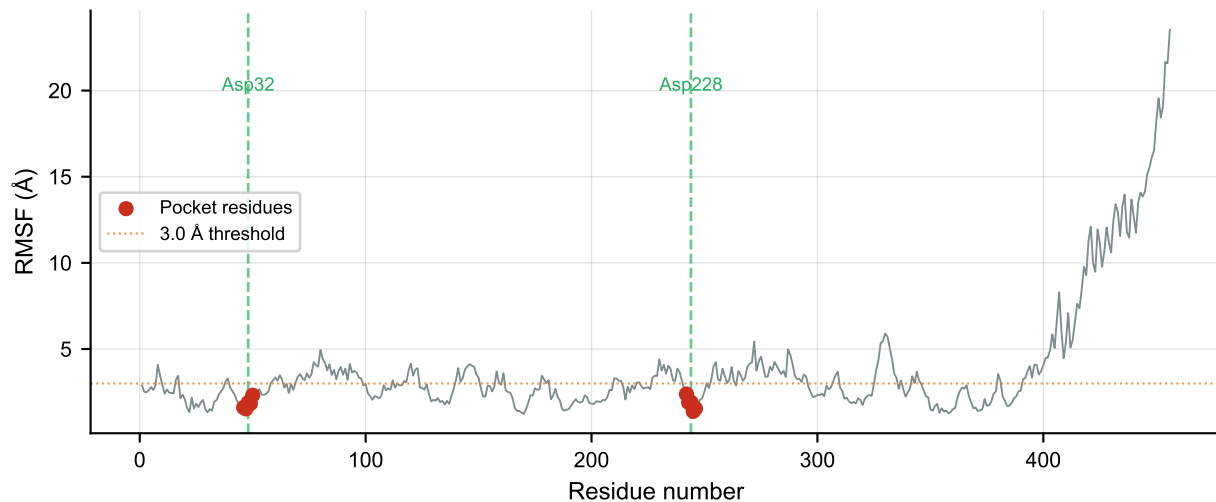
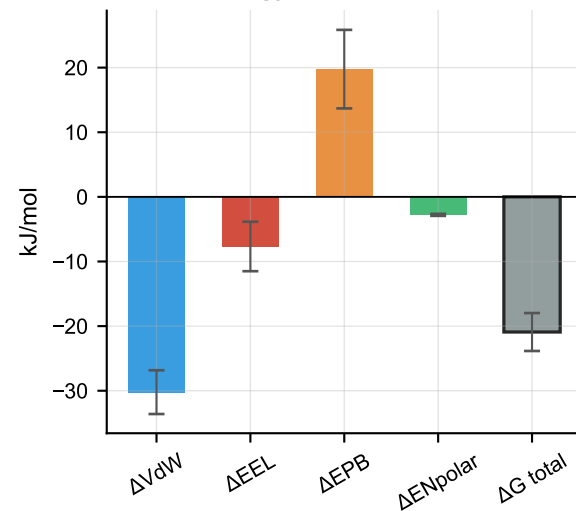


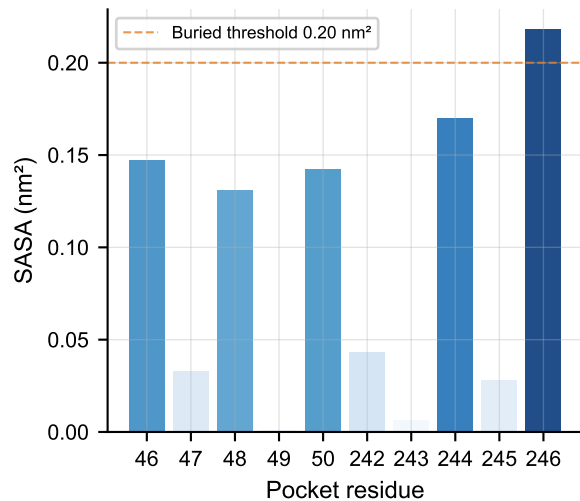
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.76 ± 0.74
H-bond pairs ≤3.5Å:	1.34
H-bonds unique:	7
Max H-bond occupancy:	0.473
Mean H-bond occupancy:	0.108
Min P-L distance:	2.31 Å
Rg (mean):	2.8788 ± 0.0636 nm
SASA protein (mean):	239.05 nm ²
RMSD ligand (mean):	8.39 ± 2.09 Å
RMSD protein (mean):	6.45 ± 2.20 Å
RMSF pocket (mean):	1.831 ± 0.316 Å

Classification

Marginal

$\Delta G = -20.91$ kJ/mol
RMSD lig = 8.39 Å
H-bonds = 0.76