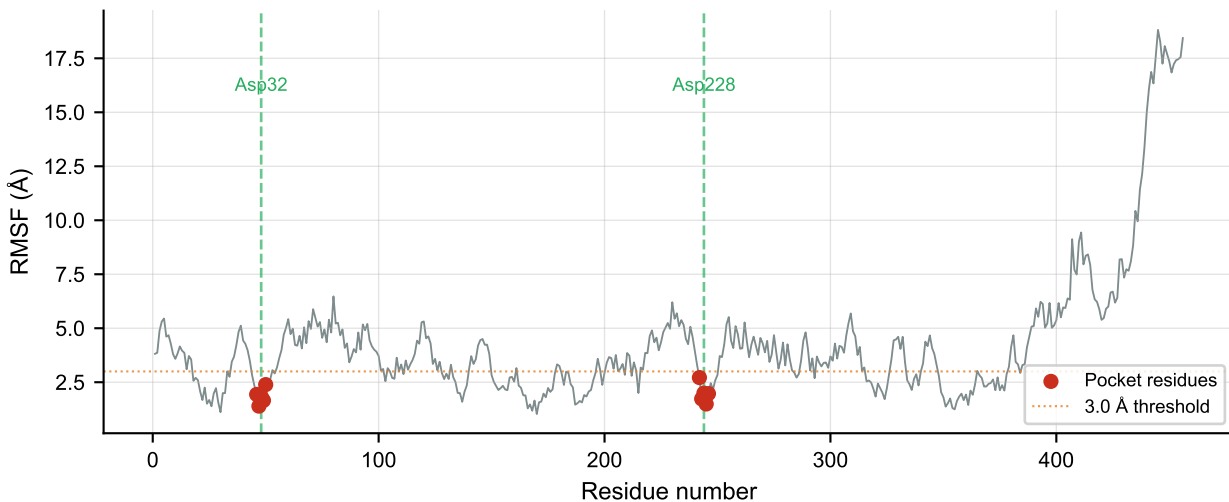
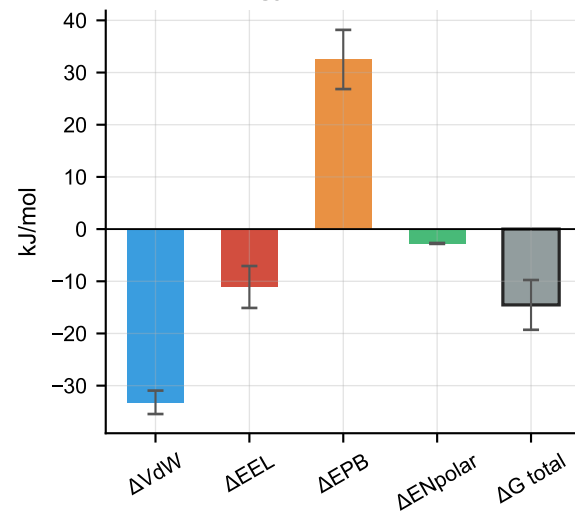


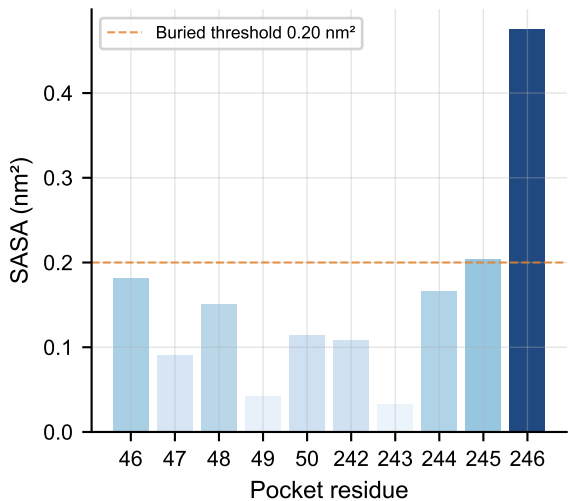
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.28 ± 0.45
H-bond pairs ≤3.5Å:	0.43
H-bonds unique:	3
Max H-bond occupancy:	0.278
Mean H-bond occupancy:	0.093
Min P-L distance:	2.46 Å
Rg (mean):	2.7513 ± 0.1123 nm
SASA protein (mean):	241.08 nm²
RMSD ligand (mean):	3.56 ± 1.76 Å
RMSD protein (mean):	7.04 ± 2.71 Å
RMSF pocket (mean):	1.912 ± 0.379 Å

Classification

Marginal

$\Delta G = -14.53$ kJ/mol
RMSD lig = 3.56 Å
H-bonds = 0.28