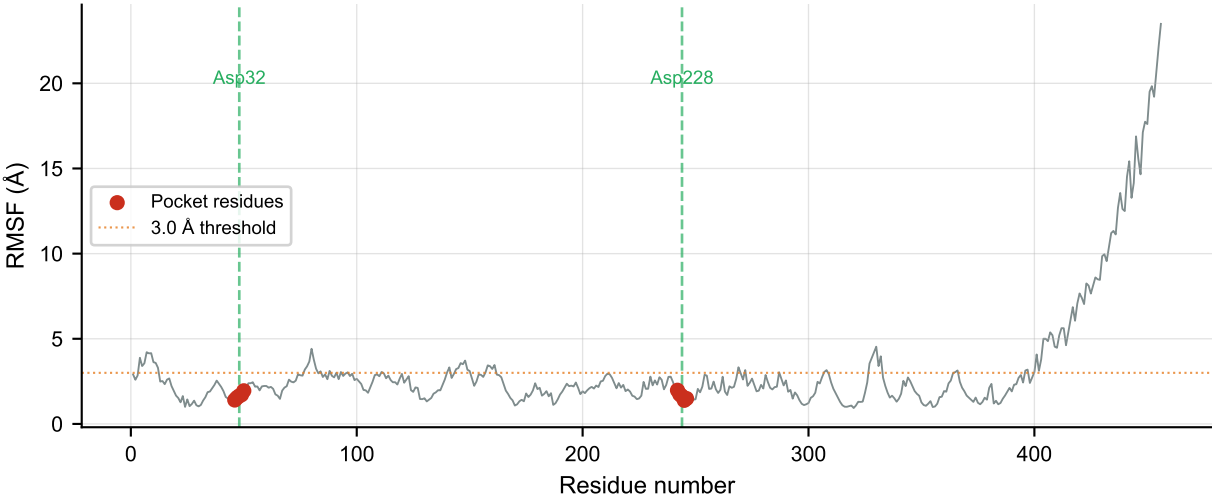
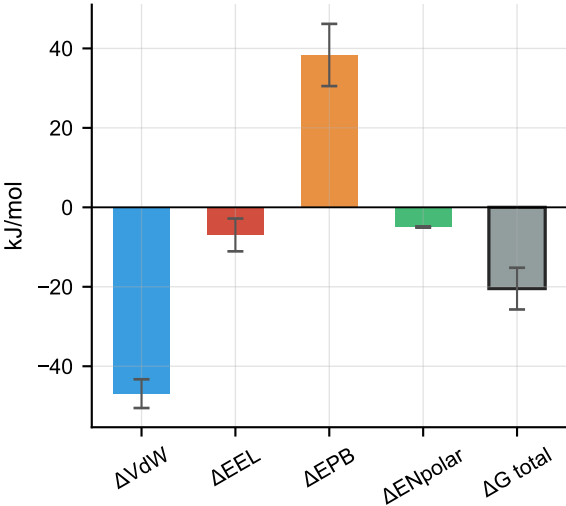


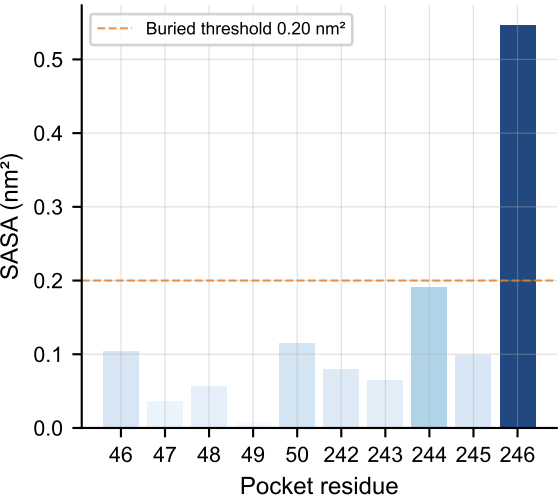
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.60 ± 0.72
H-bond pairs ≤3.5Å:	3.24
H-bonds unique:	15
Max H-bond occupancy:	0.198
Mean H-bond occupancy:	0.040
Min P-L distance:	1.94 Å
Rg (mean):	2.9517 ± 0.0859 nm
SASA protein (mean):	241.78 nm ²
RMSD ligand (mean):	4.65 ± 1.26 Å
RMSD protein (mean):	5.88 ± 2.21 Å
RMSF pocket (mean):	1.648 ± 0.194 Å

Classification

Marginal

$\Delta G = -20.46$ kJ/mol
RMSD lig = 4.65 Å
H-bonds = 0.60