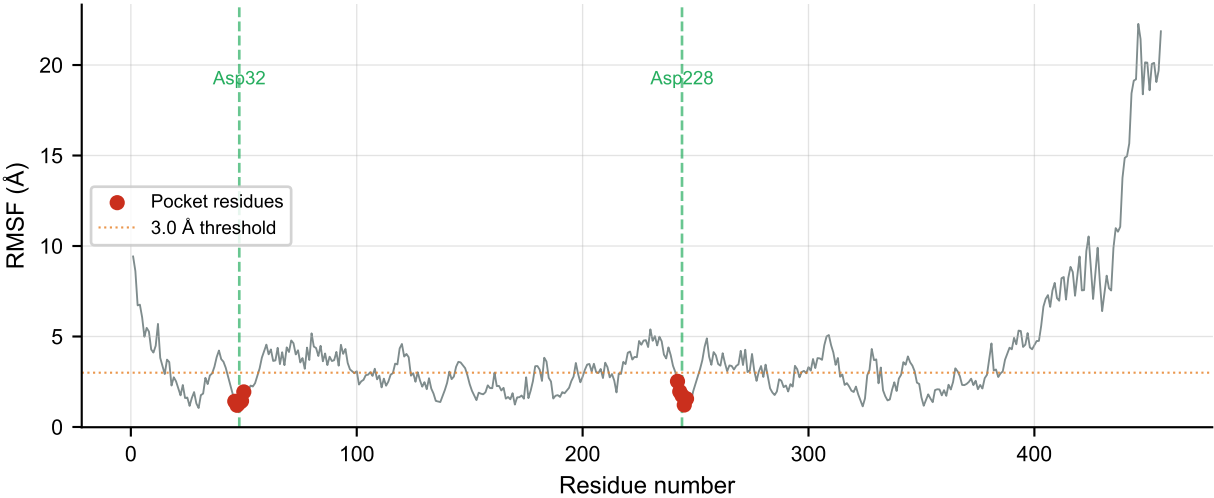
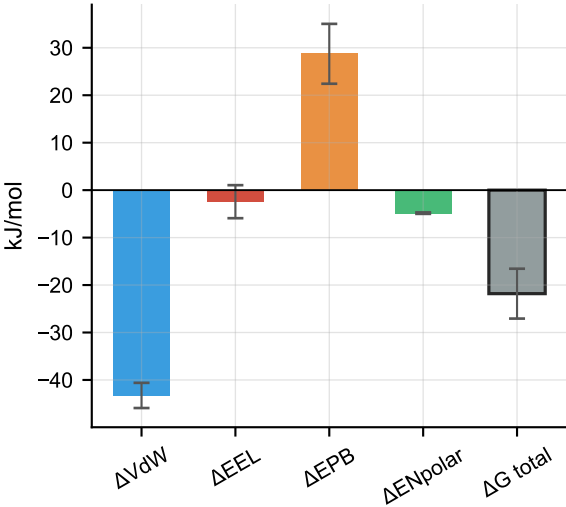


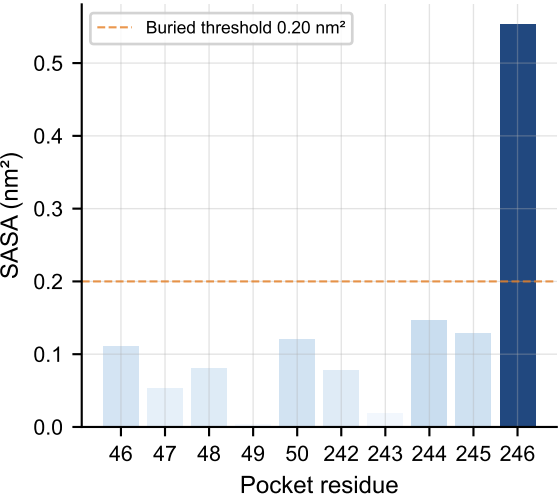
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	0.25 ± 0.47
H-bond pairs ≤3.5Å:	2.98
H-bonds unique:	8
Max H-bond occupancy:	0.108
Mean H-bond occupancy:	0.031
Min P-L distance:	2.05 Å
Rg (mean):	2.8475 ± 0.1297 nm
SASA protein (mean):	243.87 nm ²
RMSD ligand (mean):	4.87 ± 1.12 Å
RMSD protein (mean):	7.81 ± 3.26 Å
RMSF pocket (mean):	1.632 ± 0.393 Å

Classification

Marginal

$\Delta G = -21.81$ kJ/mol
RMSD lig = 4.87 Å
H-bonds = 0.25