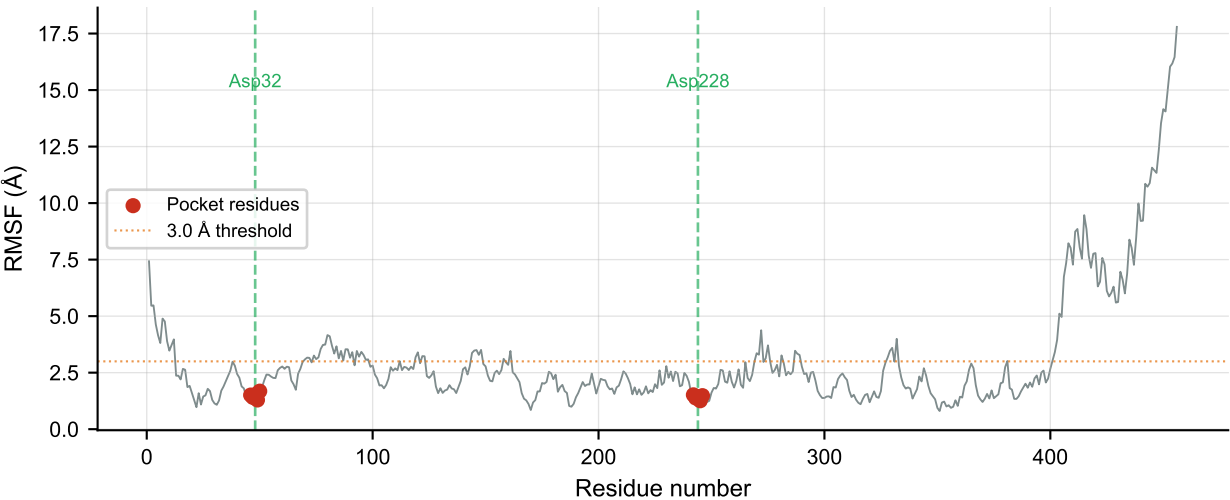
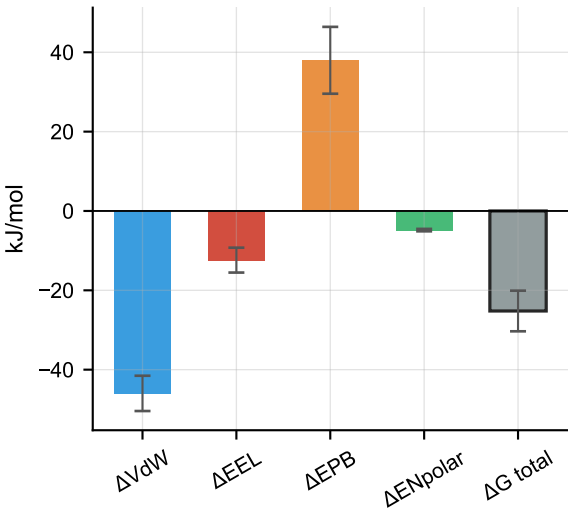


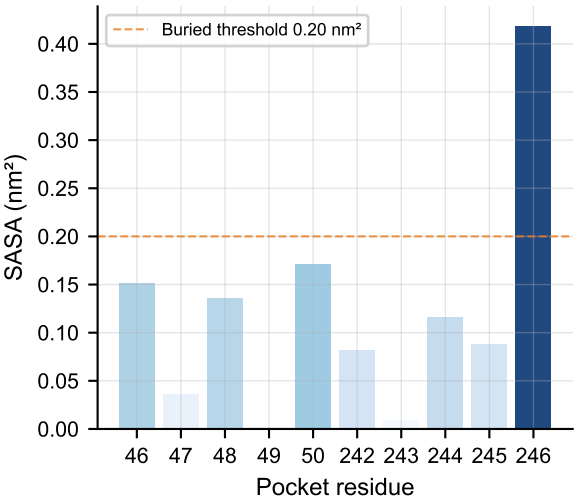
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

H-bonds (mean):	1.23 ± 0.79
H-bond pairs ≤3.5Å:	1.42
H-bonds unique:	18
Max H-bond occupancy:	0.723
Mean H-bond occupancy:	0.068
Min P-L distance:	1.99 Å
Rg (mean):	2.9585 ± 0.0616 nm
SASA protein (mean):	246.27 nm²
RMSD ligand (mean):	5.06 ± 2.00 Å
RMSD protein (mean):	6.20 ± 2.43 Å
RMSF pocket (mean):	1.449 ± 0.117 Å

Classification

Marginal

$\Delta G = -25.21$ kJ/mol
RMSD lig = 5.06 Å
H-bonds = 1.23