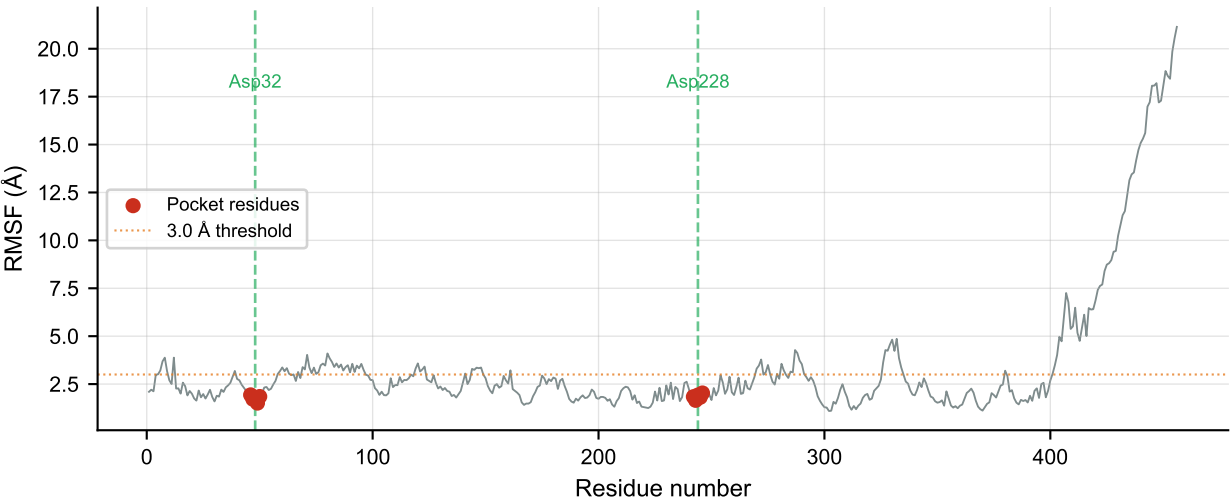
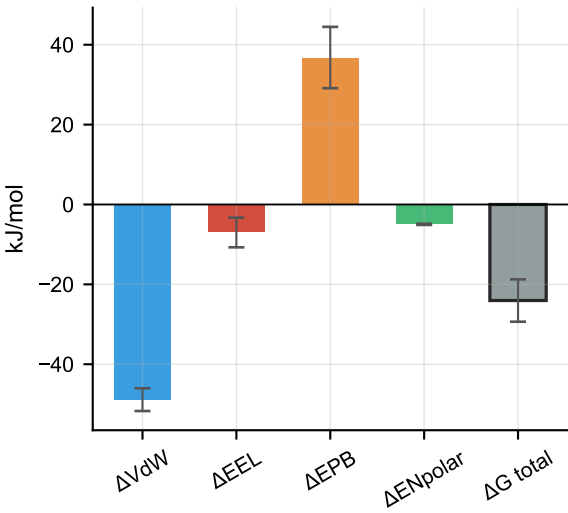


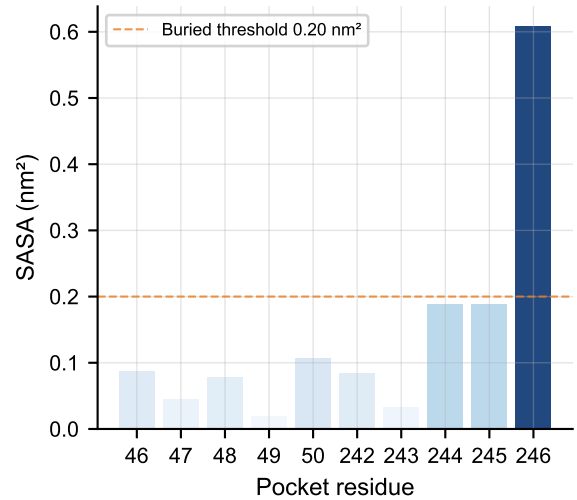
Per-Residue RMSF



Energy Decomposition



Pocket Residue SASA



Simulation Summary

|                        |                        |
|------------------------|------------------------|
| H-bonds (mean):        | 0.37 ± 0.67            |
| H-bond pairs ≤3.5Å:    | 1.02                   |
| H-bonds unique:        | 14                     |
| Max H-bond occupancy:  | 0.200                  |
| Mean H-bond occupancy: | 0.026                  |
| Min P-L distance:      | 2.02 Å                 |
| Rg (mean):             | 2.6560 ± 0.1493 nm     |
| SASA protein (mean):   | 243.66 nm <sup>2</sup> |
| RMSD ligand (mean):    | 4.86 ± 1.48 Å          |
| RMSD protein (mean):   | 7.98 ± 2.91 Å          |
| RMSF pocket (mean):    | 1.801 ± 0.145 Å        |

Classification

**Marginal**

$\Delta G = -24.05$  kJ/mol  
RMSD lig = 4.86 Å  
H-bonds = 0.37