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Supplemental Information

Influence of Protein Scaffold on Side-Chain Transfer Free Energies

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Supporting Information for:

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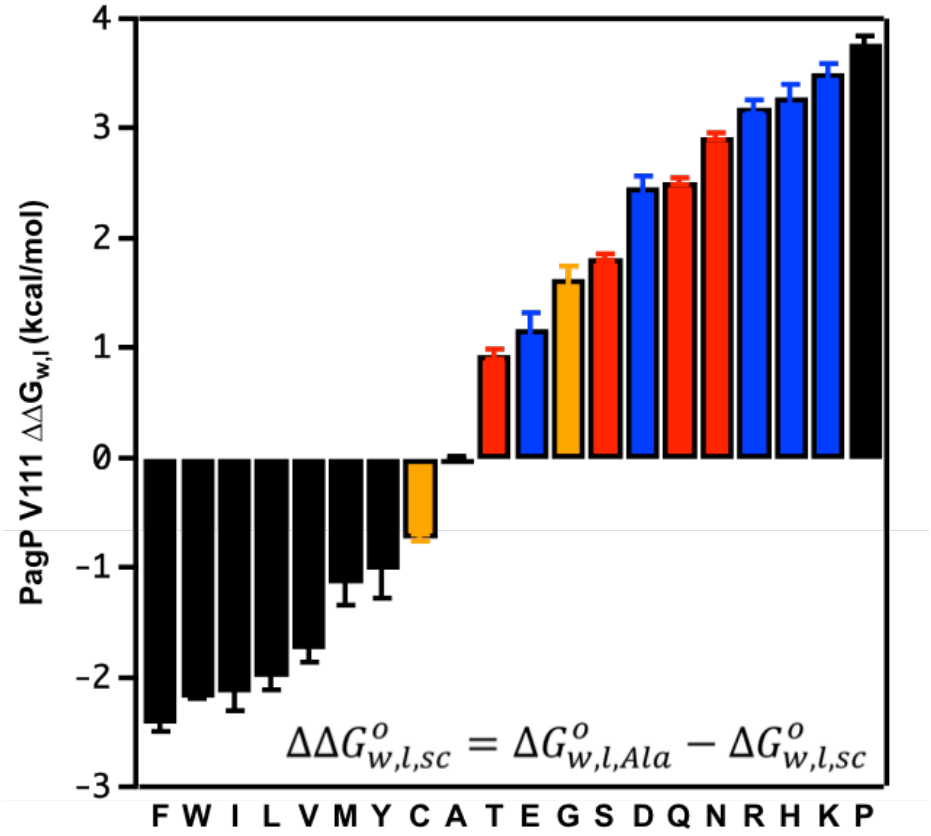
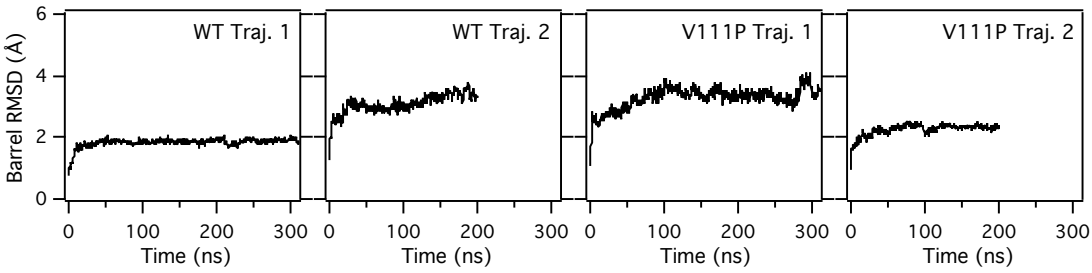
Figure S1. PagP site 111 experimentally determined side chain energy values for all twenty amino acids.



$\Delta\Delta G^{o}_{w,l}$ values were calculated by taking the difference in the stability of the V111A variant of PagP and V111X variant, where X is any amino acid (equation shown in figure). We find that most nonpolar residues are favorable at site 111 in PagP, except proline, which was the most unfavorable residue in the series. Polar residues were all unfavorable with respect to alanine, except cysteine. The coloring system is follows the same convention as Figures 2 and 5.

Figure S2. WT and V111P PagP molecular dynamics systems are equilibrated by 100 ns.



The RMSD (Å) compared to the starting structure of the backbone atoms are shown for all heavy atoms found in beta sheets. We find that all four trajectories equilibrated after 100 ns.