



Figure S5 - Family specific clusters from the *f*-PENs for selected families of the TIM fold.

Clusters obtained from *f*-PENs are highlighted as spheres in different families of the TIM fold. High energy clusters involving charged interactions at the core of the core β barrel residues that are obtained from the *f*-PENs-25(0.8) are distinguished by different shades of red. Low energy vdW clusters that are obtained from *f*-ljPEN-8(1.0) are highlighted in different shades of blue in different families of the TIM fold.