Figure 3. Interdomain flexibility in different $Vps4_{\Delta MIT}$ crystal structures.

Superposition of six independent structures of $Vps4_{\Delta MIT}$ in complex with: no ligand (2RKO, white), sulfate (crystal form 1, green), phosphate (2QPA, molecule B, blue), ADP (2QPA, molecule A, red), ATPγS (crystal form 2, molecule A, pink), and ATPγS (crystal form 2, molecule C, purple). Superposition on the large ATPase domains reveals that the small ATPase domain can rotate by up to 19° about a hinge angle located in the linker between the two domains and centered at residue Pro297. A second hinge within the small ATPase domain is also evident in the middle of the extended helix α8, centered about residue Pro350. These two hinge angles were defined by first finding the centers of masses of the large ATPase domain (residues 122-298 and 418-433), the core of the small domain (300-350; 402-414), and the β domain (358-399) using the program 6d_moleman2. Hinge angle I was then calculated as the angle between the large and small domains, with Pro297 Cα at the apex, and hinge angle II was calculated as the angle between the small domain and the β domain, with Pro350 Cα at the apex.

Figure 4. Vps4 proteins dimerize in solution

Representative equilibrium sedimentation profiles for full length Vps4 (panel 1), $Vps4_{\Delta MIT}$ (panel 2), $Vps4_{\Delta MIT,Q216A}$ (panel 3, Interface 1 mutant), and $Vps4_{\Delta MIT,L151D}$ (panel 4, Interface 2 mutant). Sedimentation data are plotted as absorbance versus the distance from the center of the axis of rotation (radius). To simplify the plot, the radius was normalized so that the data from all three sectors (i.e. three different