



**Figure S2. Related to Fig. 3. Crystal structures of the  $\alpha\text{IIb}\beta\text{3}$  headpiece in complex with inhibitors in Mg or Mn.** Structures of molecule 1 in the asymmetric unit (chains A and B) after soaking indicated compounds (1 mM) in 1 mM (or 5 mM  $\text{Mg}^{2+}$  for UR-2922) and 1 mM  $\text{Ca}^{2+}$  or 2 mM  $\text{Mn}^{2+}$  and 0.2 mM  $\text{Ca}^{2+}$  as indicated into closed  $\alpha\text{IIb}\beta\text{3}$  crystals. Structures are superimposed on the  $\beta$ -propeller and  $\beta\text{I}$  domains.  $\alpha\text{IIb}$ ,  $\beta\text{3}$ , and compounds or RGD are shown with carbons in green, cyan, and wheat, respectively. MIDAS  $\text{Mg}^{2+}$  and  $\text{Mn}^{2+}$  ions are shown as spheres in yellow and purple, respectively. Water molecule oxygens are shown as smaller red spheres. Backbone is shown as worm trace or sticks for residues that hydrogen bond to ligand. Sidechains that interact with ligand are shown in stick. Black dashes represent metal coordination, hydrogen, and pi-pi bonds. Relevant residues are labeled.