

presumably came from the 48 % ethylene glycol crystallization solution) in complex with a magnesium ion, which is coordinated by the conserved Asp232 and Ser180 side chains and a hydroxyl group of the ethylene glycol. The single unique molecule in the VPS4_{ΔMIT}-SO₄ crystal form also lacks nucleotide density, but has density within the β and γ phosphate binding sites that likely corresponds to a sulfate ion from the 1.6 M ammonium sulfate crystallization solution. A sulfate ion is also seen in the same position in the structure of human VPS4B_{ΔMIT}-SO₄²⁵.

The two different crystal forms reported here extend the range of interdomain angles seen for Vps4, and further show how the different domains can move relative to one another (Fig. 3 and Table 2). As has been noted previously²⁸, relative domain motions are centered about two different hinges. The first hinge is Pro297, which is located within the linker between the two domains of the ATPase cassette. Molecule A in crystal form 2 has the most closed hinge I angle seen to date (115°), whereas molecule C has the most open angle (134°). The second hinge is centered at Pro350 in the center of helix 8 in the small domain. This intradomain hinge is evident in overlays of the core of the small domain (Fig. 3 and data not shown). This hinge angle can vary by up to 16°, and this variation allows the β domains to project in different directions from the small ATPase domain, which may be required to accommodate different β domain packing arrangements in the two rings of the dodecamer³¹.

As in all previously reported Vps4 crystal structures, the subunits in our two crystal forms pack as continuous helices that repeat every six subunits. In crystal form 1, the helix follows the 6₅ crystallographic screw axis, and every subunit is