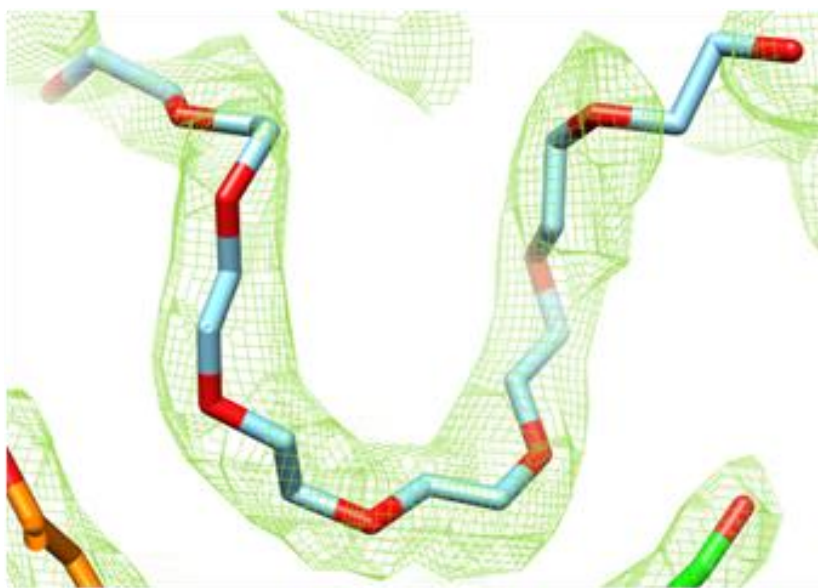


(a)



(b)

Supplementary Figure 1. Polyethylene glycol in the structure of MshB with acetate and glycerol in the active site. We report two molecules of poly-ethylene glycol (PEG) per asymmetric unit. They are located at the interface between the two protein molecules in the asymmetric unit (depicted as ribbons in dark and dark pink in Figure S1a). PEG1 (depicted as cyan coloured spheres) contributes significantly to the interface and has well defined density (Figure S1b). This PEG molecule was reported by Maynes *et al.* (2003) who observed a molecular packing in their crystal form which is very similar to that observed by us. PEG2 (depicted as blue spheres) is less well defined than PEG1 over much of its length. It contributes to the same interface as PEG1 over part of its length and it also contributes to an interface with a symmetry related molecule depicted in light blue. Both PEG molecules are far from the active site and from those residues that undergo the conformational change. The active site glycerol molecules are shown in red and green respectively. The location of Met98 in the D-*myo*-inositol binding loop is indicated by the yellow segment of the ribbon.