## Appendix 2

## **Supplemental Figures to Chapter 2**



**Supplemental Figure 1.** Crystal structures of vitamin  $B_{12}$  in the protein-free (base-on), BtuF-bound (base-on) and methionine synthase-bound (base-off) forms.



**Supplemental Figure 2.** (A) The hydrogen bond network surrounding vitamin  $B_{12}$  in the BtuF binding site. H-bonds are indicated with dashed lines. Residues from BtuF that make direct or water-mediated contacts are labeled in red. Those residues making direct contact have one asterisk (\*); aromatic residues that also make van der Waal's contacts with  $B_{12}$  have two asterisks (\*\*). Water molecules are designated with an X and a number. Interactions with the cobalamine side chain boxed in (A) are illustrated in (B) for clarity.



**Supplemental Figure 3**. (A) A GRASP electrostatic potential surface representation of BtuF looking down on the  $B_{12}$  binding slot reveals the conserved glutamate "knobs" present on the N- and C-terminal sub-domains. The distance between the alpha carbons of Glu72 and Glu202 is indicated. (B) A GRASP electrostatic potential surface representation of the periplasmic surface of BtuC reveals the conserved arginine "pockets" present on each MSD. The approximate distance between the arginine pockets is indicated.