
Article:

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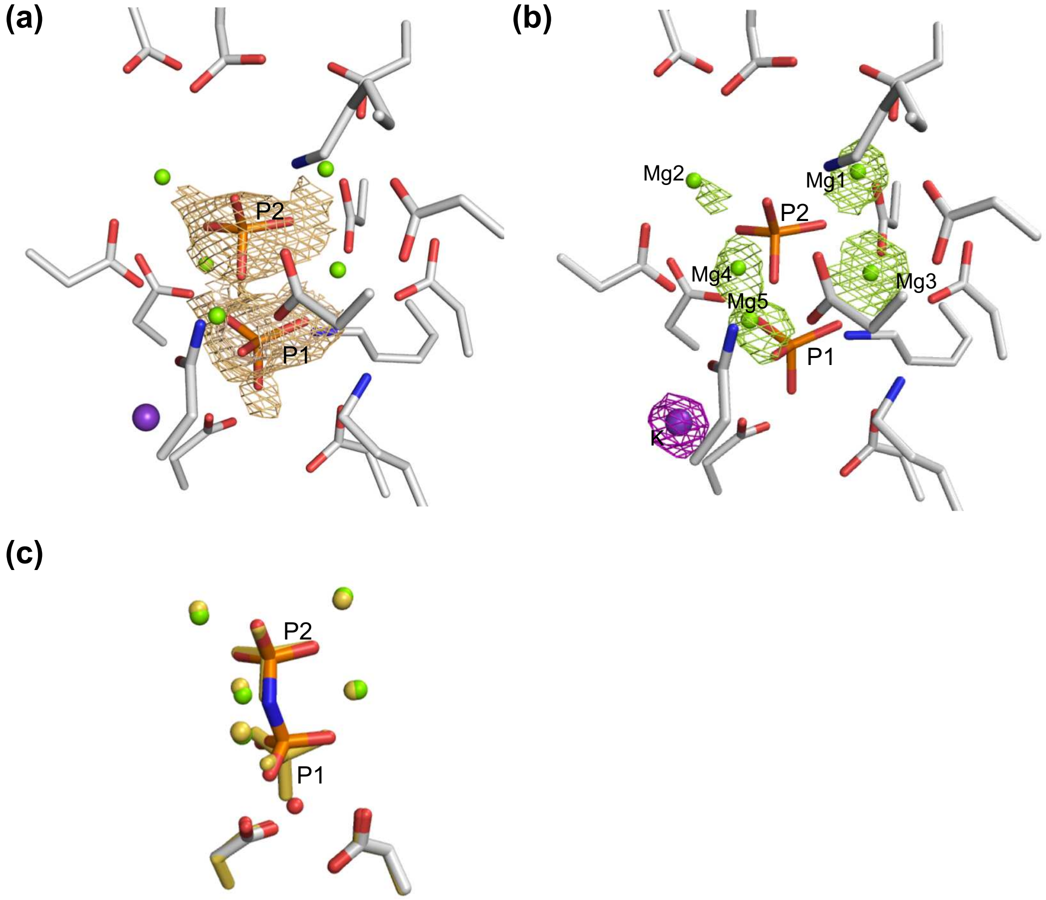

Figure S1. The F_o-F_c electron density map of the PP_i-binding pocket of the *Vr*H^+-PPase-$2P_i$.

The F_o-F_c electron density map of the PP_i-binding pocket of the *Vr*H^+-PPase-$2P_i$ complex with bound (**a**) P_i (at 4 σ), (**b**) Mg^{2+} (at 6 σ) and coordinating residues. (**c**) Superimposition of IDP and 2Pi in PPi-binding pocket. Both show the corresponding metals and the Wat_{nu}-associated Asp residues, D287 and D731. The D287 and D731 in the *Vr*H^+-PPase-IDP complex (PDB 4A01) are in CPK sticks, and the Wat_{nu} and the five Mg^{2+} ions are shown in CPK spheres. The corresponding residues and atoms in the *Vr*H^+-PPase-$2P_i$ are shown in yellow.

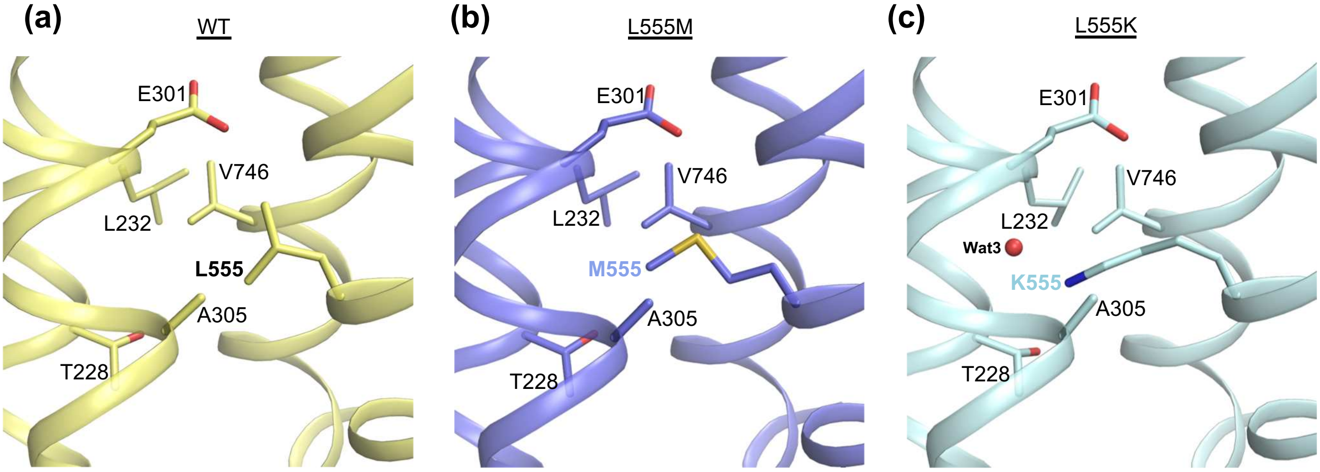

Figure S2. The view of hydrophobic gate region in the *Vr*H$^+$-PPase and mutants.

Zoom-in of the hydrophobic gate area constructed by residues, L232/TM5, A305/TM6, V746/TM16 and L555/TM12, M555/TM12 and K555/TM12 in the (**a**) wild type (WT) and two mutants (**b,c**) L555M and L555K, respectively. The area of hydrophobic gate is shrink with the side chain substitution in L555M and L555K. The residues near the gate are shown, such as E301 and T228.

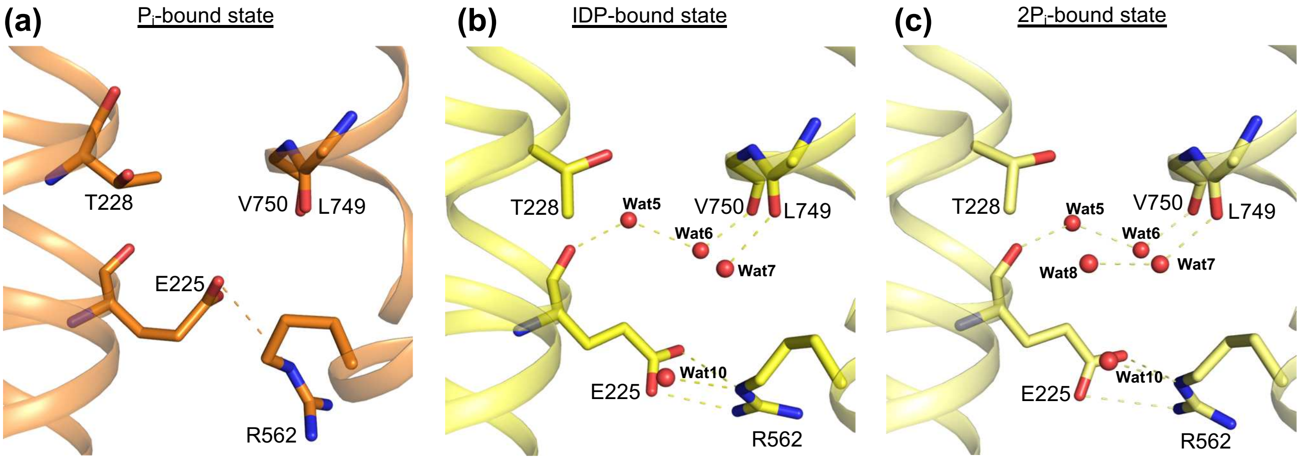

Figure S3. The view of exit channel region in the three *Vr*H$^+$-PPase complexes.

Zoom-in of the E225-R562 interaction and the water molecules around E225 in (**a**) P$_i$-bound (**b**) IDP-bound and (**c**) 2P$_i$-bound states. The colored-dash lines indicate the H-bond interactions. The residues near the exit channel and in the H-bond interactions are shown, such as T228, L749 and V750.