



UNIVERSITY OF LEEDS

This is a repository copy of *Roles of the Hydrophobic Gate and Exit Channel in Vigna radiata Pyrophosphatase Ion Translocation*.

White Rose Research Online URL for this paper:  
<http://eprints.whiterose.ac.uk/144812/>

Version: Accepted Version

---

**Article:**

Tsai, J-Y, Tang, K-Z, Li, K-M et al. (4 more authors) (2019) Roles of the Hydrophobic Gate and Exit Channel in Vigna radiata Pyrophosphatase Ion Translocation. *Journal of Molecular Biology*, 431 (8). pp. 1619-1632. ISSN 0022-2836

<https://doi.org/10.1016/j.jmb.2019.03.009>

---

© 2019 Elsevier Ltd. All rights reserved. Licensed under the Creative Commons Attribution-Non Commercial No Derivatives 4.0 International License (<https://creativecommons.org/licenses/by-nc-nd/4.0/>).

**Reuse**

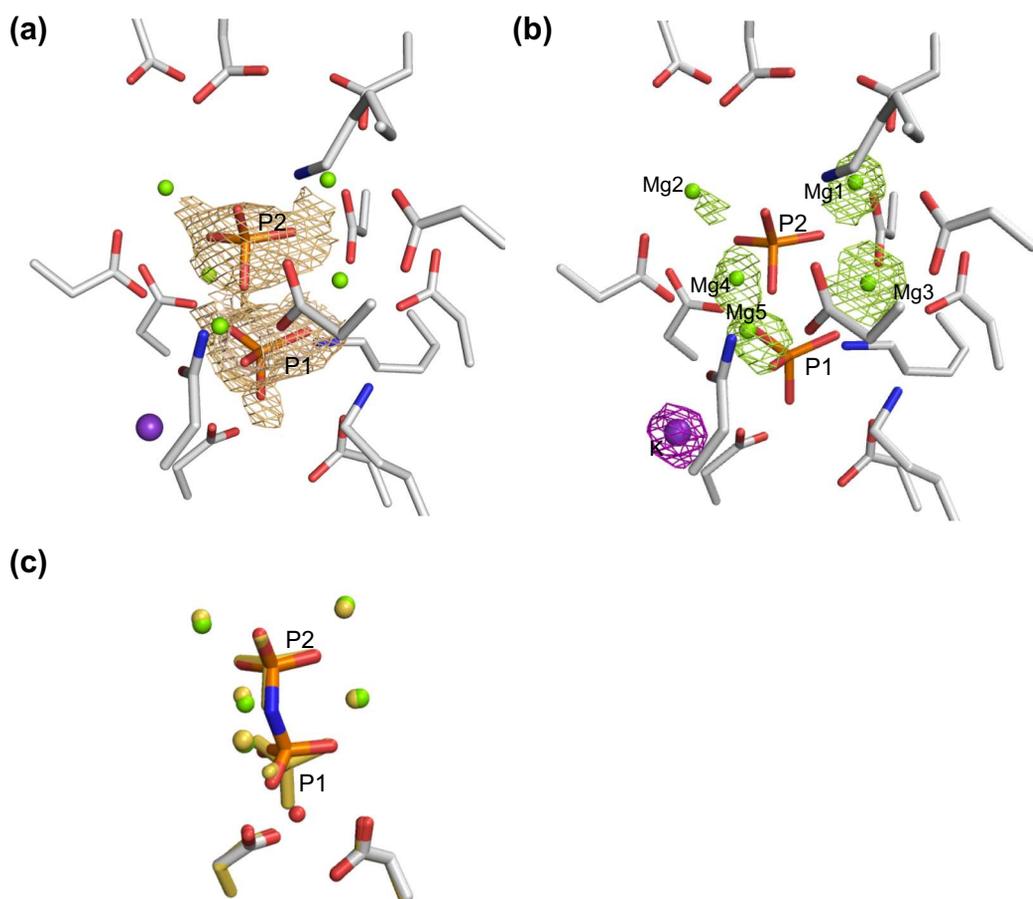
This article is distributed under the terms of the Creative Commons Attribution-NonCommercial-NoDerivs (CC BY-NC-ND) licence. This licence only allows you to download this work and share it with others as long as you credit the authors, but you can't change the article in any way or use it commercially. More information and the full terms of the licence here: <https://creativecommons.org/licenses/>

**Takedown**

If you consider content in White Rose Research Online to be in breach of UK law, please notify us by emailing [eprints@whiterose.ac.uk](mailto:eprints@whiterose.ac.uk) including the URL of the record and the reason for the withdrawal request.

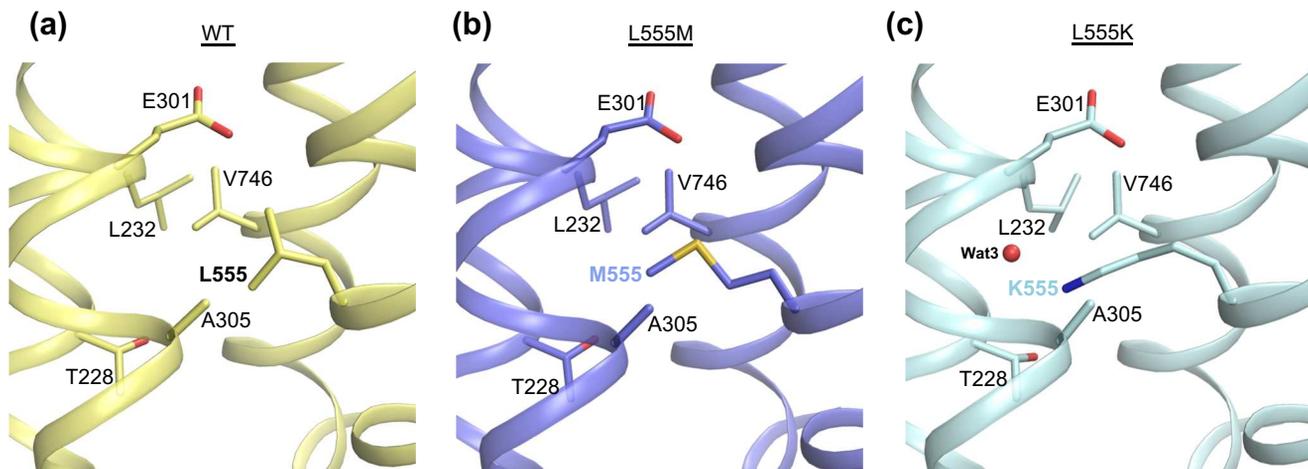


[eprints@whiterose.ac.uk](mailto:eprints@whiterose.ac.uk)  
<https://eprints.whiterose.ac.uk/>



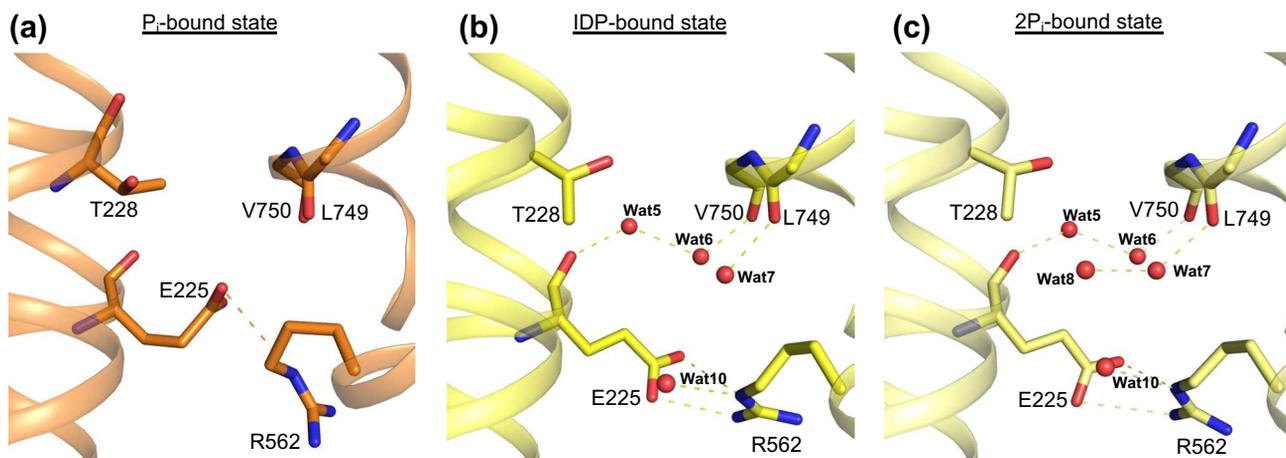
**Figure S1. The  $F_0-F_c$  electron density map of the  $PP_i$ -binding pocket of the  $VrH^+$ -PPase-2 $P_i$ .**

The  $F_0-F_c$  electron density map of the  $PP_i$ -binding pocket of the  $VrH^+$ -PPase-2 $P_i$  complex with bound (a)  $P_i$  (at  $4\sigma$ ), (b)  $Mg^{2+}$  (at  $6\sigma$ ) and coordinating residues. (c) Superimposition of IDP and 2 $P_i$  in  $PP_i$ -binding pocket. Both show the corresponding metals and the  $Wat_{nu}$ -associated Asp residues, D287 and D731. The D287 and D731 in the  $VrH^+$ -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  $VrH^+$ -PPase-2 $P_i$  are shown in yellow.



**Figure S2. The view of hydrophobic gate region in the *VrH<sup>+</sup>*-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  $Vrh^+$ -PPase complexes.**

Zoom-in of the E225-R562 interaction and the water molecules around E225 in (a) P<sub>i</sub>-bound (b) IDP-bound and (c) 2P<sub>i</sub>-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.