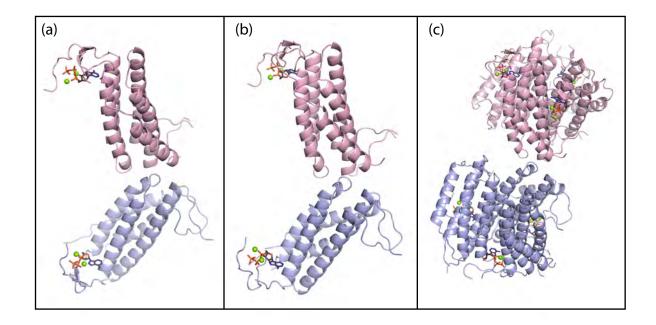


**Supplementary Figure 1**. Representative electron density. (a)  $LrPduO^{D35N}$  monomer A; (b)  $LrPduO^{D35N}$  monomer B; (c)  $LrPduO^{R132K}$  monomer A; (d)  $LrPduO^{D35N}$  monomer B. The F<sub>0</sub>-F<sub>c</sub> electron density omit map for Mg-ATP was contoured at 3.0  $\sigma$  for (a) and (b) and at 2.0  $\sigma$  for (c) and (d). The 2F<sub>0</sub>-F<sub>c</sub> electron density maps corresponding to the amino acid side chains were contoured at 1.0  $\sigma$  in all cases. ATP is illustrated in a stick representation with carbon atoms colored in gray. Mg<sup>2+</sup> ions are illustrated as green spheres.



**Supplementary Figure 2**. Ribbon representations of the asymmetric unit in the *Lr*PduO variant crystal structures. (a) The *Lr*PduO<sup>D35N</sup> variant monomers, with monomer A in *blue* and monomer B in *pink*. (b) The *Lr*PduO<sup>R132K</sup> variant monomers, with monomer A in *blue* and monomer B in *pink*. (c) The *Lr*PduO<sup>R132K</sup> variant trimer structures, formed by crystallographic symmetry operations.