

Figure S2. Omit-map Densities of Important Regions in Dda_ykkC

- (A) Guanidinium in the binding pocket.
- (B) Rotated view of guanidinium in the binding pocket.
- (C) P3 A-loop (orange) in the L1 minor groove (pink). .
- (D) Coordinated Mg²⁺ ions (green spheres) between L1 (violet) and P3 (orange) backbones.