Supplemental Information

(A)



(C)



Figure S1 Unmodeled electron density of overhang DNA in the solvent channel for crystal form 1 (**A**, **B**) and hairpin DNA in crystal form 2 (**C**, **D**). The *2Fo-Fc* map is shown in blue and contoured at 1.0σ , and the *Fo-Fc* maps are shown in green and red and contoured at +/- 3.0σ . Active site zinc ions are labeled and proximity to unmodeled DNA density are shown (B and D).



Figure S2 (A) Superposition of Artemis structures from crystal form 1 (grey), molecule A of crystal form 2 (lilac), and molecule B of crystal form 2 (light blue). The root mean square deviations of C α are 0.37Å (form 1 – A of form 2), 0.60Å (form 1 – B of form 2), and 0.50 (A – B of form 2). (**B**) Superposition of Artemis structure from crystal form 1 (grey) and PDB 6TT5 (yellow).



Figure S3 (**A**) Experimental map (blue) contoured at 1.0 σ and anomolous map (orange) contoured at 15.0 σ of the zinc ion in the active site of the Metallo- β -Lactamase domain. (**B**) Experimental map (blue) contoured at 1.0 σ and anomolous map (orange) contoured at 15.0 σ of the zinc ion in the novel, structural binding site in the β -CASP domain.