Supplemental information

Structural analysis of the OXA-48 carbapenemase bound to a "poor" carbapenem substrate, doripenem

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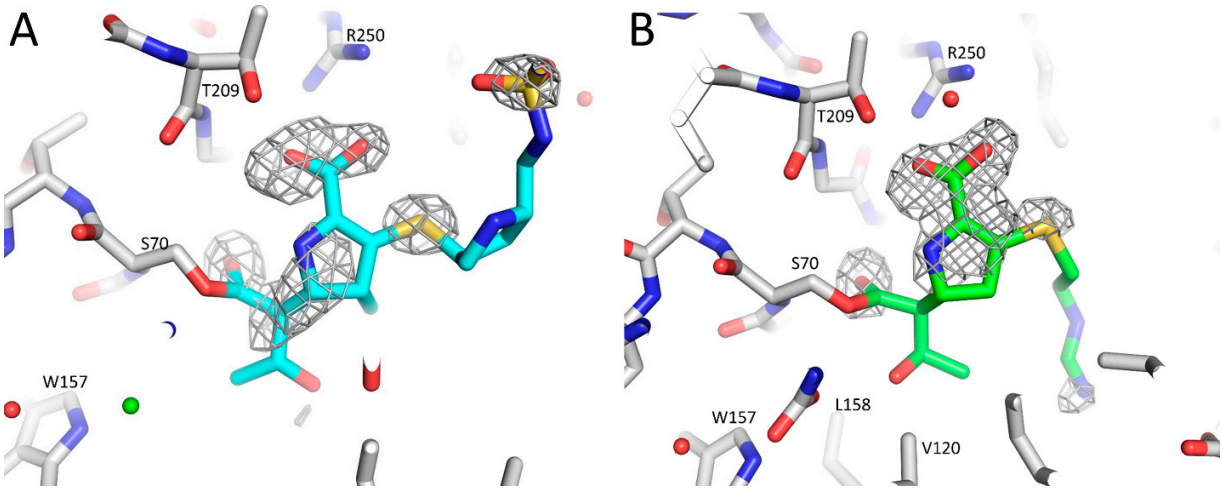

Figure S1. Electron density maps of the active sites of wild-type OXA-48 with doripenem and imipenem bound. To remove ligand bias prior to the map calculation, a 10-cycle refmac crystallographic refinement was carried out with the ligands removed from the coordinates. (A) Unbiased |Fo|-|Fc| Polder omit map of the active site of wild-type OXA-48 showing a poorly ordered doripenem molecule (PDBid = 6P9C molecule A; density contoured at 3 σ). The doripenem ligand was added back to the coordinates prior to the map calculation to allow Polder to adjust the solvent mask. A regular unbiased omit map showed similar results. (B) Unbiased |Fo|-|Fc| omit map of the active site of wild-type OXA-48 showing a poorly ordered imipenem molecule (PDBid = 5QB4 molecule A; density contoured at 3 σ). Electron density in the other molecules in the asymmetric units was equal or worse than the depicted doripenem and imipenem density.

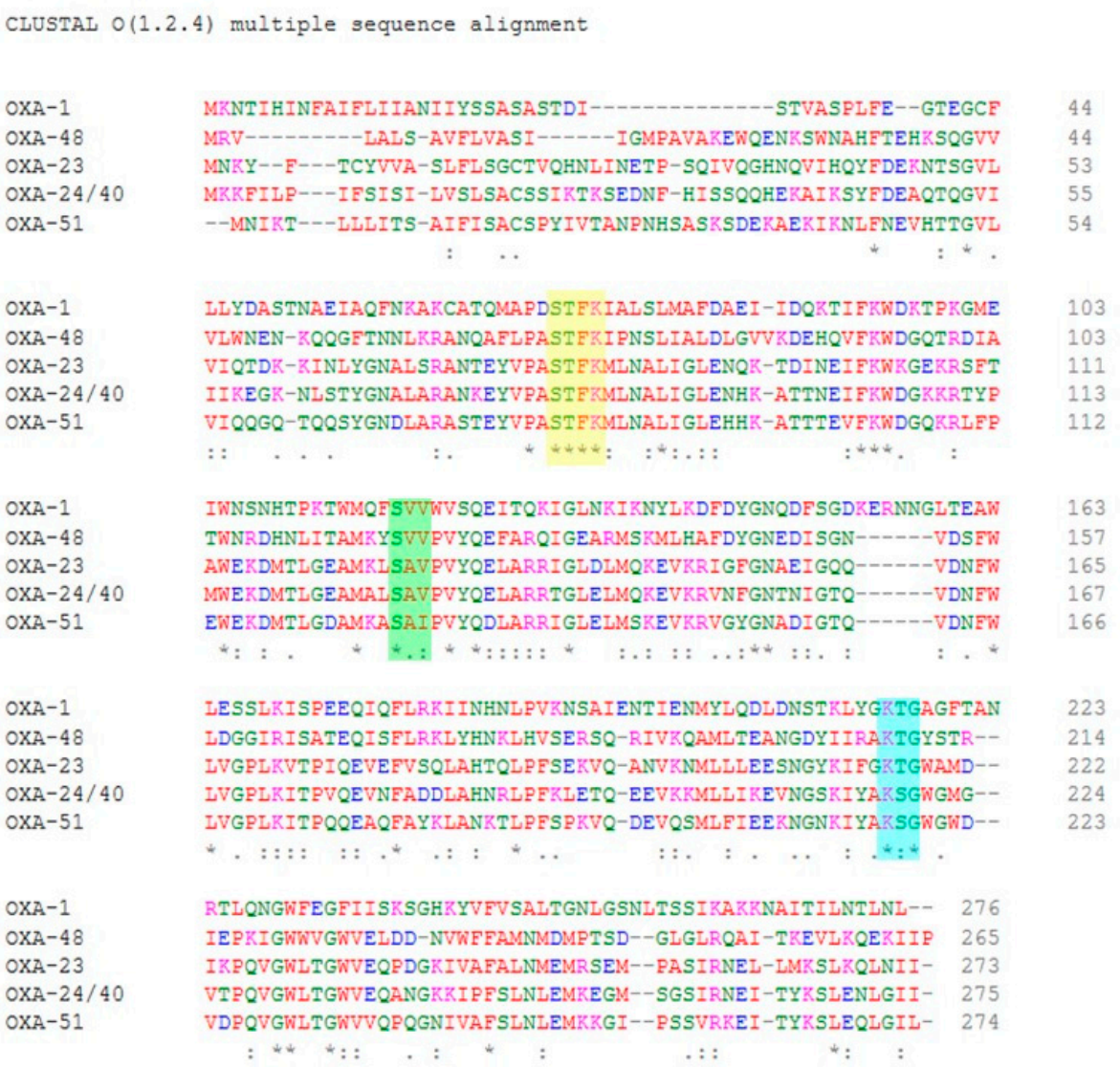

Figure S2. Multiple sequence alignment using Clustal Ω using wild-type enzymes of OXA-1, OXA-23, OXA-24/40, OXA-48, and OXA-51. The catalytic serine and carboxylated lysine residues encompassing the STFK motif are highlighted by the yellow box. The S-A/V-V/I motif is represented by the green box and the K-T/S-G motif is highlighted in blue.