Protein production: see https://www.thesgc.org/structures/6nft

Structure Determination:

Ligand: 3-(5-phenyl-1,3,4-oxadiazol-2-yl)propanoate

Concentration: protein: 12 mg/mL

Crystallization: Crystals of the complex were grown at 291 K using vapor diffusion sitting drop by mixing equal volumes of 1:2.5 protein (12 mg/mL, 1.1% DMSO (v/v)): ligand and crystallization buffer (1.5 M ammonium sulfate, 0.1 M bis-tris pH 7.0). The crystals were cryoprotected in 25% ethylene glycol (v/v) and cryo cooled in liquid nitrogen.

Data Collection & Processing: X-ray diffraction data was collected at 100 K at a Rigaku FR-E Superbright copper source. Diffraction data were processed with the XDS and AIMLESS, using the Xia2 interfaces and were solved by direct refinement of protein chains A and B of the isomorphous PDB entry 2G43