

Protein production: see <https://www.thescg.org/structures/6nft>

Ligand: 4-(4-tert-butylphenyl)-4-oxobutanoate

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 1:5 protein (12 mg/mL, 2.25% 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 was processed with the XDS and AIMLESS, using the Xia2 interfaces. The complex structure was solved by molecular replacement with Phaser and coordinates from chain A of PDB entry 2G43.