

A STRUCTURAL BASIS FOR CAFFEINE BIOSYNTHESIS

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Supplemental Fig. 1.

Stereo view of the ligand binding sites showing a $2F_o - F_c$ omit electron density map contoured at 2σ and coloured in blue for the DXMT and XMT. A. Tb bound to DXMT in the 7mX like conformation; B. Tb bound to DXMT; C. XR bound to XMT (molecule A), the O5' hydroxyl was only visible at 1σ .