



STRUCTURAL BIOLOGY
COMMUNICATIONS

Volume 73 (2017)

Supporting information for article:

Structural insights into the mechanism of the drastic changes in enzymatic activity of the cytochrome P450 vitamin D₃ hydroxylase (CYP107BR1) caused by a mutation distant from the active site

Yoshiaki Yasutake, Tomoshi Kameda and Tomohiro Tamura

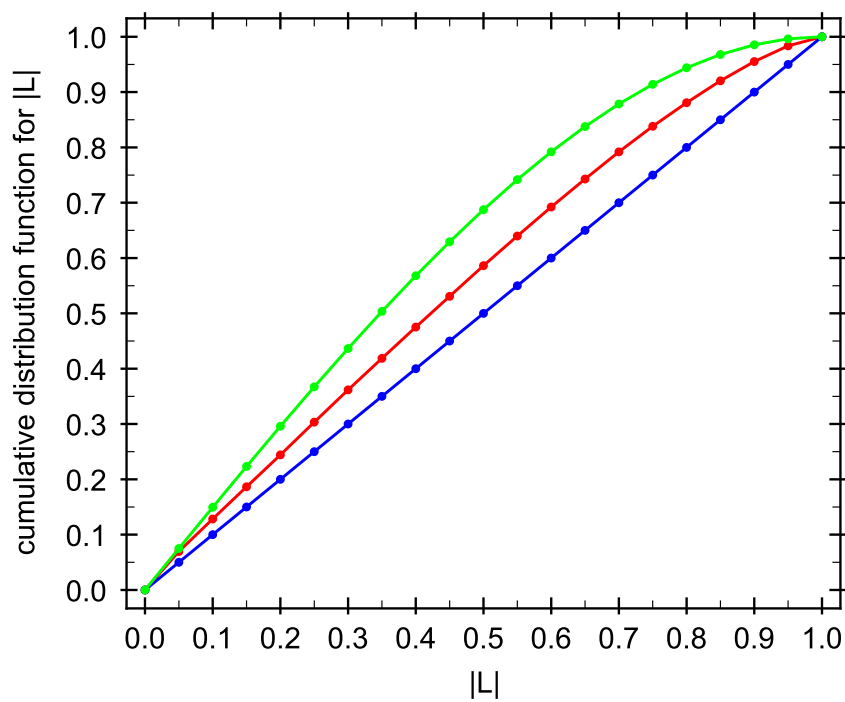


Figure S1. The L-test analysis (Padilla & Yeates, 2003) using the data of Vdh-L348M processed in space group $P22_12_1$. $L = I_1 - I_2 / (I_1 + I_2)$, where I_1 and I_2 represent the intensities of independent reflections. The blue and green lines represent the theoretical distribution of L for untwinned and twinned data, respectively. The red line represents the observed distribution of L for Vdh-L348M.

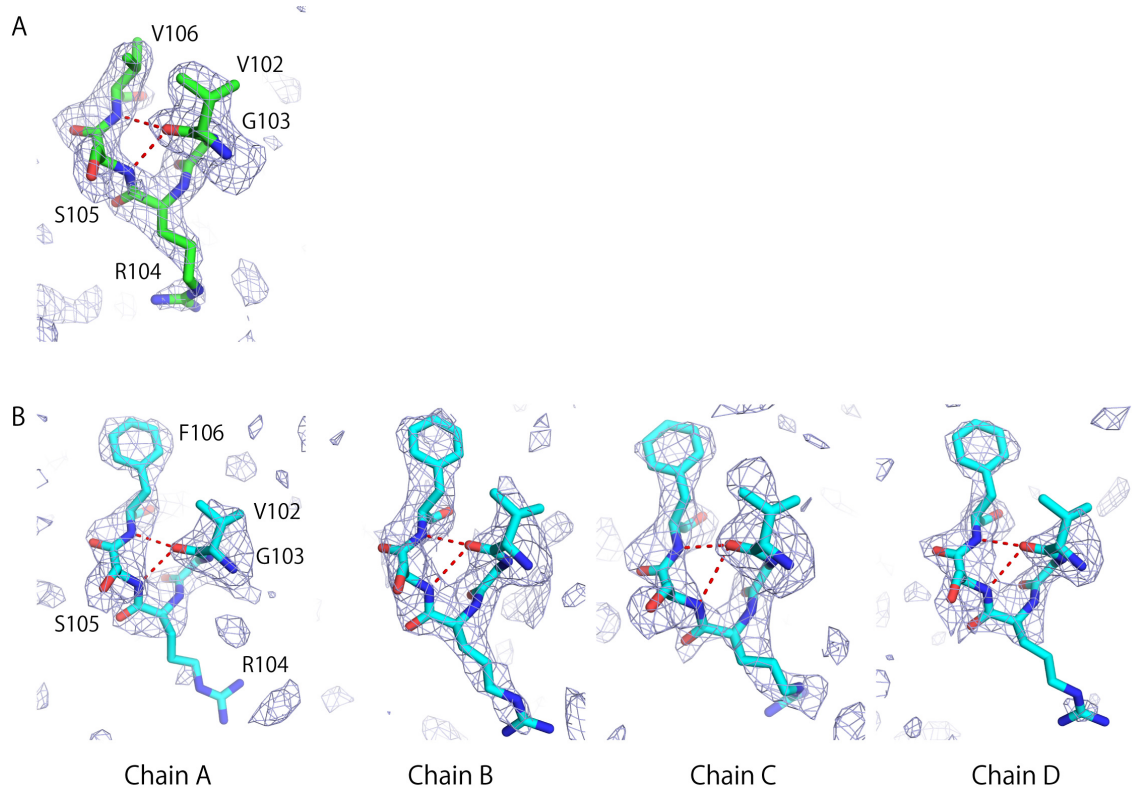


Figure S2. The $mFo - DFc$ omit map for the residues 102-106 of Vdh-F106V contoured at 2.5σ level (A) and of Vdh-L348M at 2.2σ level (B). The maps were calculated at early stage of model refinement using the model without the residues 102-106. The final refined models are also shown. Red dashed lines represent hydrogen bonds between main-chain O of V102 and main-chain N of F106/V106/S105.