

## SUPPLEMENTAL DATA

Exploring the structural basis of substrate preferences in Baeyer-Villiger  
monooxygenases: insight from steroid monooxygenase

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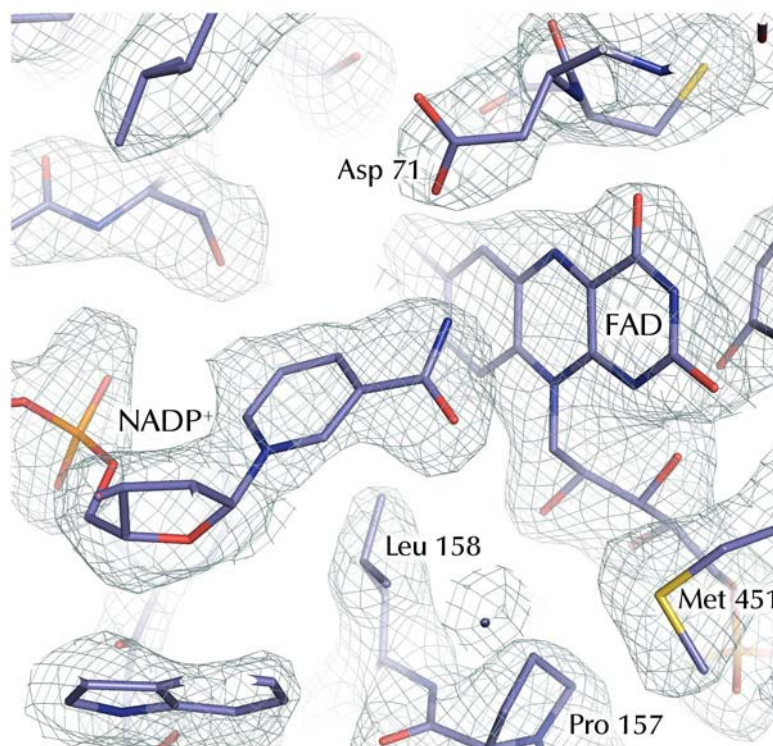
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**Running Title:** Steroid monooxygenase from *Rhodococcus rhodochrous*

## SUPPLEMENTARY FIGURES

**Figure S1.** Quality of the final electron density with reference to the crystal structure of STMO bound to NADP<sup>+</sup> (Table 1). The density was calculated with weighted 2Fo-Fc coefficients and is contoured at 1.3  $\sigma$  level. Carbons are in purple, nitrogens in blue, oxygens in red, sulfurs in yellow, and phosphorous in orange.



**Figure S2.** Superposition of STMO (blue ribbon) and CHMO (green ribbon; open conformation; PDB entry 3GWF) active sites. FAD and NADP<sup>+</sup> of STMO are depicted with yellow and orange carbons, respectively. The C $\alpha$  atoms of the STMO residues targeted by mutagenesis are shown as blue spheres (Table 3).

