Crystal Structure of CYP2B6 in Complex with an Efavirenz Analog

Supporting Information

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Figure S1: The *Fo–Fc* electron density map (contoured to 3σ, green mesh) obtained before modeling the ligand in the CYP2B6-efavirenz analog. The protein is shown in orange ribbons, ligand in yellow sticks, and heme in red sticks.

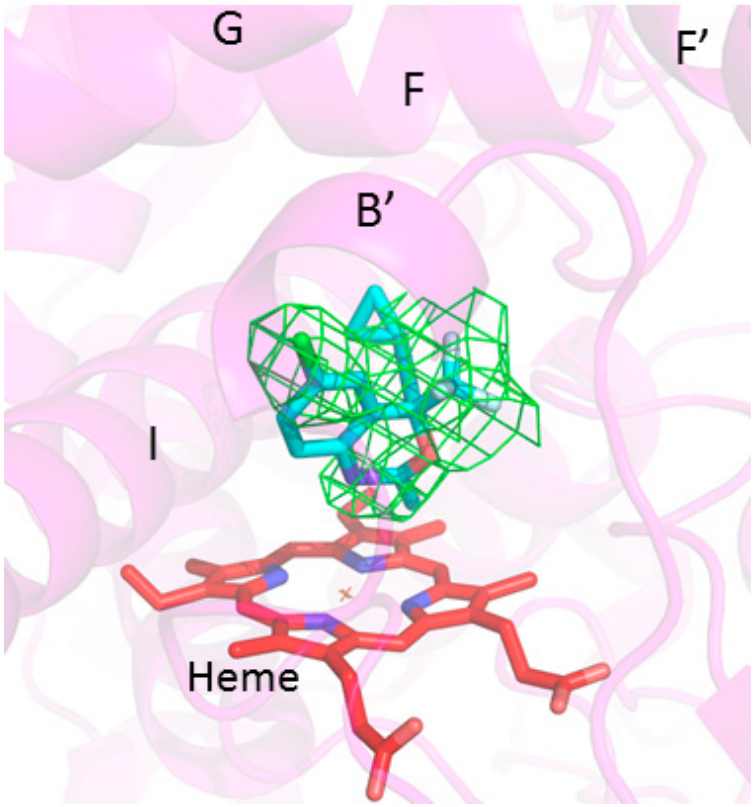

Table S1: Crystallographic data collection and refinement statistics.

Protein	CYP2B6dH
Ligand	Efavirenz Analog
PDB ID	5WBG
Crystal Space group	$P12_11$
Crystal Unit Cell Parameters	
a (Å) b (Å)	103.29 197.78
c (Å)	119.22
$\alpha = \gamma$ (°)	90
β (°)	98.51
Data Collection Statistics. Values for highest resolution shell are shown in parentheses.	
Lightsource and beamline	SSRL 14-1
Wavelength (Å)	1.18
Resolution range (Å)	50.0-2.99 (3.06-2.99)
Completeness (%)	98.9 (96.7)
Redundancy	3.3 (3.2)
R_{merge}	0.18 (0.1)
Mean I/sigma (I)	6.4 (1.6)
Total reflections	89926
Refinement Statistics. Values for highest resolution shell are shown in parentheses.	
R-factor (%)	22 (33)
R_{free} (%)	26 (37)
RMS Deviations	
Bond lengths (Å)	0.01
Bond angles (°)	1.65
Average B factor (Å^2)	49.63
Ramachandran Plot	
Favored (%)	91.1
Outliers (%)	1.1
Number of Atoms	
Protein[a]	21849 (50.3)
Heme[a]	258 (41.3)
Solvent[a]	156 (39.5)
Efavirenz 2-desoxo, 2-methyl[a]	126 (97.1)
CYMAL-5[a]	181 (116.3)

[a]Average *B*-factors (Å^2) are in parentheses.