Table S1. Data collection and refinement statistics for the human MAO B-inhibitor complexes

	Rosiglitazone Complex	Pioglitazone Complex
PDB Code	4a7a	4a79
Space group	C222	C222
Unit cell axes (Å)	a = 131.5, b = 223.2, c = 86.5	a = 131.9, b = 223.7, c = 86.8
Resolution (Å)	1.7	1.9
R_{sym}[a,b] (%)	8.2 (42.1)	8.2 (30.7)
Completeness[b] (%)	99.2 (98.7)	100 (100)
Unique reflections	140,773	102,915
Redundancy	3.4 (3.3)	4.2 (4.1)
I/σ[b]	10.5 (2.6)	12.7 (4.6)
N° of atoms protein/FAD/ligand/water	7914/2x53/2x19/791	7914/2x53/2x25/695
Average B value for ligand atoms (Å^2)	28.8	26.5
R_{cryst}[b, c] (%)	18.6 (26.9)	17.8 (21.8)
R_{free}[b, c] (%)	21.4 (30.8)	20.8 (25.6)
Rms bond length (Å)	0.009	0.010
Rms bond angles (°)	1.15	1.2

[a] $R_{sym}=\sum|I_i-\langle I\rangle|/\sum I_i$, where I_i is the intensity of i^{th} observation and $\langle I\rangle$ is the mean intensity of the reflection.

[b] Values in parentheses are for reflections in the highest resolution shell.

[c] $R_{cryst}=\sum|F_{obs}-F_{calc}|/\sum|F_{obs}|$ where F_{obs} and F_{calc} are the observed and calculated structure factor amplitudes, respectively.

R_{cryst} and R_{free} were calculated using the working and test sets, respectively.