Supporting Information

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SI Text

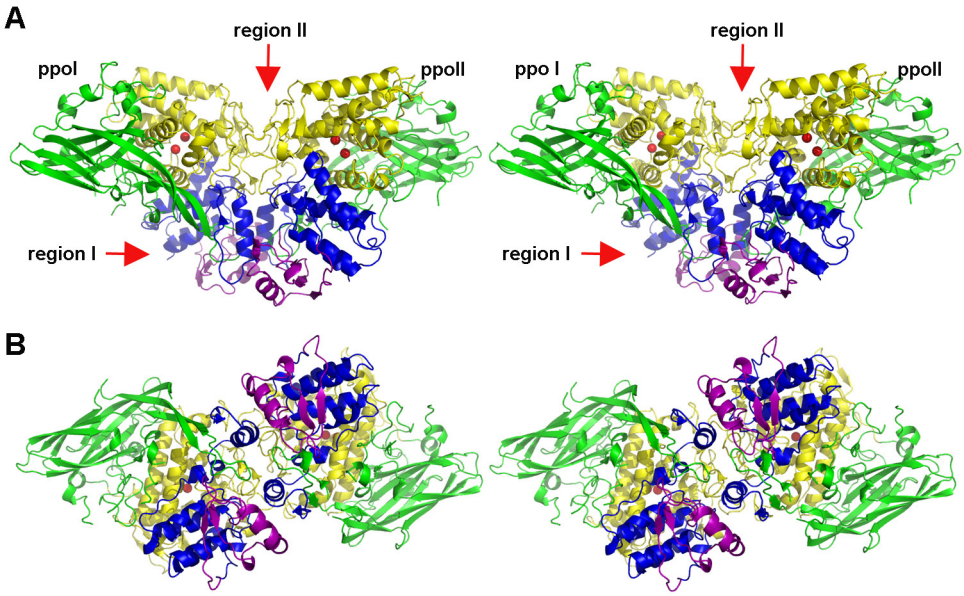

Fig. S1. Dimer interface of *M. sexta* PPO. The heterodimeric PPO is formed in a back-to-back mode. The secondary structures are colored differently according to individual domains: pro-region, purple; domain I, blue; domain II, yellow; domain III, green. The di-copper atoms are located in domain II and are shown as red spheres. There are 2 regions at the dimer interface, as indicated by the red arrow. Region I interactions involve mainly the pro-region, domain I, and domain III. Region II interactions predominantly involve domain II. (*A*) Stereo side view. (*B*) Stereo top view along the pseudo–2-fold axis.

Table S1. Data and statistics

Crystal data	
Beam-line	19-ID APS
Wavelength, Å	1.07177
Space group	P 2_12_12
Cell constants	a = 148.8 Å, b = 153.7 Å, c = 75.8 Å, α = 90.0°, β = 90.0°, γ = 90.0°
Resolution, Å	1.97
Total reflections	976,846
Unique reflections	117,346
Completeness	100.0 (100.0%)
I/S	27.8 (2.3)
R_{sym}	7.4 (79.4%)
Refinement statistics	
Reflection range used, Å	1.97–50.0
No. reflections used	115,234
R_{work}/R_{free}, %	15.4/19.4
rmsd bonds, Å	0.016
rmsd angle, °	1.516
No. atoms/average B, Å^2	
Protein	10,803
Metal ions	4
Waters	1,225
Ramachandran plot (preferred/allowed), %	96.87/3.13

$R_{sym} = \Sigma\, |I_{obs} - I_{avg}| \,/\Sigma\, I_{avg}$; $R_{work} = \Sigma||F_{obs} - F_{calc}||/\Sigma\, F_{obs}$.
R_{free} was calculated using 5% data.
APS, Advanced Photon Source; I/S, Intensity/Sigma(Intensity). Values in parentheses are for the highest-resolution shell.