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Supporting information for article:

Crystal structures of the disulfide reductase DsbM from *Pseudomonas aeruginosa*

Inseong Jo, Nohra Park, In-Young Chung, You-Hee Cho and Nam-Chul Ha

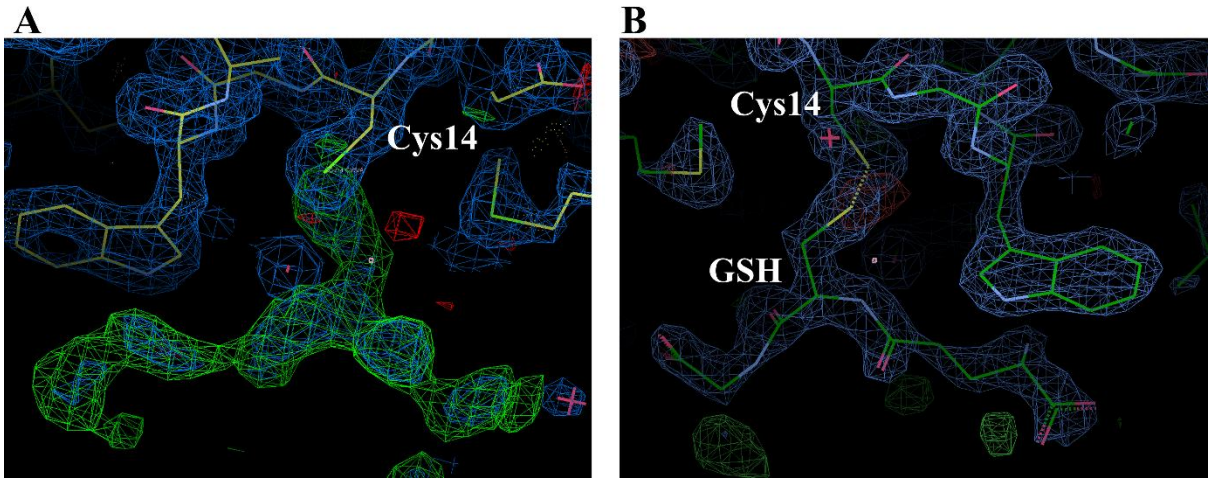

Figure S1 2Fo-Fc (blue, 1.50 σ) and Fo-Fc (green, 3.00 σ) difference electron density map around GSH binding site before (A) and after GSH fitting (B).

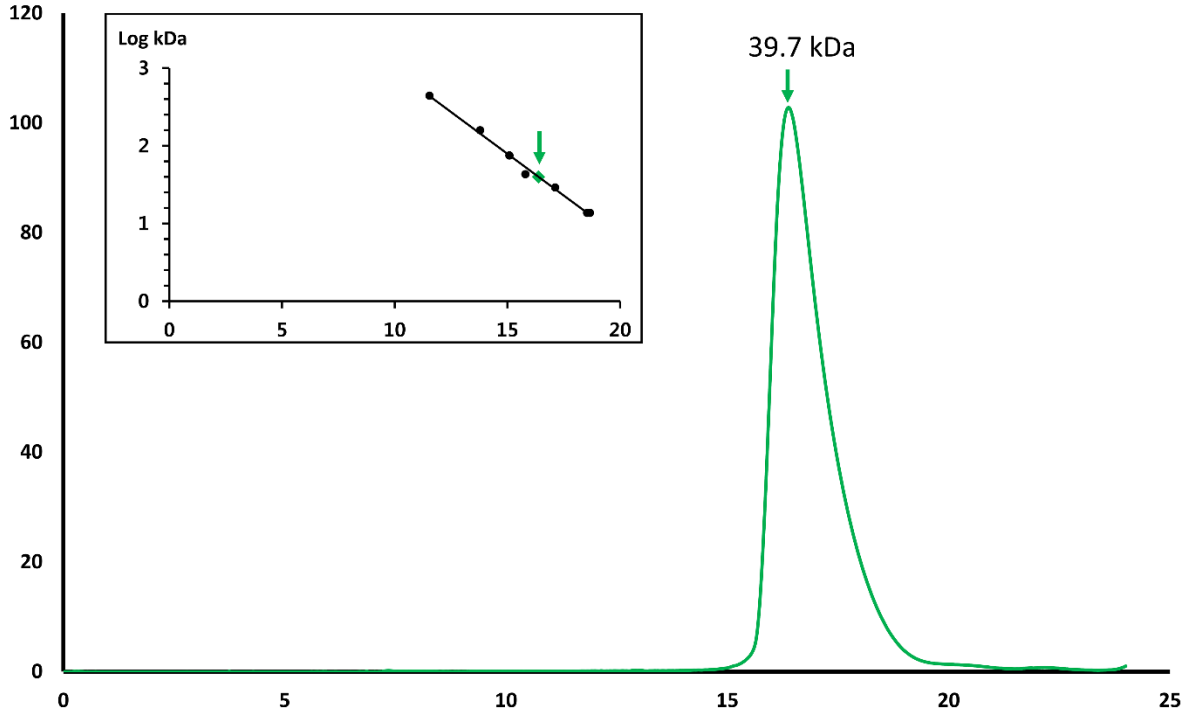

Figure S2 The size profile of the apo-DsbM. To confirm the oligomer state of apo-DsbM, size-exclusion chromatography was performed using the Superdex 200 HR 10/30 column (GE Healthcare). The peak indicates 39.7 kDa, which is larger than monomer but smaller than dimer size (green). The molecular weight was calculated using a standard curve (inset).

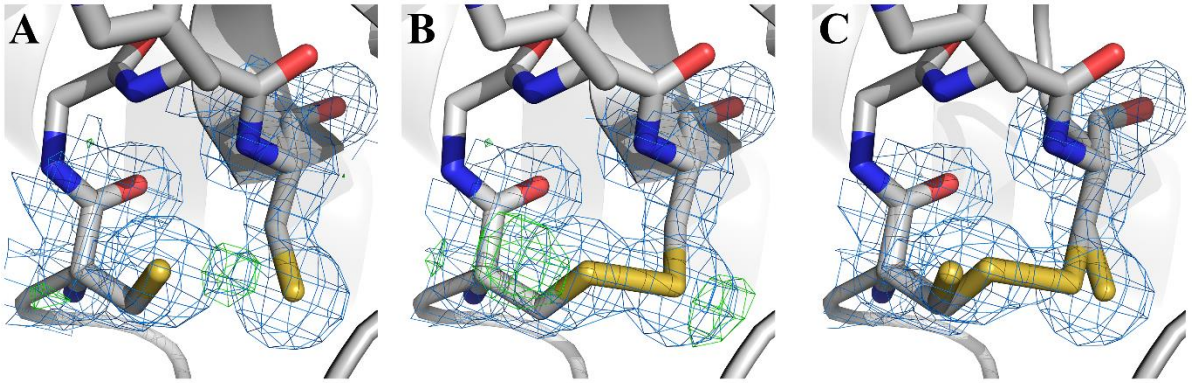

Figure S3 Electron density maps of the CXXC motif in DsbM. The apo-DsbM structures around the Cys14 and Cys17 residue superposed onto the *2Fo-Fc* (blue) and *Fo-Fc* (green) maps contoured at 1.0 σ and 3.0 σ, respectively. The *Fo-Fc* (green) electron density map could not be dissipated in either the reduced (A) or the oxidized (B) form. A model with the mixed conformations was well fitted to the electron density map (C).

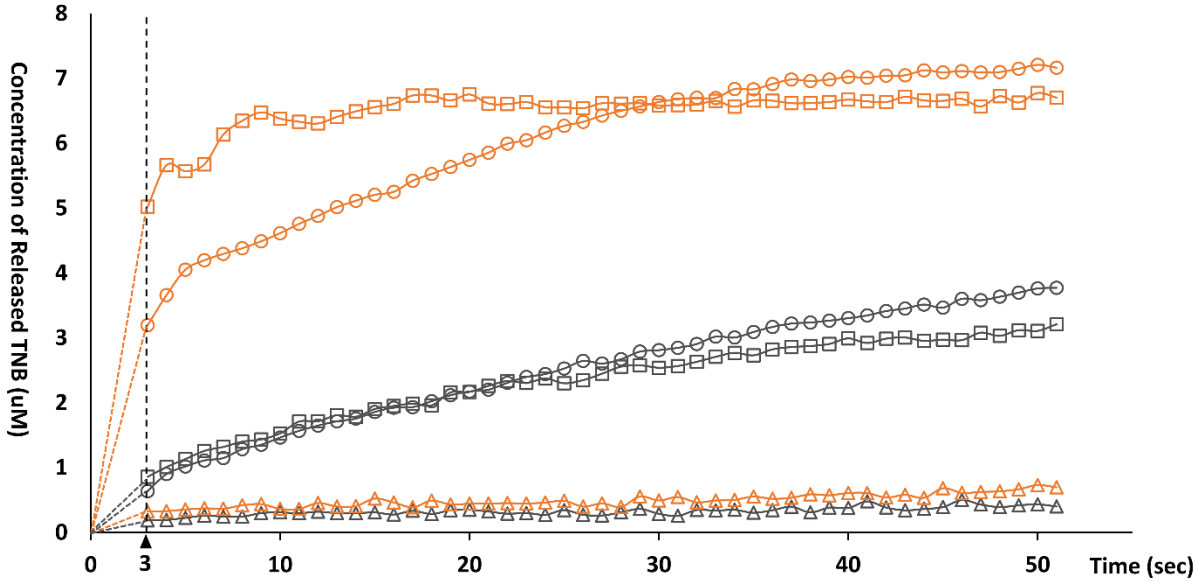

Figure S4 Kinetic measurement of the thiol reduction activity of DsbM C17S (orange) and GSH (gray) with TNB-labeled OxyR variants (C25-TNB (△), C199-TNB (□) and C208-TNB (○)). Both DsbM C17S and GSH were at a concentration of 50 μM in 50 mM Tris-HCl (pH 7.5) buffer containing 10 μM TNB-labeled OxyR variants. The absorbance of the liberated TNB^{2-} was measured at 412 nM. Five independent measurements were performed, and the average lines are presented. This figure is related to Fig. 5C.

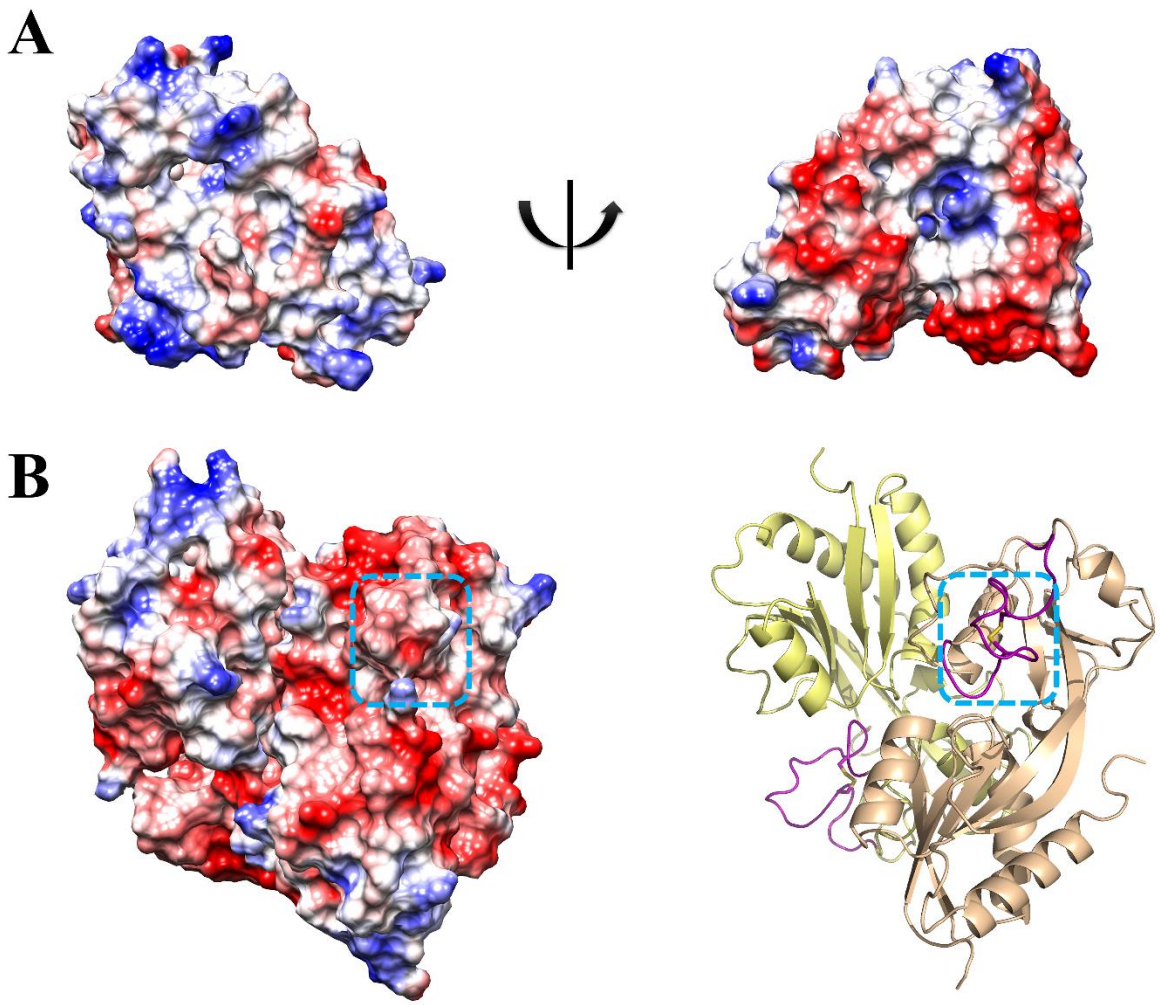

Figure S5 The surface electrostatic potential of DsbM and PaOxyR, related to Fig. 6. (A) The electrostatic potential of both sides of the surface of DsbM. (B) The dimer structure of the oxidized *E.coli* OxyR was present in the surface representation colored by the electrostatic potential (left) and in the ribbon representation (right). The disulfide-bridged loop (shown in magenta in the right panel) was marked by dashed boxes. The electrostatic potential was calculated with a coulombic surface in the program Chimera. The potential contours are shown on a scale from -10.0 kBT (red) to +10.0 kBT (blue).