Supplementary Material for

Structural features promoting dioxygen production by *Dechloromonas aromatica* chlorite dismutase

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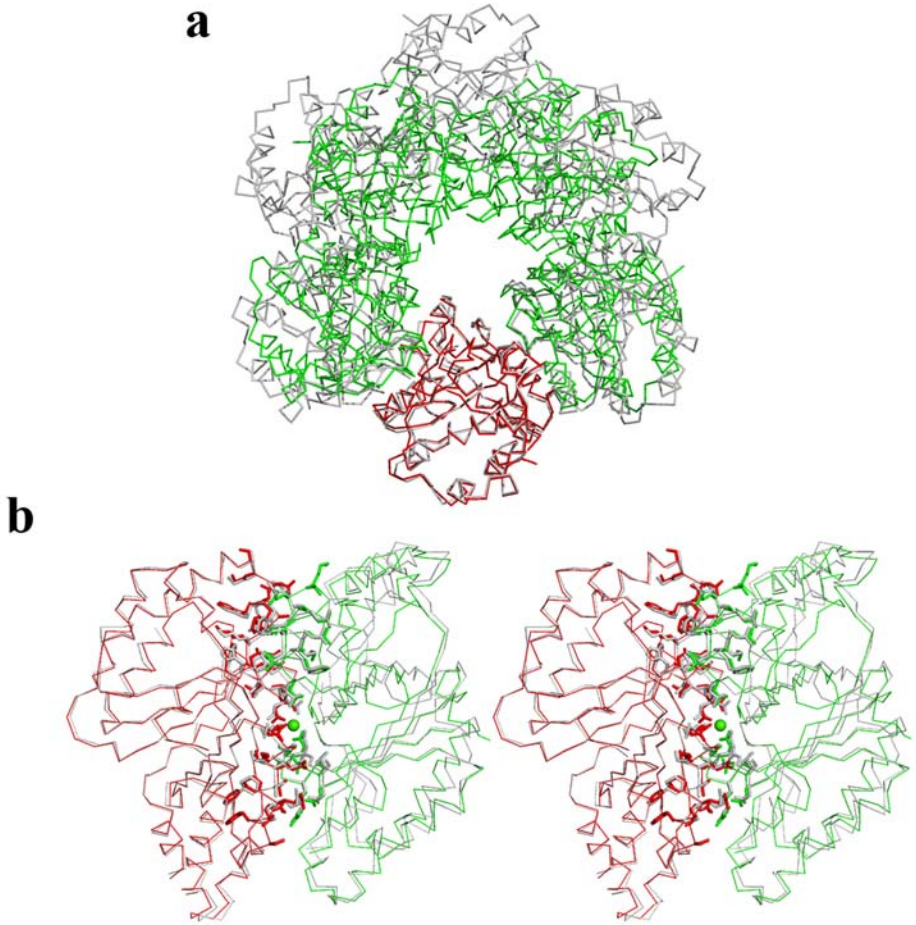

Fig. S1. Overlay of *D. aromatica* chlorite dismutase and *A. oryzae* chlorite dismutase (PDB entry: 2vdx). The *D. aromatica* pentamer is drawn as a green and red colored Cα trace and the *A. oryzae* hexamer as a grey Cα trace. The Figure was generated by overlaying the red *D. aromatica* monomer onto an *A. oryzae* monomer. **(a)** Superimposition of *D. aromatica* chlorite dismutase pentamer on *A. oryzae* chlorite dismutase hexamer. **(b)** Stereo representation of the chlorite dismutase monomer/monomer interface. The calcium ion found in *D. aromatica* chlorite dismutase is shown as a green sphere. This figure was generated using PyMOL (http://www.pymol.org/).

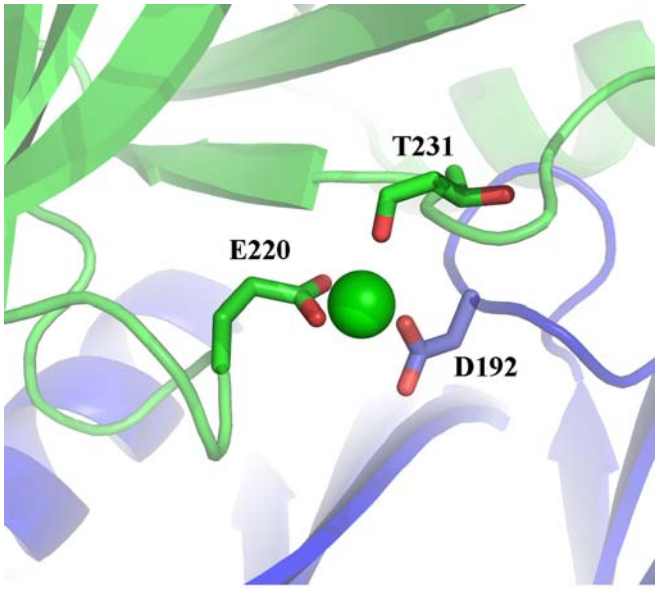

Fig. S2. Calcium binding site at the monomer/monomer interface of the chlorite dismutase pentamer. The two monomers are shown as green and blue cartoon respectively, and the calcium ion is shown as a green sphere. This figure was generated using PyMOL (http://www.pymol.org/).

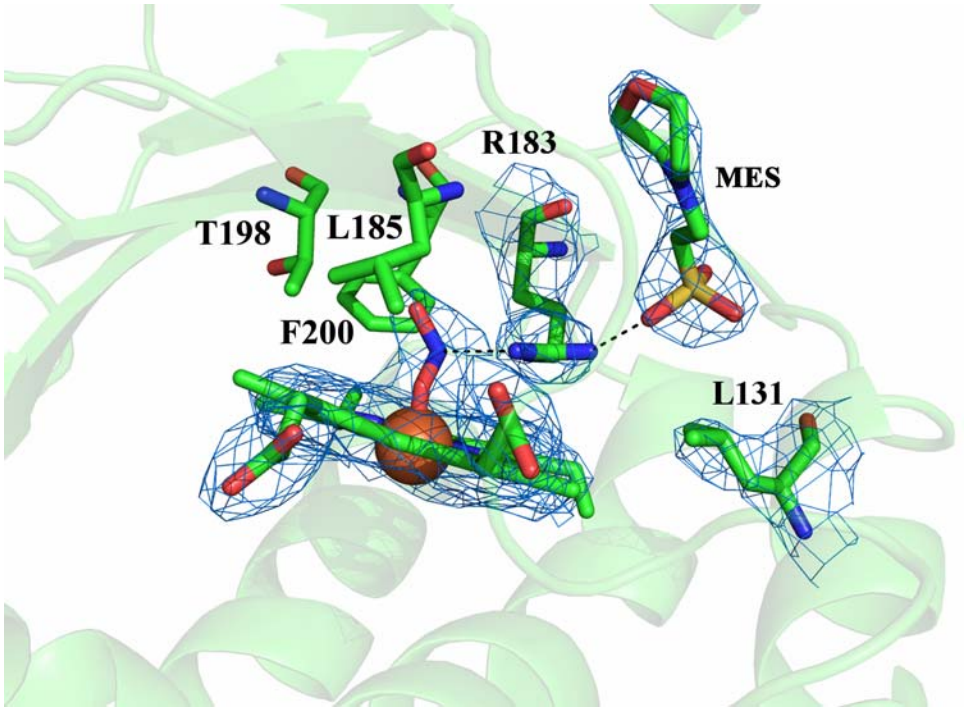

Fig. S3. Molecule of MES buffer bound close to the chlorite dismutase active site at pH=6.5**.** Electron density shown in blue is 20-fold NCS averaged 2Fo-Fc maps contoured at 3 σ. The heme, MES, nitrite and residues are drawn as stick colored by atom (carbon, green), with the Fe as an orange sphere. This figure was generated using PyMOL (http://www.pymol.org/).

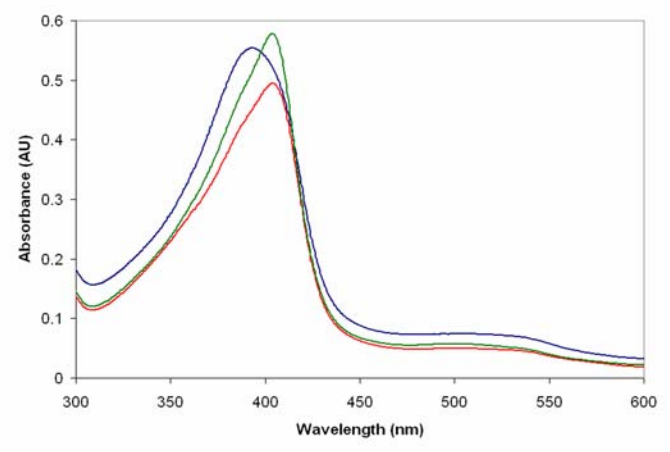

Fig. S4. UV-visible absorbance spectra of nitrite and acetate binding to chlorite dismutase. Ligand concentrations are equivalent to those in the crystallization; nitrite 47-fold excess per active site, and acetate 373-fold excess per active site. Spectra are colored as follows; chlorite dismutase alone, blue (λ_{max} = 392 nm); chlorite dismutase + nitrite, red (λ_{max} = 405 nm); chlorite dismutase + acetate, green (λ_{max} = 404 nm).

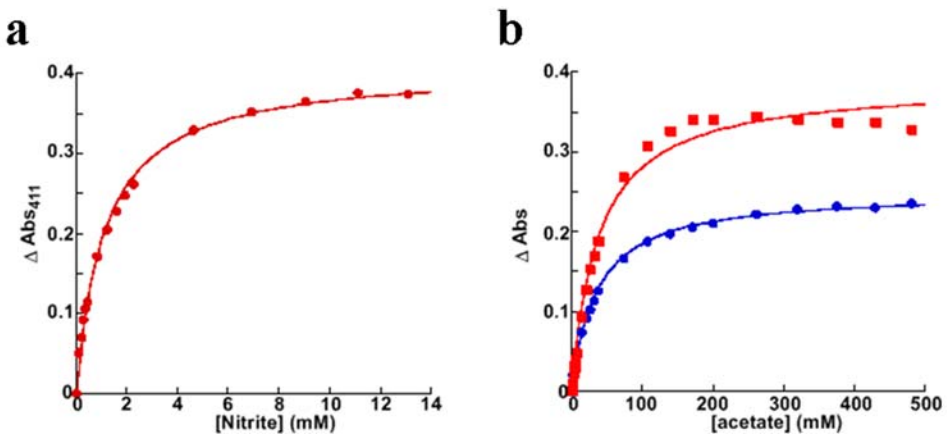

Fig. S5. Nitrite and acetate binding curves to Cld at pH 6.5. **(a)** Change of the absorbance at 411 nm as a function of nitrite added. The data were fit to the equation described in Materials and Methods, and yield a apparent K_d value of 1120 $\pm$ 50 µM. **(b)** Change in absorbance at 407 nm (red) or 381 nm (blue) as a function of acetate added. A fit of the data to the equation described in Materials and Methods yields an apparent K_d value of 38 $\pm$ 3 mM (407 nm) or 35 $\pm$ 1 mM (381 nm).