## SUPPLEMENTARY MATERIAL

## Structure and function of the lanthanide-dependent methanol dehydrogenase XoxF from the methanotroph *Methylomicrobium buryatense* 5GB1C

Yue Wen Deng,<sup>\*</sup> Soo Y. Ro,<sup>\*</sup> and Amy C. Rosenzweig $^{\boxtimes}$ 

Departments of Molecular Biosciences and of Chemistry, Northwestern University, Evanston, IL

## 60208, USA

<sup>\infty</sup>To whom correspondence should be addressed. Email: amyr@northwestern.edu; Phone: (847) 467-5301; Fax: (847) 467-6489

\*These authors contributed equally to this work.

PDB accession code: 6DAM



**Fig. S1** Purification of 5G-XoxF. **a** Anion exchange chromatogram of *Mm. buryatense* 5GB1C soluble protein fraction (50 mM-400 mM NaCl gradient shown as a *green* slope) and **b** Superdex 200 size exclusion trace. 5G-XoxF is present in the peaks indicated by black arrows. The absorbance at three wavelengths, 280 nm, 345 nm, and 415 nm, is shown in *blue*, *pink*, and *red*, respectively.



**Fig. S2** SDS-PAGE of 5G-XoxF purified. Lane 1, molecular weight markers; lane 2, XoxF after the final purification step.



**Fig. S3** 5G-XoxF absorbance spectrum. Monitoring 5G-XoxF during column chromatography is based on the peak around 345 nm corresponding to the PQQ cofactor [50]. The peak around 415 nm is indicative of cytochrome contamination. A high 345 nm to 415 nm ratio indicates the presence of 5G-XoxF.



**Fig. S4** SDS-PAGE of pMMO purified from *Mm. buryatense* 5G. The three subunits of 5G-pMMO are labeled; PmoA and PmoC run closely together on a 15% SDS-PAGE gel.



**Fig. S5** Purification of 5G-pMMO. Anion exchange chromatogram of 5G-pMMO using Source 15Q. The absorbance at 280 nm is shown in *blue*. A 50-800 mM NaCl gradient is shown as a *green* slope (corresponding to 0-40%).



**Fig. S6** 5G-XoxF crystal packing. The 5G-XoxF monomer (*pink*) shown with its symmetry mate forms the standard dimer of other MDHs. The Na(III) ion is shown as a yellow sphere, the PQQ is shown as sticks, and a modeled sodium ion is shown as a cyan sphere.