Supporting Information for:

Structural Characterization of *Porphyromonas gingivalis* Enoyl-ACP Reductase II (FabK)

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Figure Notes.

1. Figures S1, S2, and S3 were generated using the PrimeX software included in the Schrodinger molecular modeling package; Schrödinger Release 2017-3: PrimeX, Schrödinger, LLC, New York, NY, 2017.

- Bell JA, Cao Y, Gunn JR, Day T, Gallicchio E, Zhou Z, Levy R and Farid R, "PrimeX and the Schrödinger Computational Chemistry Suite of Programs," *International Tables for Crystallography*, **2012**, 534-538.

2. Figure S4 was generated using the UCSF Chimera package. *Chimera is developed by the Resource for Biocomputing, Visualization, and Informatics at the University of California, San Francisco (supported by NIGMS P41-GM103311).*

- Pettersen EF, Goddard TD, Huang CC, Couch GS, Greenblatt DM, Meng EC, Ferrin TE, “UCSF Chimera--a visualization system for exploratory research and analysis,” *J Comput Chem*. **2004**, 25(13):1605-12.

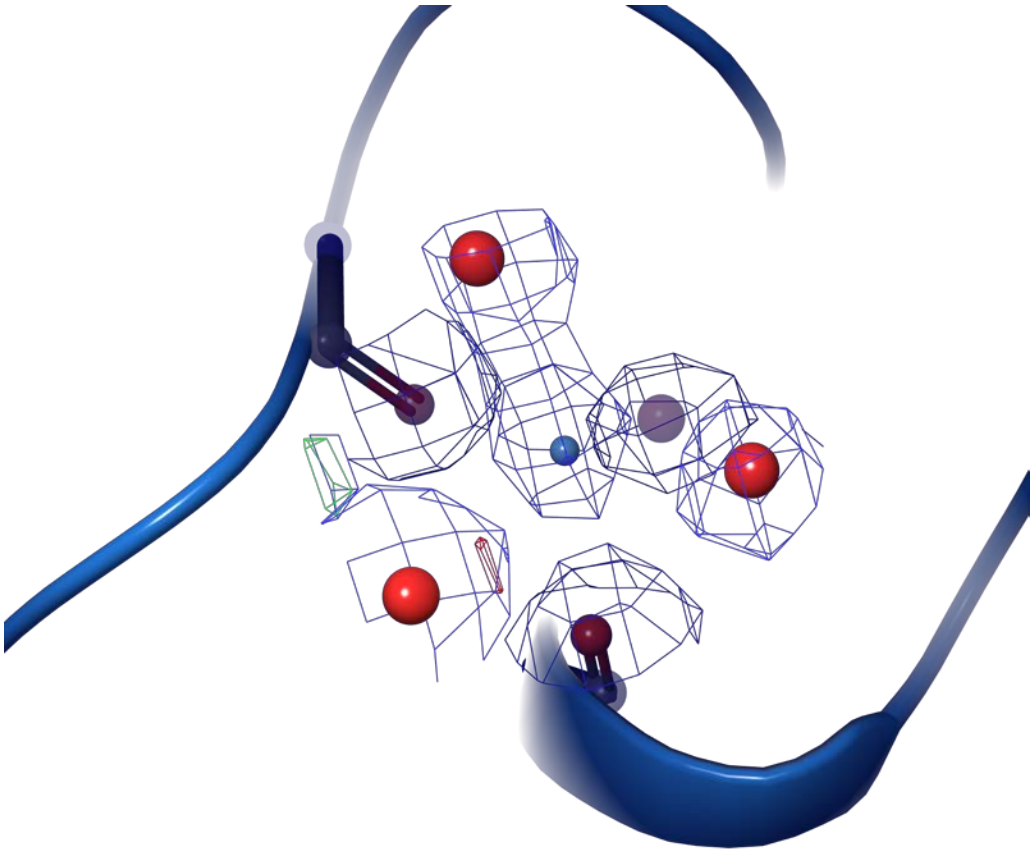

Figure S1. Sodium ion (B-405) contour map and difference map overlay. A sodium ion and its associated water molecules and coordinating residues are shown with both 2Fo-Fc (at 1 r.m.s.d.) and Fo-Fc (at 3 r.m.s.d.) maps. The maps have been truncated at a 2 Å distance from the displayed sodium atom (blue). Octahedral coordination geometry is discernable from the electron density which is consistent with a metal ion at this position rather than water.

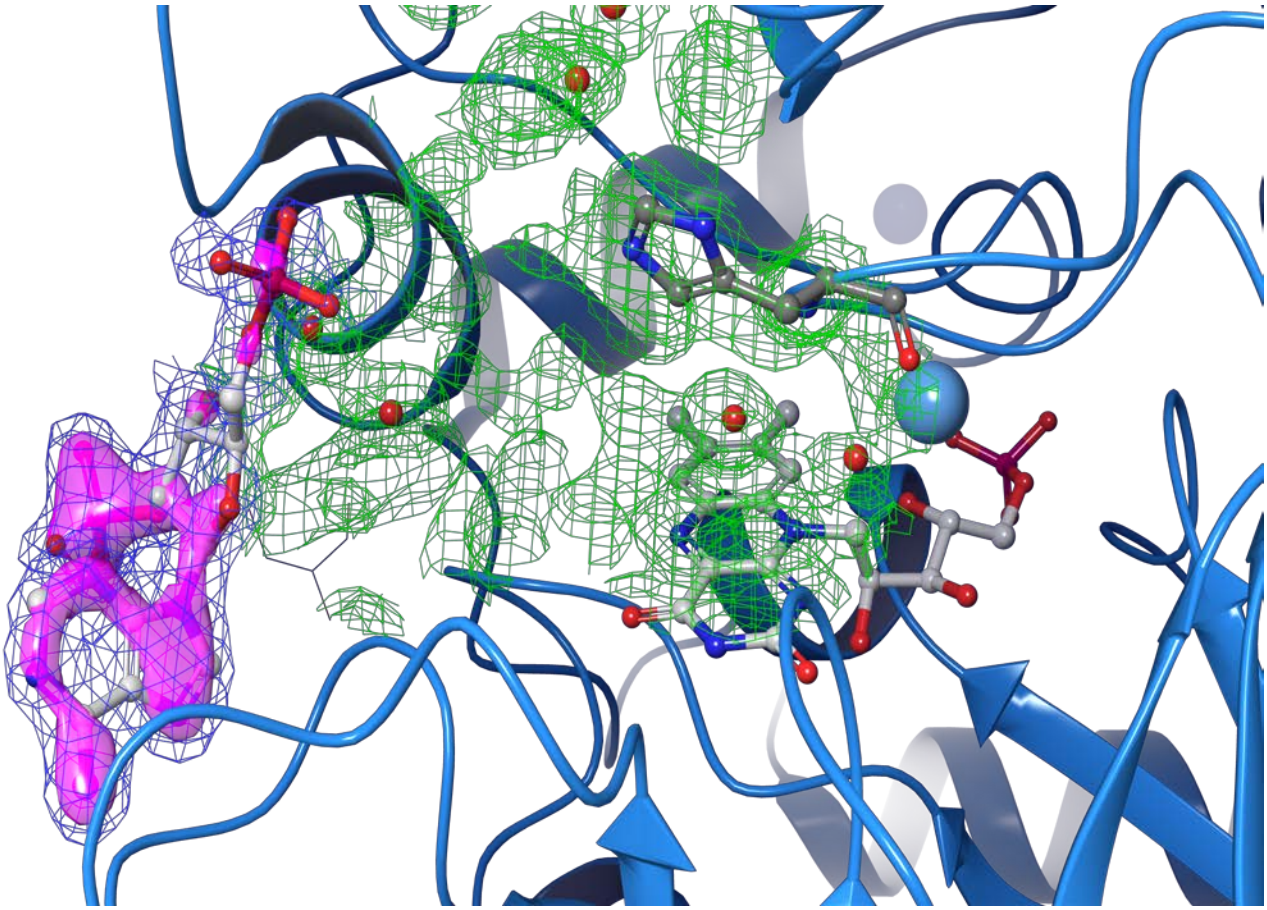

Figure S2. NADP and *Pg*FabK Active Site Electron Density. Shown is the *Pg*FabK active site with NADP (left), FMN (right), and modeled active site waters and sodium ion. 2Fo-Fc contour maps are shown at r.m.s.d. of 1 (blue mesh) and 2 (purple solid) for NADP with truncation at 1 Å from the NADP atoms. A 2Fo-Fc contour map at r.m.s.d. of 0.5 (green mesh) is shown for the active site region spanning NADPH and the FMN prosthetic group, selected by centering between the two ligands.

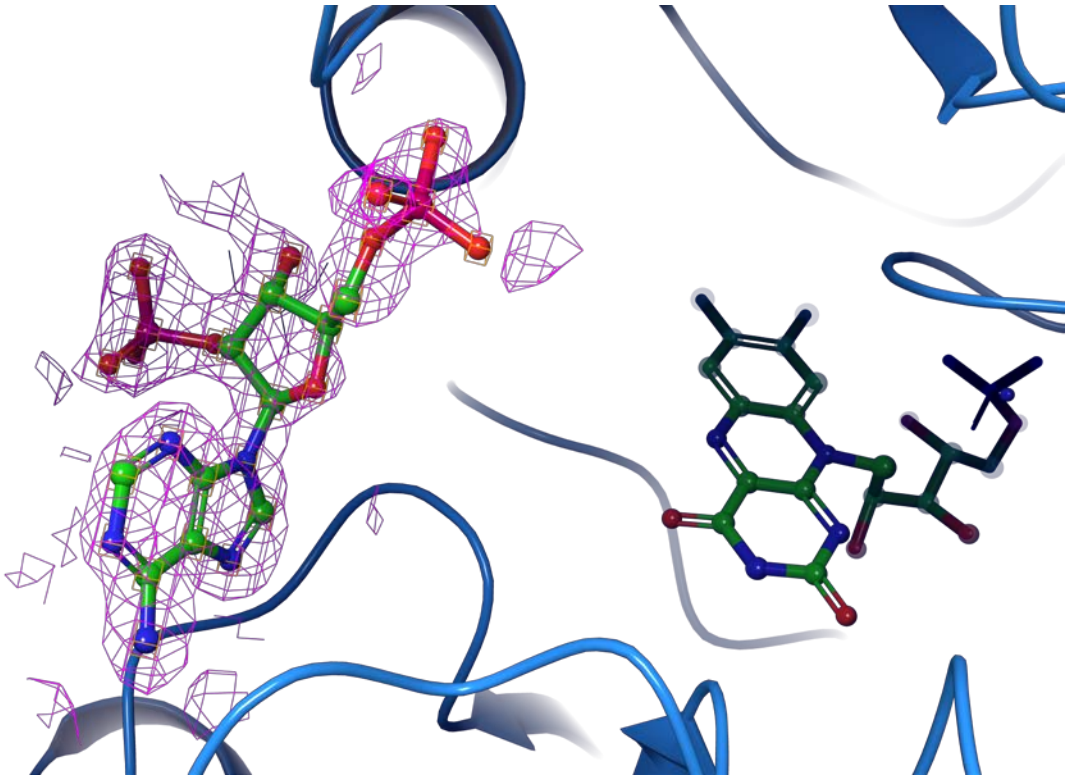

Figure S3. 2Fo-Fc Omit Map. Shown is a 2Fo-Fc omit map calculated by omitting the active site NADP molecule. The r.m.s.d. is 1 with truncation of the map at 2 Å from the NADPH atoms.

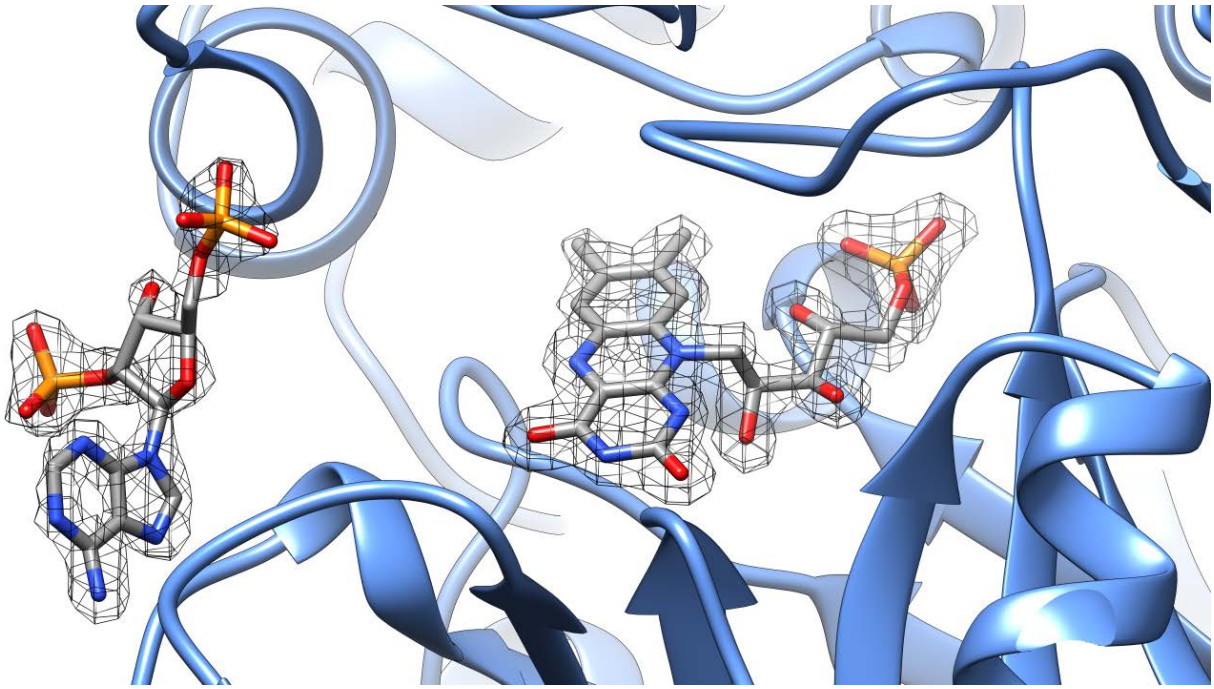

Figure S4. FabK Cofactor FMN and NADPH Electron Density. 2Fo-Fc contour map showing electron density of FMN prosthetic group and NADPH fragment spanning the *Pg*FabK active site (shown at 1.25 r.m.s.d. with a zone radius cutoff of 1.5 Å from the FMN and NADPH ligands).

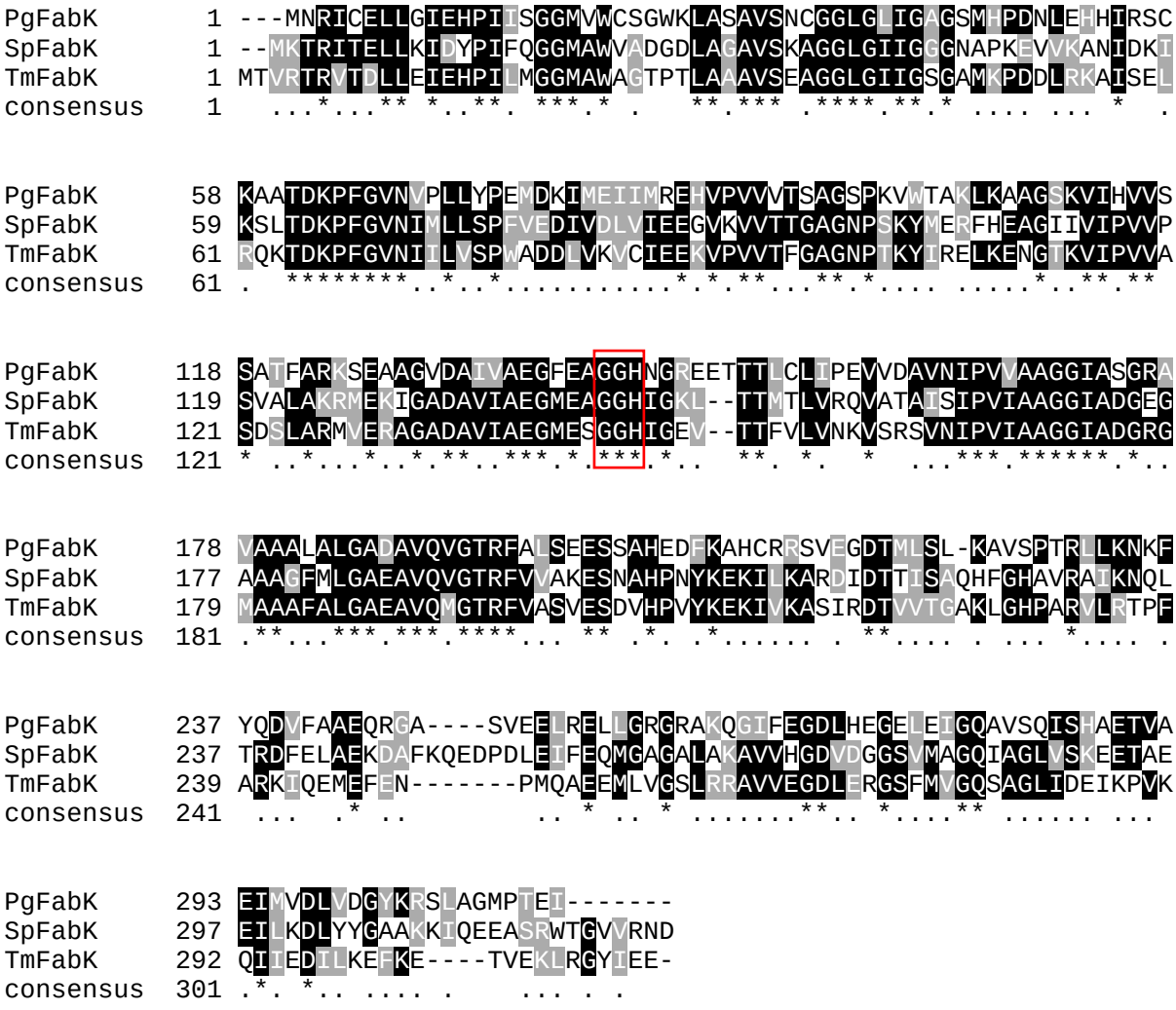

Figure S5. FabK Multiple Sequence Alignment. Multiple sequence alignment of *P. gingivalis*, *S. pneumoniae*, and *T. maritima* FabK enzymes. Produced using Clustal Omega at EMBL-EBI (Sievers, F., et al. (2011). *Mol. Syst. Biol.* **7**, 539.) and rendered using the BoxShade program at the ExPASy Bioinformatics Resource Portal. Conserved active site structural motif of the NMO family of flavoproteins is shown in red box.