

- 2 Volume 71 (2015)
- 3 Supporting information for article:
- 4 Structure of *Plasmodium falciparum* orotate phosphoribosyltransferase
- 5 with autologous inhibitory protein-protein interactions
- 6 Shiva Kumar, Kalyanaraman Krishnamoorthy, Devaraja G. Mudeppa and Pradipsinh K.
- 7 Rathod

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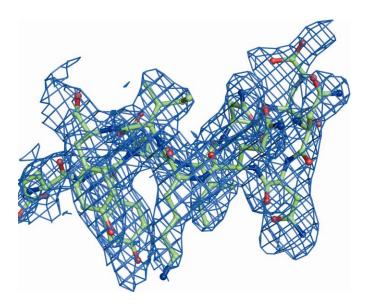
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100 \*\* 80 90 4FYM\_P.fal IYIDLR 2WNS Human 1STO\_S.typhimur 2PRY\_S.cerevisi Substrate Pocket 130 4FYM\_P.fal NITC 2WNS\_Human 1STO\_S.typhimur 1ORO E.coli 2PRY\_S.cerevisi Inhibitory Loop 250 4FYM P.fal EYEINENNQKIYF 2WNS\_Human Q....GGKDKLQA E...RGRGEISA E...RGRGEISA 1STO\_S.typhimur 10RO E.coli EVVSTDDKEGLSA 2PRY\_S.cerevisi

Hood Domain

**Figure S1** Multiple sequence alignment of OPRTase homologues with available structures. Sequence similarity around the hood domain, substrate binding pocket and inhibitory loop is depicted in separate boxes. PDB id and the organism names are shown for each sequence. Residues are numbered according to the *Plasmodium falciparum* sequence. Conserved residues are shown with red background, while the semi-conserved residues are shown in red fonts in white background. Residues that are expected to make contacts with the ligand, based on the human structure (PDB id: 2WNS), are denoted with a black star.



**Figure S2** Simulated annealing omit map of the *P. falciparum* OPRTase inhibitory loop. Blue mesh depicts the 2fo-fc map calculated using the simulated annealing omit-map procedure and contoured to 1σ. The entire inhibitory loop (<sup>243</sup>EYEINENNQKIY<sup>254</sup>) from all the eight chains were omitted for the calculation. Quality of the map shows that the inhibitory loop is modeled entirely within an unbiased electron-density.