

# 1 Acta Crystallographica Section D

2 Volume 70 (2014)

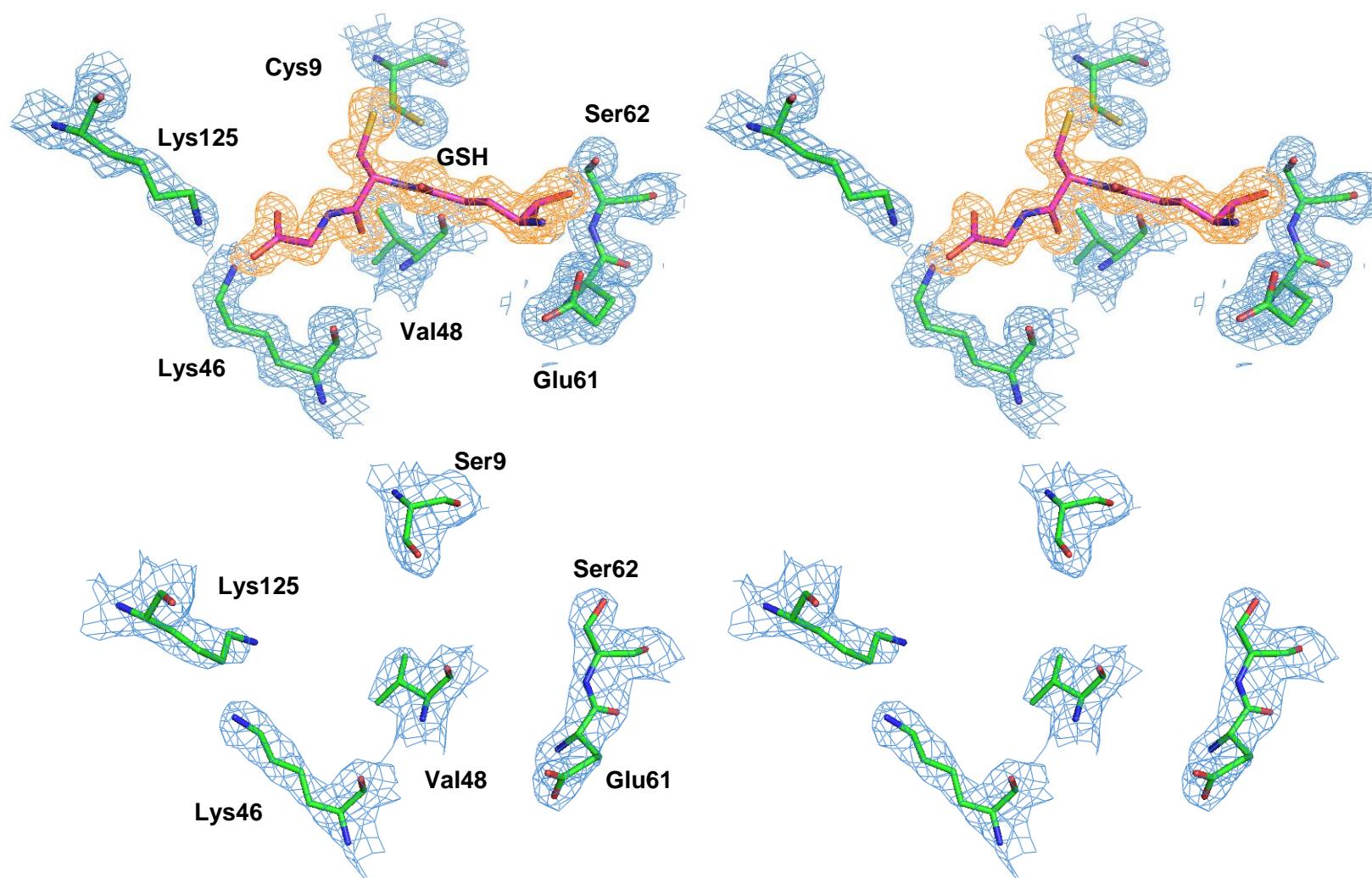
3 Supporting information for article:

4 Structure of *Escherichia coli* Grx2 in complex with glutathione: a dual-function hybrid of glutaredoxin  
5 and glutathione S-transferase

6 Jun Ye, S. Venkadesh Nadar, Jiaojiao Li and Barry P. Rosen

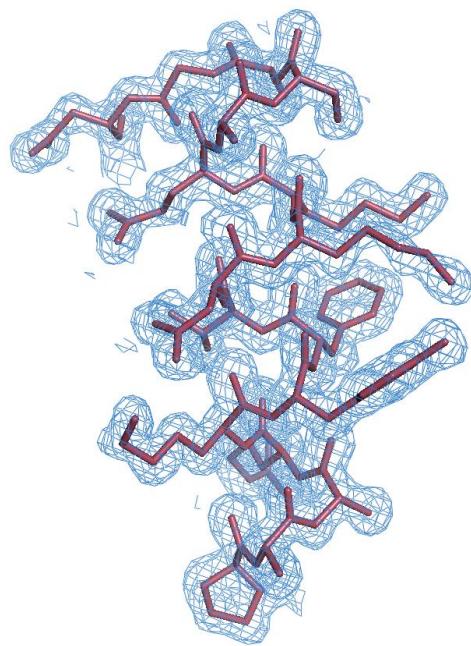
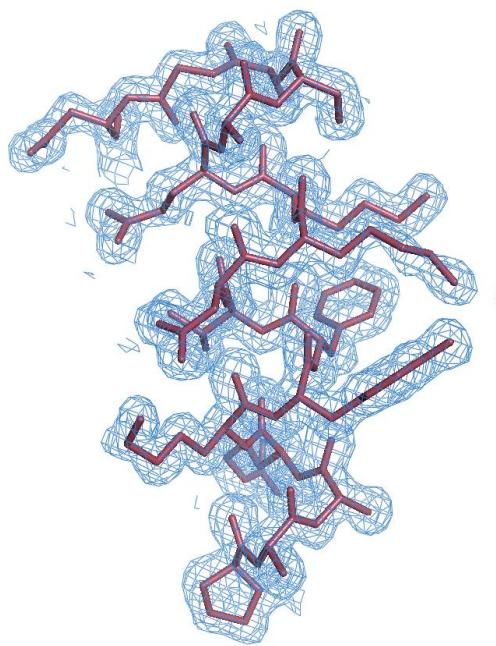
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10 **Figure S1** Stereo view of active site residues of Grx2-GSH (top) and Grx2 C9S/C12S mutant (bottom) with electron density map.  
11 The 2Fo-Fc map contoured at 1σ level shown in blue mesh and omit map (Fo-Fc) at 3σ level shown in orange mesh.



(a)

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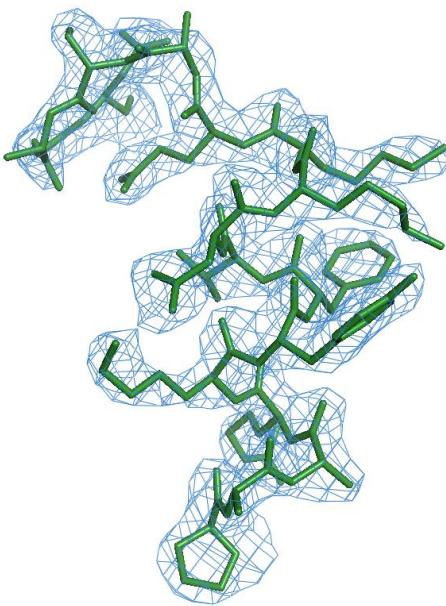
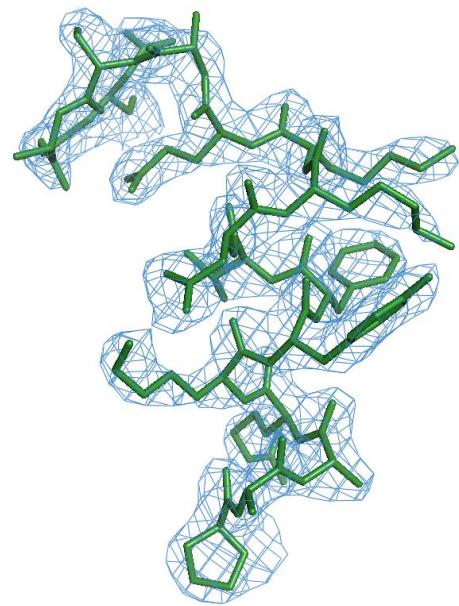
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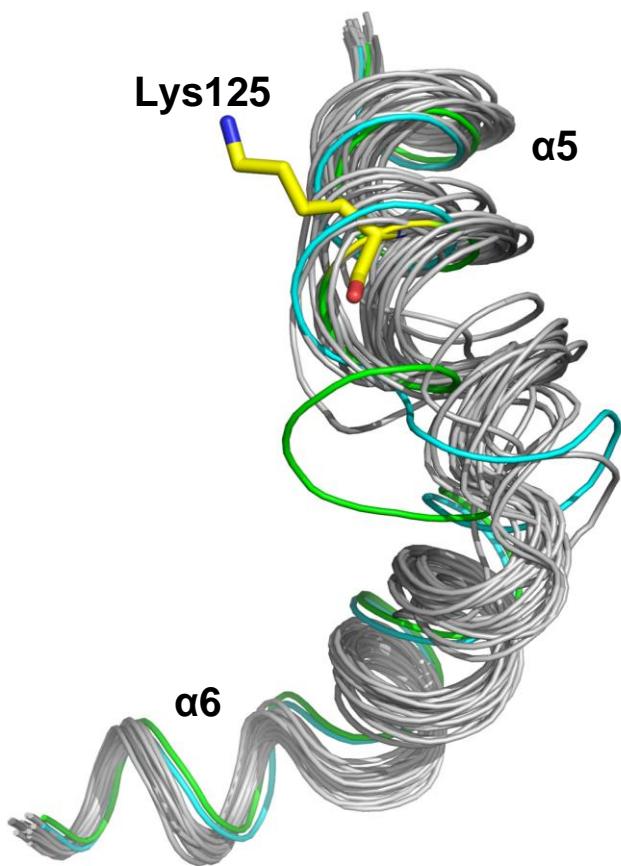
(b)

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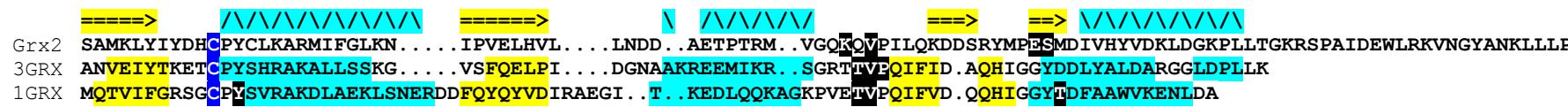
20 **Figure S2** Stereo view of helix  $\alpha$ 5 (Pro116 to Asn132) with 2Fo-Fc map contoured at  $1\sigma$  level. (a) Grx2-GSH and (b) Grx2 C9S/C12S mutant structure.

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23 **Figure S3** Superimposition of helices  $\alpha$ 5 and  $\alpha$ 6 of Grx2 structures. The wild type Grx2-GSH structure is shown in green. The Grx2 C9S/C12S mutant  
24 structure is shown in cyan. The 21 models of the NMR structure of Grx2 (PDB ID: 1G7O) are shown in gray. Lys125 of the wild type Grx2-GSH structure  
25 are shown in grey.

**26 Figure S4**

27 Structure-based sequence alignment of Grx2 with *E. coli* glutaredoxins Grx1 (1GRX) and Grx3 (3GRX). The active site cysteine residues are highlighted  
28 in blue, and glutathione binding residues are highlighted in black. The cyan and yellow shaded residues represent  $\alpha$  helices and  $\beta$  sheets, respectively.

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31 **Figure S5** Structure-based sequence alignment of Grx2 with members of different classes of GSTs. Each GST is labeled by its PDB ID. Glutathione-  
 32 binding residues are highlighted in black. The shaded residues represent  $\alpha$  helices (cyan) and  $\beta$  sheets (yellow).