

Article

A Novel Substrate-Binding Site in the X-Ray Structure of an Oxidized E. coli Glyceraldehyde 3-Phosphate Dehydrogenase Elucidated by Single-Wavelength Anomalous Dispersion

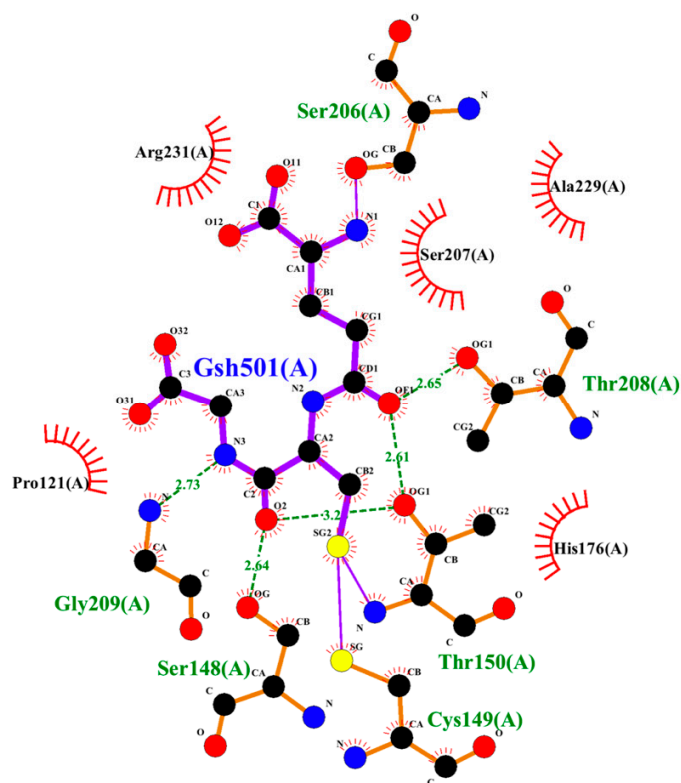
Rodríguez-Hernández Annia ^{1,*}, Enrique Romo-Arévalo ², Adela Rodríguez-Romero ^{1,*}

¹ Instituto de Química, Universidad Nacional Autónoma de México, Circuito exterior s/n, Ciudad Universitaria, Coyoacán, 04510, Ciudad de México, México

² Facultad de Odontología, Universidad Nacional Autónoma de México, Investigación Científica 1853, Ciudad Universitaria, 04360, Ciudad de México, México

* Correspondence: arodriguezh@iquimica.unam.mx (A.R.-H.); adela@unam.mx (A.R.-R.)

Supplementary Material



Supplementary Figure 1. Possible interactions of GAPDH and GSH. The likely oxidizer, GSH was built into the electron density map (initially Fo-Fc, later into the 2Fo-Fc). Despite our attempts, several

clashes with the protein occurred. A LigPlot [1] of the GSH modification, was obtained to show likely interactions with the protein. GSH is shown in purple, residues at hydrogen bond distance, and their distances are in green. Electrostatic and hydrophobic interactions are shown as red semi-circles with sparks. Three purple lines show atoms that are too close to form non-covalent interactions, logically the sulfur atom of Cys149 is one of them. However, the side-chain oxygen of Ser206 and the main chain nitrogen of Thr150 clash with the GSH. Thus, we decided to remove the ligand from the final model.

[1] Laskowski, R.A, Swindells, M.B LigPlot+: multiple ligand-protein interaction diagrams for drug discovery. *J. Chem. Inf. Model.* **2011**, *51*, 2778–2786.