



BIOLOGICAL
CRYSTALLOGRAPHY

Volume 71 (2015)

Supporting information for article:

The structure of apo ArnA features an unexpected central binding pocket and provides an explanation for enzymatic cooperativity

Utz Fischer, Simon Hertlein and Clemens Grimm

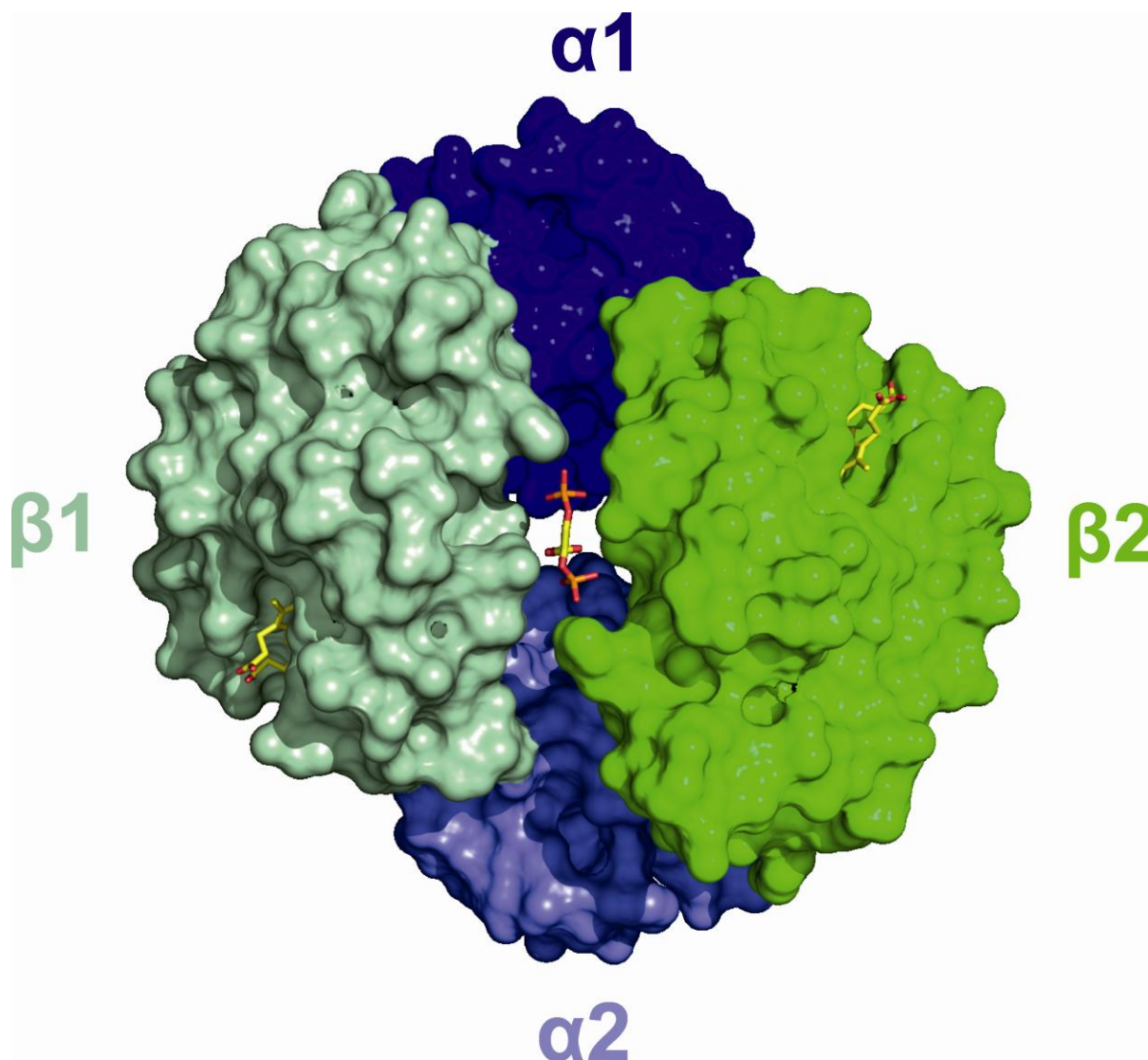
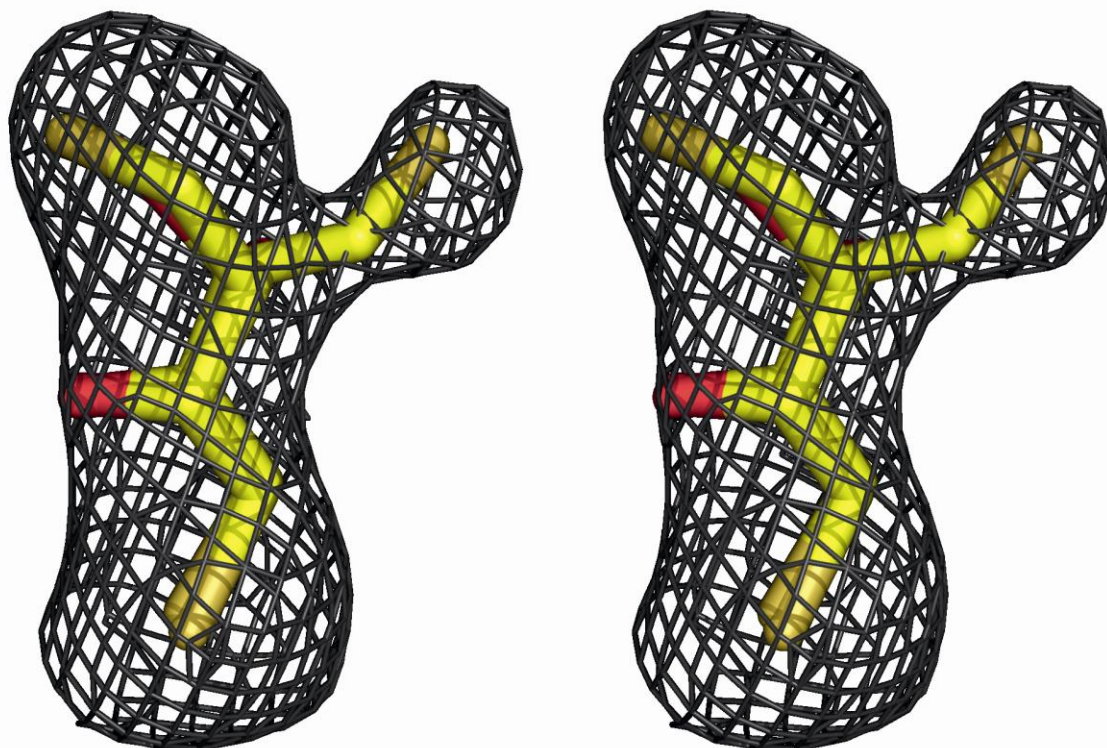


Figure S1 Two Cross-eyed Stereo views of the DTT ligand fitted in two alternative conformations within the ArnA central binding pocket. The $2F_{\text{obs}} - F_{\text{calc}}$ simulated annealing electron density map is shown as a grey mesh isosurface contoured on 0.8σ level. The upper view is along the trimeric NCS axis, the lower view is perpendicular to the trimeric NCS axis.

View perpendicular to threefold NCS axis



View along threefold NCS axis

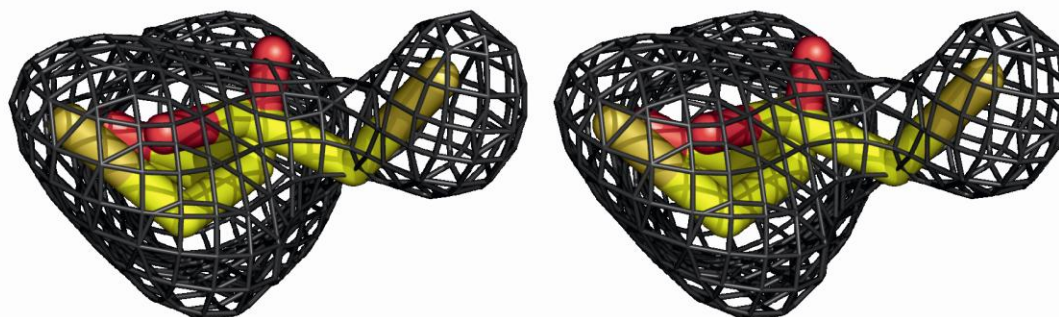


Figure S2 Crystal structure of the complex between deoxyhemoglobin and 2,3-BPG (PDB ID code 1B86). The two α subunits are shown in shades of blue, the two β subunits in shades of green. The two heme groups bound to the two β subunits, each, are shown as stick model. In the center of the molecule, the bound 2,3-BPG effector is shown as a ball-and-stick model.