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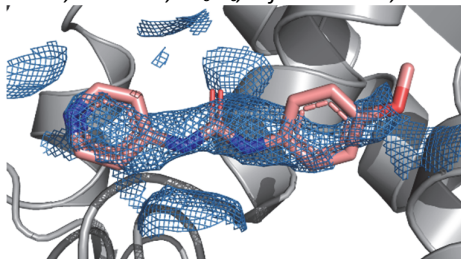
Supporting information for article:

Structures of the *Plasmodium falciparum* heat-shock protein 70-x ATPase domain in complex with chemical fragments identify conserved and unique binding sites

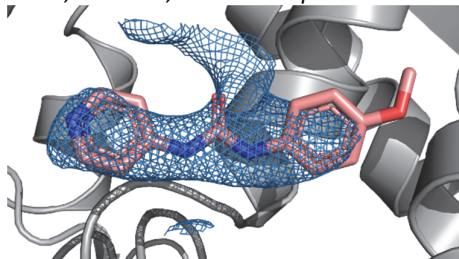
Nada Mohamad, Ailsa O'Donoghue, Anastassia L. Kantsadi and Ioannis Vakonakis

Supporting Figures

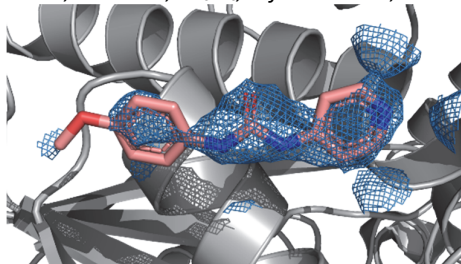
700E, JHJ A509, 2F_o-F_c, B-factor 81 Å², Occ 0.73, RSR 0.21



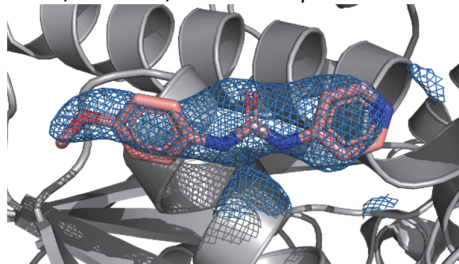
700E, JHJ A509, PanDDA map



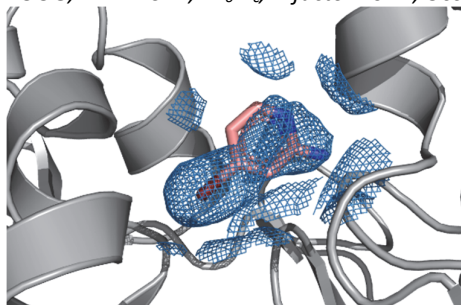
700E, JHJ A515, 2F_o-F_c, B-factor 68 Å², Occ 0.66, RSR 0.32



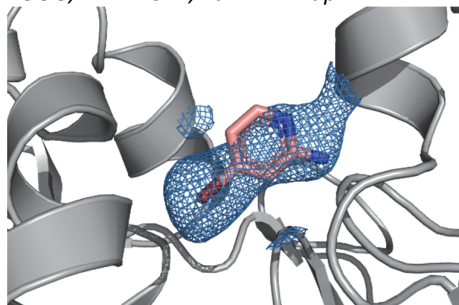
700E, JHJ A515, PanDDA map



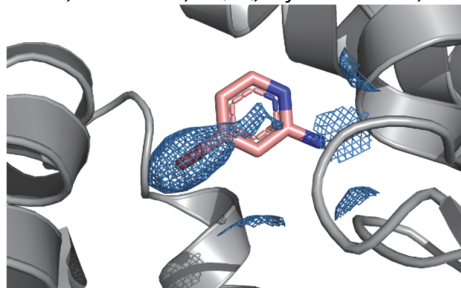
700G, HEW A511, 2F_o-F_c, B-factor 70 Å², Occ 0.7, RSR 0.2



700G, HEW A511, PanDDA map



700G, HEW B511, 2F_o-F_c, B-factor 125 Å², Occ 0.72, RSR 0.2



700G, HEW residue B511, PanDDA map

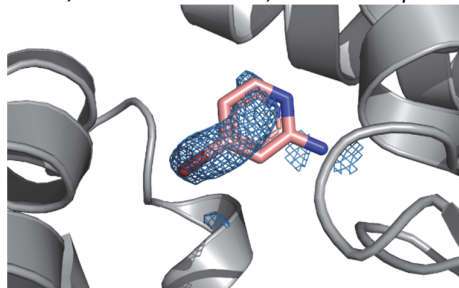


Fig. S1: Electron density of fragments. Shown here are (left column) 2F_o-F_c electron densities and (right column) PanDDA difference densities of fragments bound to the PfHsp70-x ATPase domain, truncated at 3 Å distance from any ligand atom. The structure PDB IDs, ligand residue numbers, B-factors, occupancies (Occ) and real-space R values (RSR) are indicated. For ligand PYZ (entry 7P31, next page) reported occupancies exclude the iodine atom. 2F_o-F_c densities were plotted at 1 r.m.s.d. level; PanDDA densities at 2 r.m.s.d. level. Figure continues on the next page.

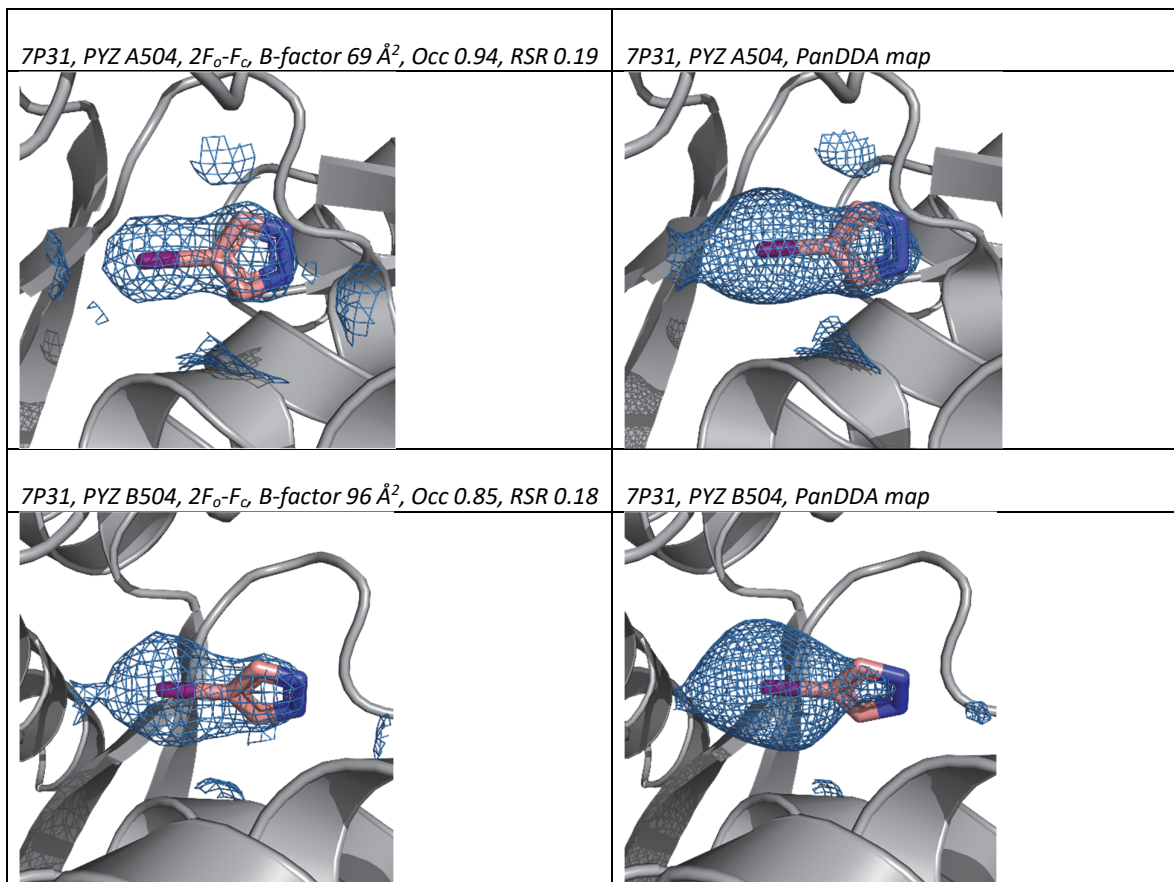


Fig. S1 continued

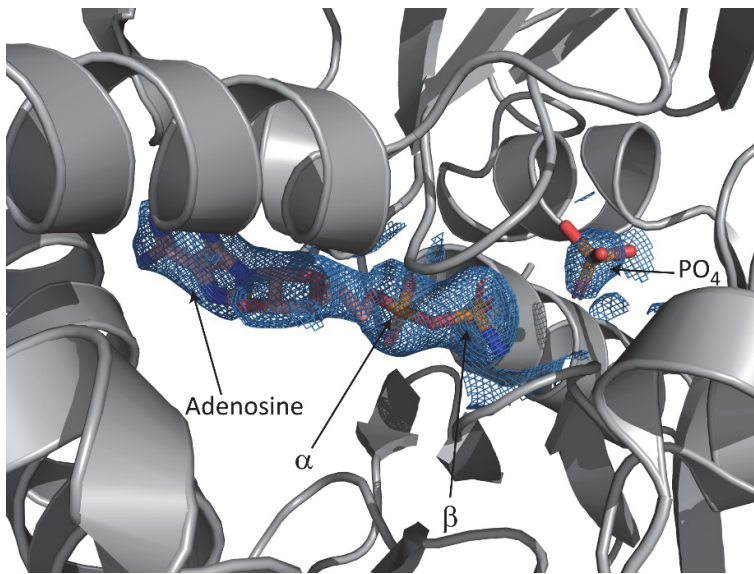
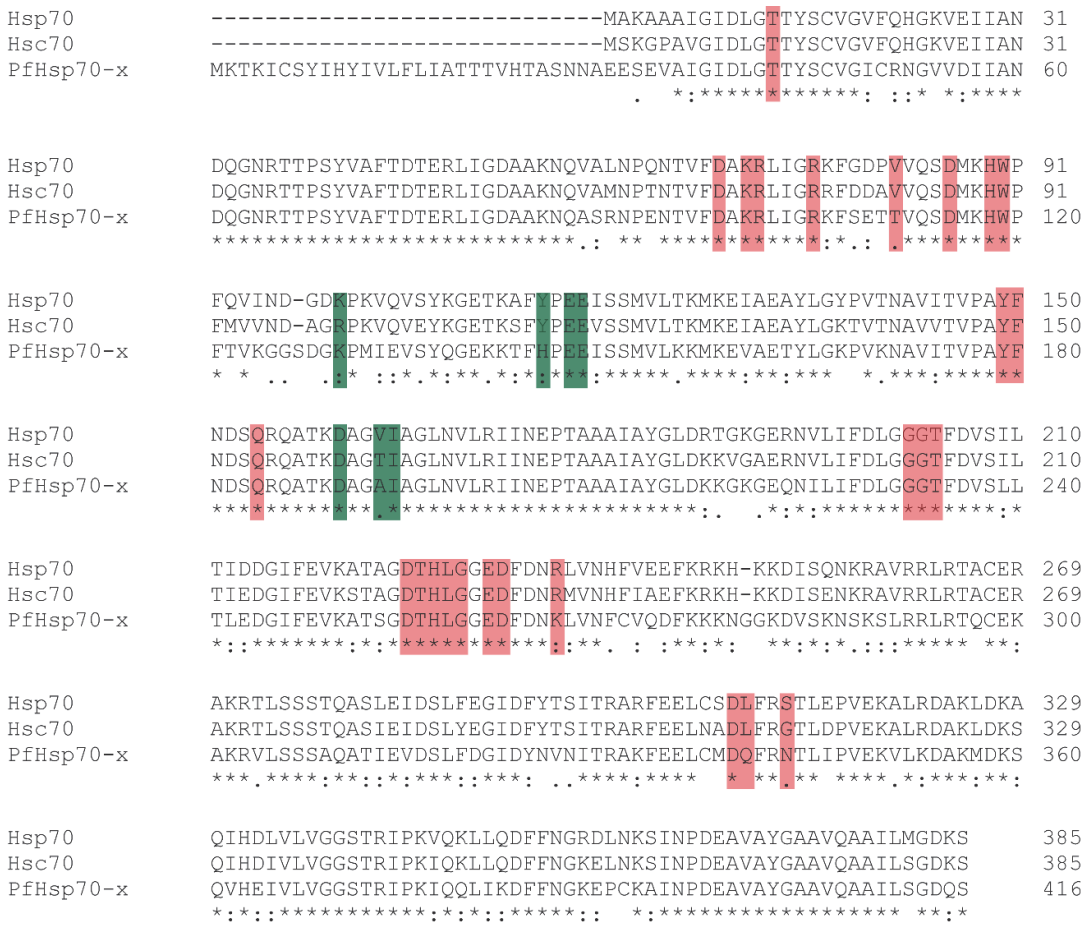


Fig. S2: Nucleotide electron density in PfHsp70-x ATPase domain crystals. Shown here is exemplar 2F_o-F_c electron density for the bound nucleotide in PfHsp70-x ATPase domain crystals and its surrounding environment, drawn from entry 7OOE chain A. The electron density was plotted at 2 r.m.s.d. level. As seen, PfHsp70-x crystals trapped a hydrolysed nucleotide state with clear density for the leaving phosphate group.





 Interaction site 1
 Interaction site 2

Fig. S3: Sequence alignment of PfHsp70-x and human erythrocytic chaperones. Shown here is a Clustal Omega multiple sequence alignment of the ATPase domain of PfHsp70-x (UniProt ID K7NTP5) with the equivalent domains of human Hsp70 (P0DMV8) and Hsc70 (P11142). Residues up to 5 Å away from fragment ligands in the PfHsp70-x crystallographic structures are colour coded by binding site.