Supplemental Information for

# Crystal structures of cytochrome P450 2B4 in complex with the inhibitor 1-biphenyl-4-methyl-1H–imidazole: ligand induced structural response through α-helical repositioning[†‡]

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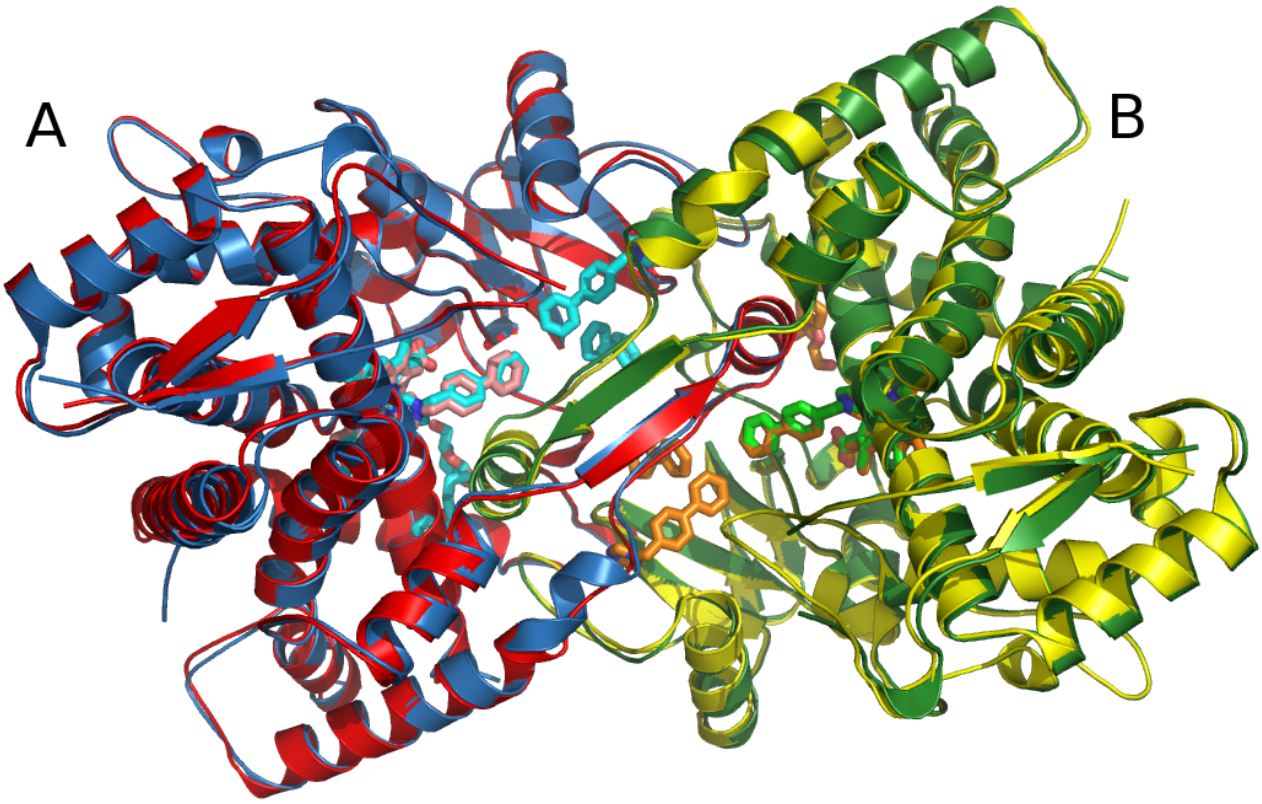



**Figure S1a**

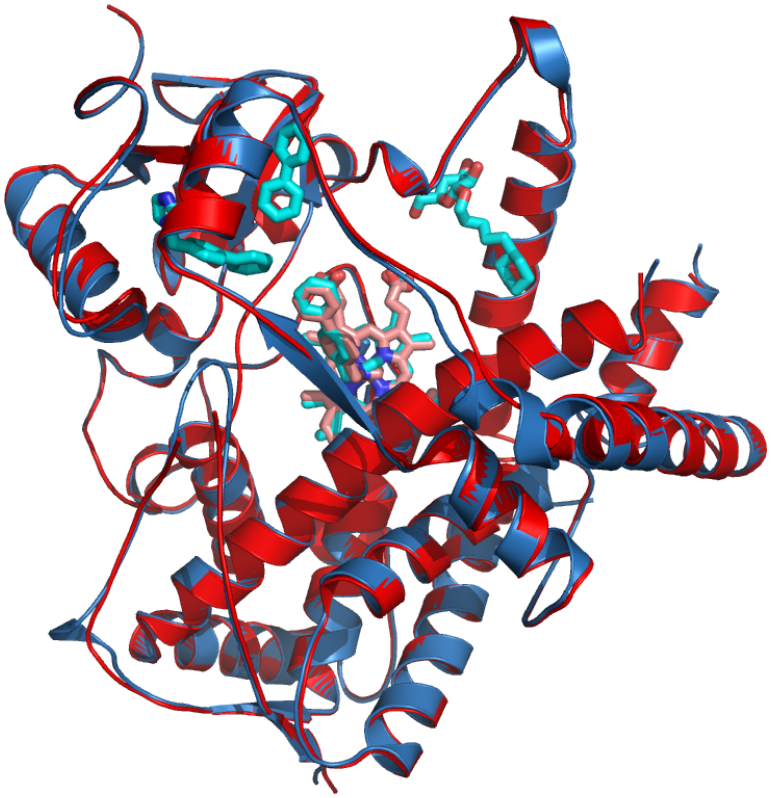


**Figure S1b**

**Supplemental Figure 1.** Ribbon diagram overlay of both CYP2B4:1-PBI structures. The triple ligand occupancy complex is colored blue and yellow with cyan and orange ligands. The single ligand occupancy complex is colored red and green with salmon and light green ligands. **a**. An overlay of the dimer yields an RMSD of 0.6 Å. The A chain is shown on the left and the B chain on the right. **b.** An overlay of the monomer yields an RMSD of less than 0.5 Å for each chain. The single ligand occupancy complex does not show electron density for the dimer interface 1-PBI molecules. The active site 1-PBI is in essentially the same orientation in both models.

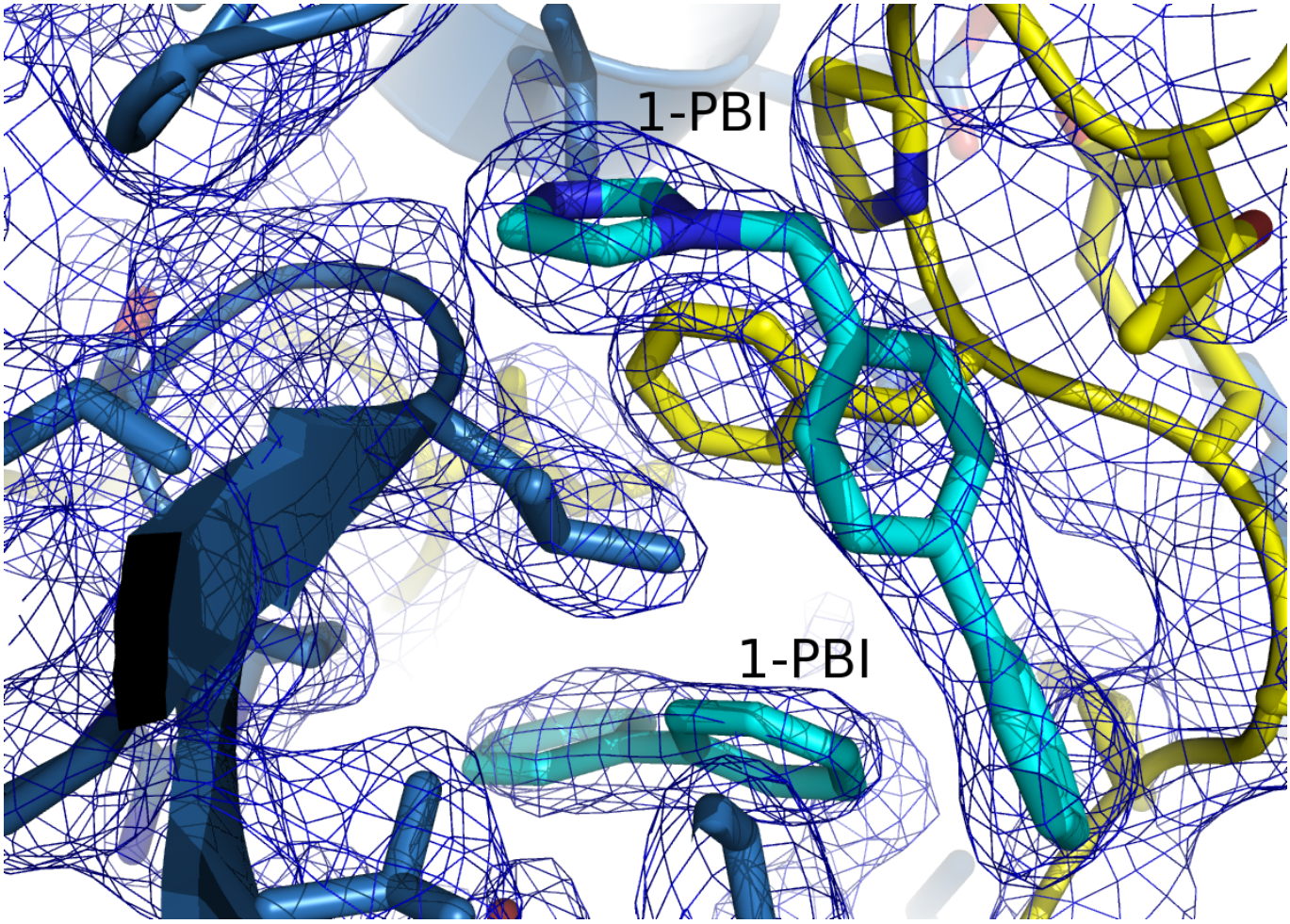



**Figure S2a**

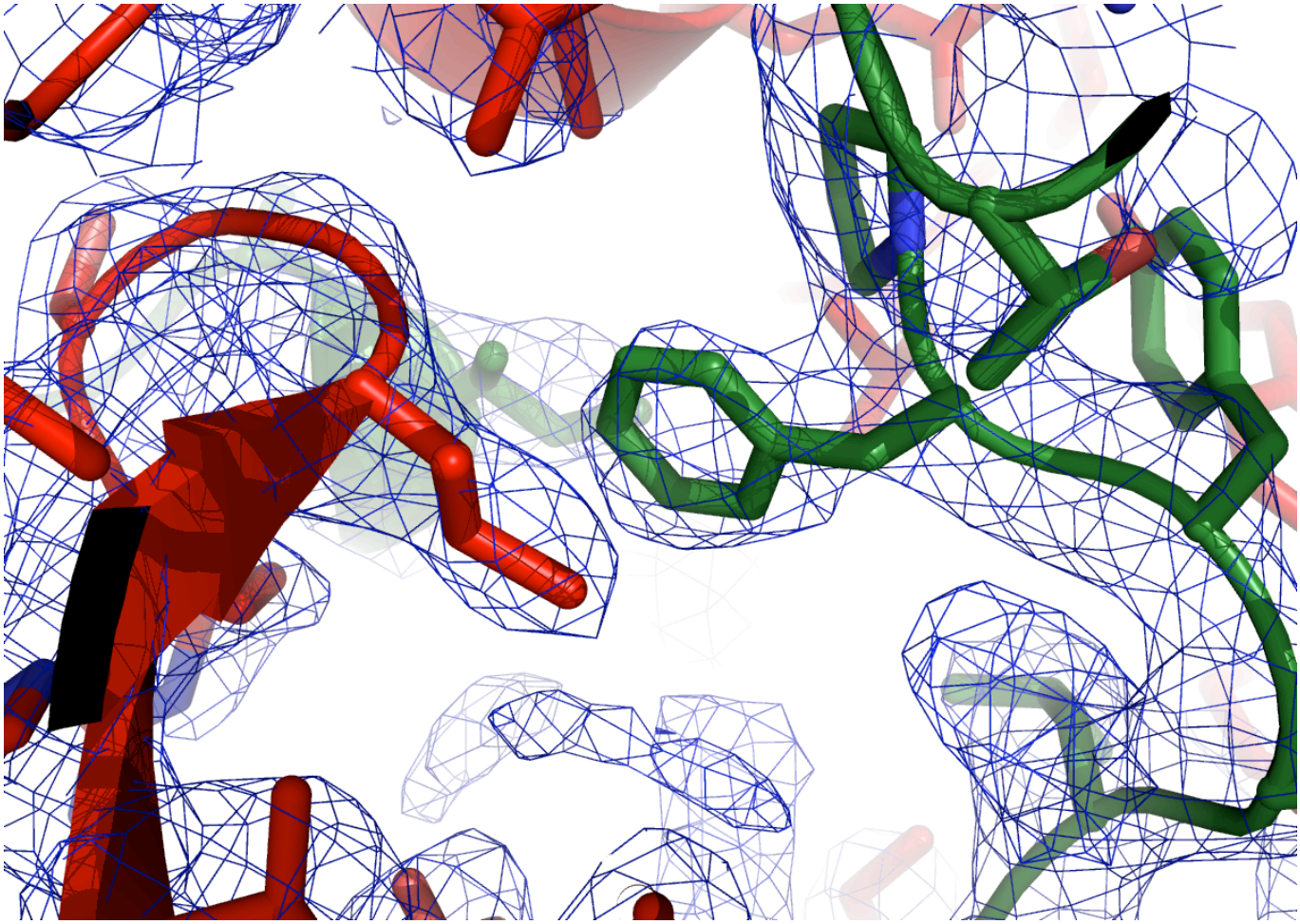
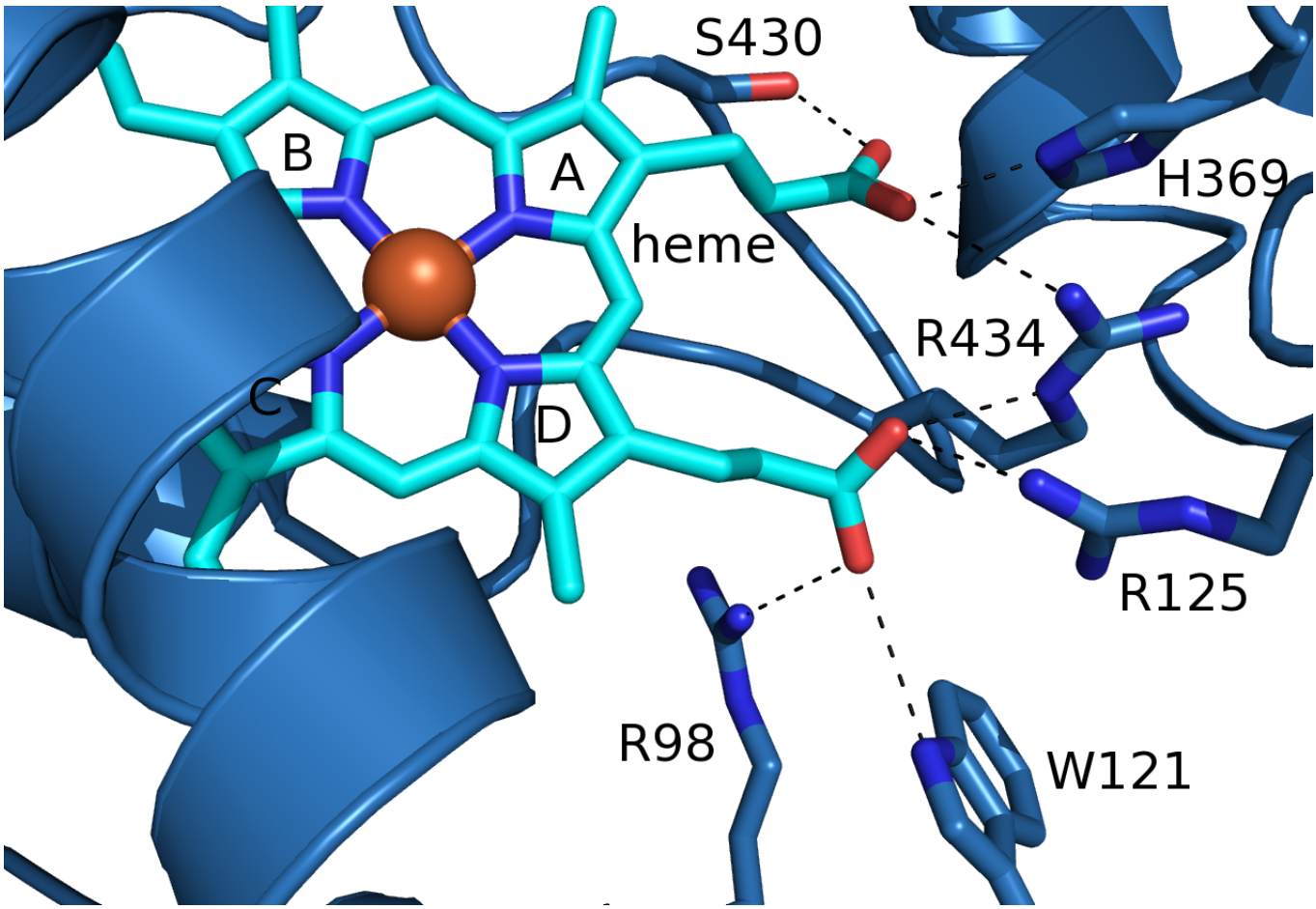


**Figure S2b**

**Supplemental Figure 2.** Ribbon and stick diagram with electron density maps showing the peripheral inhibitor binding site. Colors are the same as in Supplemental Figure 2. **a.** The triple ligand occupancy structure shows clear density for one extra 1-PBI molecule as well as the biphenyl moiety for another. **b.** The same region of the protein in the single ligand occupancy structure does not show any definitive density for peripheral ligands.




**Supplemental Figure 3.** Ribbon and stick model showing heme propionate interactions. Protein side chains are shown as blue sticks, heme is shown as cyan sticks with a ball depiction of the chelated iron. The A ring is held into place through hydrogen bonds to His, 369, Ser 430 and Arg 434. Arg 98, Trp 121, Arg 125 and Arg 434 secure the D ring.