

Reflections on Resolution and Revolution – the PDB and me

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The Protein Data Bank (PDB) tracks with my own scientific career. I was at the Cold Spring Harbor symposium where the concept was hatched, my data were in the first PDB release, and I continue to this day – both as a depositor and as a user of PDB data. During this half century, much has transpired with respect to the resolution of maps from which atomic models have been built, in my case from 5.5 Å for the initial myohemerythrin model to 0.935 Å resolution for crambin. Progress continues for interpretations at both ends of this scale. There have been revolutions in how these atomic models are generated as well. Notable advances are in recombinant-DNA expression, crystallogensis, graphics-assisted and automated model building, robust refinement procedures, MAD and SAD phasing, synchrotrons and FELs, multi-dimensional NMR, and cryo-EM most recently. I will relate these developments to our current projects on the analysis of Hsp70 molecular chaperones, where we refine a novel conformational state at 7.7 Å resolution and visualize the in crystallo ATP hydrolysis reaction down to 1.29 Å resolution, and on transmembrane ion channels, where we compare populations of open and closed pores by cryo-EM and can observe hydrogen atoms at 1.90 Å resolution.