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Generation of Atomic Coordinates from Time-Resolved X-ray Diffraction Data. George N. Phillips, Jr., Elena J. Levin, Roman Aranda, IV, Dept. of Biochemistry, Univ. of Wisconsin-Madison, Wisconsin 53706.

New methods of refinement of time-resolved crystallography have been used to follow the dissociation of carbon monoxide from the heme pocket of sperm whale myoglobin and its mutants and to quantify the resultant conformational changes.

Electron density maps were previously created at various time points and used to describe amino acid side-chain and carbon monoxide movements. In this work, specially designed implementations of difference refinements were employed to generate atomic coordinates at each time point in order to create an explicit, quantitative representation of the photo-dissociation process. After photolysis the carbon monoxide moves to various docking sites, causing rearrangements in the heme pocket residues whose coordinate changes can be plotted as a function of time. These include rotations of the heme pocket phenylalanine, concomitant movement of the distal histidine, and proximal displacement of the heme iron. The degree of relaxation toward the intermediate and deoxy states could then be probed by analysis of the coordinate movements in the time-resolved models, revealing a non-linear progression to the unbound state and return to the bound state over time.

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