CDCS CENTER FOR DATA AND COMPUTING IN NATURAL SCIENCES

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Interactive TEMPy

Cryo-EM is a popular technique for understanding the structure of biological molecules. At intermediate resolutions (worse than ~4.5 Å), building and assessing the quality of atomic models derived from cryo-EM data is particularly difficult. At this resolution range, existing X-ray models or models derived from machine-learning based structure prediction approaches such as AlphaFold2 offer information about local geometry, but may require adjustment to be well fit to the cryo-EM data. *Interactive TEMPy* is a plugin for ChimeraX which facilitates fitting such models to density maps using a variety of methods.

The combination of manual placement, global search and density-based fitting offers a flexible platform for model refinement.

Integration with RIBFIND offers a flexible approach to decomposing structures hierarchically, a method which has seen success in automated fitting tools such as Flex-EM.

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