## MS01 MX/Cryo-EM software development

MS01-2-2 Efficient automated matching of protein structural entities from a database to partitioned cryo-EM maps #MS01-2-2

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## Abstract

Cryo-electron microscopy (Cryo-EM) has undergone a recent resolution revolution; however, the majority of maps deposited are below 3.0Å resolution. The current methods for model generation, such as ARP/wARP, rely on high resolution maps (<4.0Å) and take hours to complete. Here is proposed a pipeline that takes an input Cryo-EM map and returns a protein structure. The input map could be over a range of resolutions and will be sequence independent. The proposed pipeline starts by model segmentation, a method of splitting Cryo-EM map files into components of a larger macro assembly or 'Segments'. Once the map has been segmented, each segment will be run in a database search to find corresponding protein structures. The two search methods currently being investigated are 3D Zernike Descriptors: describing the shape of the protein map which is invariant to rotation; and FTIP, a software which finds representative points on the map to describe its shape. The top ranking matches for each segment will then undergo fitting and metrics from this process will determine a correct match or not. From this matching models will be determined and a structure realting to the input map will be outputted.