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ISOLDE: Building High Quality Macromolecular Models into Low Resolution Experimental Maps

ISOLDE is a ChimeraX plugin (installable via its built-in Tool Shed) designed to ease the task of building high quality macromolecular models into low to medium resolution electron density maps where experimental information alone is insufficient to place individual atoms precisely.

ISOLDE is unique in that it allows the model building task to be re-imagined as a truly interactive experience akin to working with a real physical molecule. It achieves this by combining the AMBER molecular dynamics forcefield (providing a high-fidelity description of the forces governing most macromolecules and small molecule ligands) with the GPU-accelerated molecular dynamics engine OpenMM, solving Newton's laws of motion for these forces hundreds of times per second on systems of a few thousand atoms.

Advantages of ISOLDE include real-time geometric validation, automatic fixing of simple errors thus reducing time spent on manual model building, and native compatibility with cryo-EM maps and/or crystallographic data. ISOLDE can generate maps directly from crystallographic F/sigF or I/sigI data in MTZ or CIF format (and automatically re-calculate them when the model changes), as well as "static" maps from pre-calculated F/phi data.

Further information can be found at the ISOLDE website and in the following publication:

Croll, Tristan Ian. 2018. "ISOLDE: A Physically Realistic Environment for Model Building into Low-Resolution Electron-Density Maps." Acta Crystallographica Section D: Structural Biology 74 (6):519–30. doi: 10.1107/S2059798318002425.

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