MS01 MX/Cryo-EM software development

MS1-01

Fitting, refinement and validation of atomic models in cryo-EM maps using TEMPy2

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Abstract

As the resolutions of cryo-EM reconstructions of macromolecular assemblies are being improved, there is a need for better fitting and refinement methods of atomic models in medium-to-high resolutions. There is also a strong need for robust approaches for model assessment. Here, we present the current capabilities of our software TEMPy2 to fit, refine and validate atomic models in cryo-EM maps. We demonstrate it on a large benchmark of assemblies from EMDB (at 1.8-7.1 Å resolution) and CASP14 cryo-EM targets (2.1-3.8 Å resolution). We also present new capabilities of TEMPy2 to process cryoEM maps.

References

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2. Cragnolini T, Kryshtafovych A, Topf M (2021) Cryo-EM targets in CASP14. Proteins 89(12):1949-1958.