The Use of Checkmymetal for Modeling Metal Binding Sites in Low-Resolution Protein Structures

Michal Gucwa[1], Joanna Lenkiewicz[2], Michal Szczygiel[2], Aziza Aripova[3], Wladek Minor[2]
[1]University of Virginia, Jagiellonian University, [2]University of Virginia, [3]Jagiellonian University, University of Virginia
michal_g@iwonka.med.virginia.edu

Improving the accuracy of metal binding site modeling can contribute to a better understanding of metal-mediated biological processes. Many structural experiments result in low-resolution structures, making it challenging to identify and model metal binding sites in the electron density or potential map. We have improved CheckMyMetal, a web server that validates metal ions in metal-binding sites, to provide better guidance for modeling metal binding sites in low-resolution structures. The new version of CheckMyMetal provides information about the optimal geometry and metal-ligand distances based on the type of metal ion in the structure. Such easy guidance can have significant educational value.
CheckMyMetal is available at https://cmm.minorlab.org.