Modeling and Refinement of Metal Coordination Environments with MetalCoord

Kaveh H. Babai[1], Fei Long[2], Martin Maly´[2], Keitaro Yamashita[3], and Garib N. Murshudov[2,1]

[1]Institute of Molecular Biology and Biotechnology, Ministry of Science and Education, Baku, Azerbaijan, [2]MRC Laboratory of Molecular Biology, Francis Crick Avenue, Cambridge CB2 0QH, United Kingdom, [3]Structural Biology Division, Research Center for Advanced Science and Technology, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8904, Japan

Accurate modeling of metal coordination environments remains a challenge in macromolecular crystallography due to the complexity and variability of metal-ligand interactions. We present *MetalCoord*, a computational tool designed to address this issue by systematically extracting and analyzing coordination geometries from the Crystallography Open Database (COD) [1]. *MetalCoord* uses a statistical framework, including Procrustes analysis and the symmetrized von Mises distribution [2], enabling reliable determination of metal-ligand bond lengths and angles. The software is freely available at https://github.com/Lekaveh/MetalCoordAnalysis. Our analysis involved extracting coordination geometry data from over 228,000 metal environments in the COD, leading to the classification of various coordination geometries and improvements in metal-containing ligand dictionaries within the CCP4 monomer library [3, 4. Integration of *MetalCoord* into macromolecular structure refinement workflows, such as Servalcat and AceDRG [5, 3], has improved refinement accuracy, particularly for complex metal-ligand interactions like heme groups and iron-sulfur clusters.

The application of *MetalCoord* has updated stereochemical parameters for metal-containing ligands across many Protein Data Bank (PDB) entries, resulting in clearer metal environments and chemically accurate macromolecular models [6]. This development contributes to refining metal-containing macromolecular structures and enhances structural biology computations.

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