Modeling and Refinement of Metal Coordination Environments with MetalCoord

Kaveh H. Babai1, Fei Long2, Martin Maly´2, Keitaro Yamashita3, and Garib N. Murshudov2,1

1Institute of Molecular Biology and Biotechnology, Ministry of

Science and Education, Baku, Azerbaijan

2MRC Laboratory of Molecular Biology, Francis Crick Avenue, Cambridge CB2 0QH, United Kingdom

3Structural Biology Division, Research Center for Advanced

Science and Technology, The University of Tokyo, 4-6-1 Komaba,

Meguro-ku, Tokyo 153-8904, Japan

**Abstract**

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.](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.

1

# References

1. Graˇzulis, S. et al. (2009). *J. Appl. Cryst.*, **42**, 726-729.
2. Dryden, I. L. & Mardia, K. V. (2016). *Statistical Shape Analysis, with Applications in R*. John Wiley & Sons.
3. Long, F. et al. (2017). *Acta Cryst. D*, **73**, 112-122.
4. Vagin, A. A. et al. (2004). *Acta Cryst. D*, **60**, 2184-2195.
5. Yamashita, K. et al. (2021). *Acta Cryst. D*, **77**, 1282-1291.
6. Babai, K. H. et al. (2024). *Acta Cryst. D*, **80**, 821-833.

2