Poster Presentation

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Which metal or ion? Identification of metals and ions in protein structures

J. Dohnalek[1]

[1]*Institute of Macromolecular Chemistry AS CR, Department of Structural Analysis of Biomacromolecules, Prague, Czech Republic*

Identification of ligands in single crystals of biomolecules is often uneasy. The target molecules undergo expression, purification, and special pre-crystallization treatment and even trace impurities in known chemicals become a source of potential ligands. The final "binders" belong to a large set of both natural cofactors and chemicals encountered before the diffraction experiment. Some promiscuous metal binding sites can bind different types of metals of the fourth period and activity towards the same substrate can be measured with different divalent metals in active sites of nucleases, anhydrolases, etc. Therefore, 1) Not all structures have correct ions; 2) Ion identification in all structures requires high attention, especially in metal-dependent proteins. To date 98% of X-ray structures in the PDB have the high diffraction limit of 1.2 Å or worse. Thus we must rely on other indicators as for the ion type than just the height of electron density because our data often provide an accurate picture of a mixture of states. Therefore, essential determinants (relative heights of unbiased electron density maxima, anomalous signal, the shortest interatomic distances, stability of atoms in refinement, nature of coordinating atoms) must be distinguished from marginal factors which can be smeared by worse data quality, resolution limits, position in protein chain or local disorder (atomic displacement parameters, occurrence of longer coordination distances, missing vertices of the first coordination sphere). We have applied the described approach to identify cations, such as Cu2+, Mn2+, Zn2+, Ni2+, Ca2+, Mg2+, Na+ and other ionic ligands, for instance Cl-, PO43-, SO42- [1]. The available tools for identification of metals/ions also include statistics on coordination and bonding distances [2], absorption edge detection and fluorescence [1] or microbeam proton induced X-ray emission [3]. The work was supported by MEYS CR (EE2.3.30.0029) and BIOCEV (CZ.1.05/1.1.00/02.0109).

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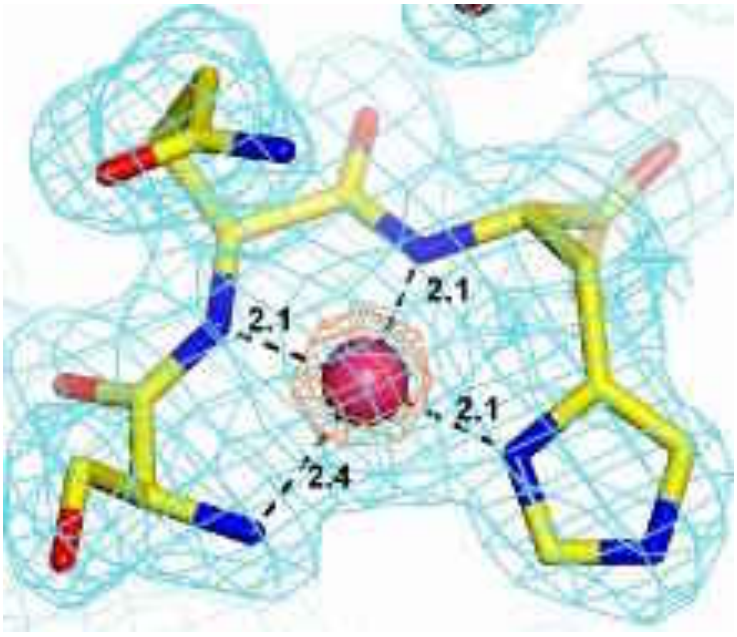

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