

Abstract Submitted
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Monatomic Ion Coordination in Proteins KATHLEEN CLARK¹,
Arizona State University — In order to understand the role of ions in proteins,
it is important to have an accurate description of the interactions between bound
ions and atoms common in proteins. An automated analysis method was developed
to analyze monatomic ions contained in crystal structures in the RCSB Protein
Data Bank (PDB). The coordination characteristics of the most prevalent monova-
lent cations in the PDB were analyzed through the radial distribution functions of
oxygen atoms around ions. It is known that sodium ions coordinate oxygen atoms
within about a 6 Å radius, with a clear first coordination shell, similar to a hydration
shell in bulk water, and a secondary shell also typically visible. However, oxygen
atoms are not the only atoms that can coordinate cations, and coordinating atoms
for anions are far less understood than those for cations. The analysis was extended
to explore the distributions of other coordinating atoms, namely nitrogen, sulfur,
and carbon, as well as anions and multivalent cations. It was observed that many
ions are preferentially coordinated by certain atoms, for example, zinc specifically is
largely coordinated by sulfur. Additionally, quantitative values were calculated to
describe the locations and strengths of the coordination shells for each ion.

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