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Figure S1. Distribution of secondary structure elements (α helices, β strands, and random coil) around: a) His residues from inner spheres of Mg²⁺ complexes; b) His residues from outer spheres of Mg²⁺ binding sites; c) His residues that are not involved in Mg²⁺ binding



Figure S2. Distribution of secondary structure elements (α helices, β strands, and random coil) around: a) His residues from inner spheres of Mn²⁺ complexes; b) His residues from outer spheres of Mn²⁺ binding sites; c) His residues that are not involved in Mn²⁺ binding



Figure S3. Distribution of secondary structure elements (α helices, β strands, and random coil) around: a) Asp residues from inner spheres of Mg²⁺ complexes; b) Asp residues from outer spheres of Mg²⁺ binding sites; c) Asp residues that are not involved in Mg²⁺ binding.



Figure S4. Distribution of secondary structure elements (α helices, β strands, and random coil) around: a) Asp residues from inner spheres of Mn²⁺ complexes; b) Asp residues from outer spheres of Mn²⁺ binding sites; c) Asp residues that are not involved in Mn²⁺ binding.



Figure S5. Distribution of secondary structure elements (α helices, β strands, and random coil) around: a) Glu residues from inner spheres of Mg²⁺ complexes; b) Glu residues from outer spheres of Mg²⁺ binding sites; c) Glu residues that are not involved in Mg²⁺ binding.



Figure S6. Distribution of secondary structure elements (α helices, β strands, and random coil) around: a) Glu residues from inner spheres of Mn²⁺ complexes; b) Glu residues from outer spheres of Mn²⁺ binding sites; c) Glu residues that are not involved in Mn²⁺ binding.