**Supplemental Material for Finding high-quality metal ion-centric regions across the worldwide Protein Data Bank**

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Supplemental Table S1: A list of high-quality metal ion list that passes all four criteria in CSV format.

Filename: TableS1.txt

Column Descriptions:

* pdbid - PDB id
* resolution - resolution of x-ray structure
* chainID - chain ID of the metal ion
* resNum - residue number of the metal ion
* metal - the metal name
* occupancy - the occupancy of the metal
* symmetry - whether or not there are symmetry atoms nearby. -1: no symmetry atom nearby (~5 angstrom range); 0: no symmetry atoms within 3 angstroms; 1: symmetry atoms exist within 3 angstroms sphere.
* totalDensity - the total electron densities within 3 angstroms sphere of the metal, in the unit of e/Å3 (same as .ccp4 density map).
* electronNum - the total number of discrepancy electrons after the conversion, in the unit of e.



**Figure S1.** Distribution of average absolute discrepancy sum within a 3.5 Å radius sphere volume. The red line indicates the discrepancy cutoff criterion used to filter out low quality metal binding site regions.

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**Figure S2.** Distribution of electron discrepancy within 3.5 Å of the metal ion for metal ions within 3 Å of another metal ion. The red line indicates the discrepancy cutoff criterion used to filter out low quality metal binding site regions.