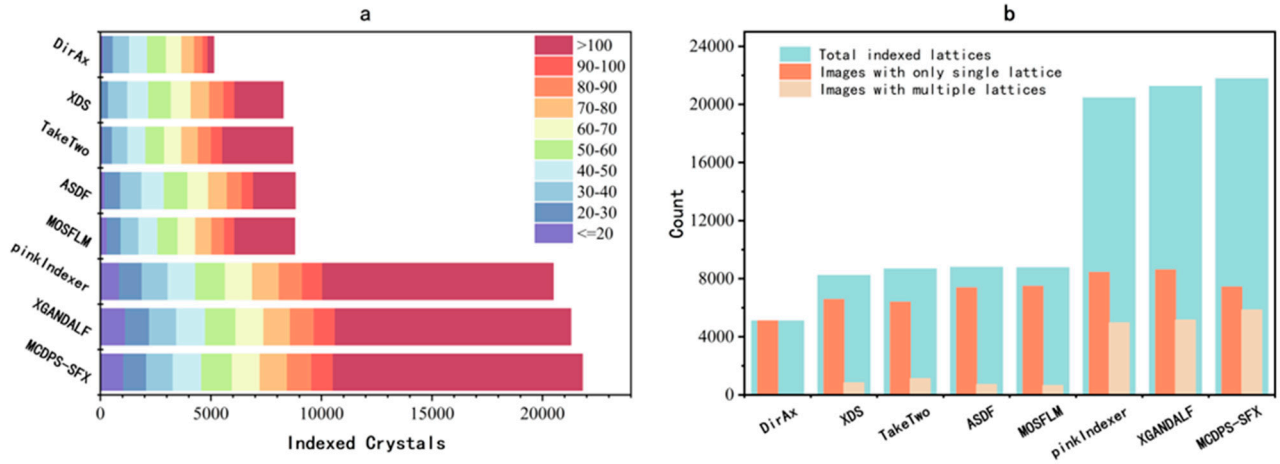


Figure S1. Performance benchmark of MCDPS-SFX and comparative algorithms on the AcNiR dataset. (a) Breakdown of indexed crystal hits categorized by the number of reflections per diffraction pattern. The stacked horizontal bars illustrate the performance of eight indexing programs. Colors represent distinct reflection count intervals, ranging from ≤ 20 (purple) to > 100 (dark red). MCDPS-SFX exhibits a superior indexing yield across all intervals, particularly for images with higher reflection density. (b) Analysis of lattice recovery according to image complexity. For each algorithm, the bars represent the Total indexed lattices (light blue), which are partitioned into Images with only single lattice (orange) and Images with multiple lattices (beige). Notably, MCDPS-SFX achieves the highest total lattice count by effectively resolving "multiplets" (multi-lattice images), where it shows a significant improvement over traditional methods like MOSFLM and XDS.

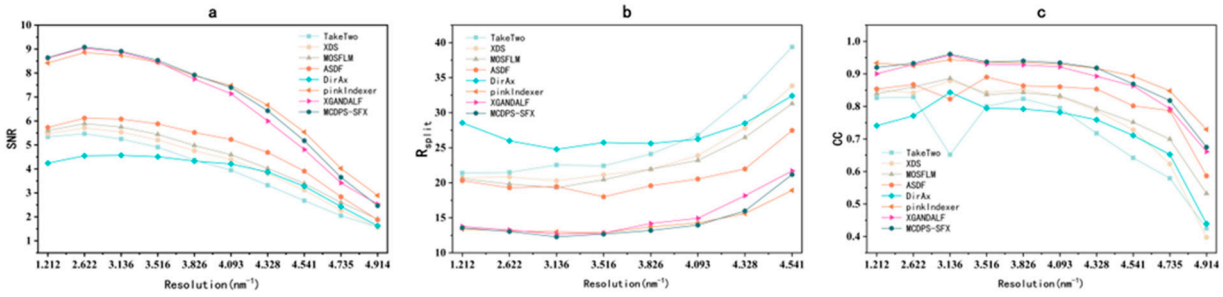


Figure S2. Evaluation of data quality metrics as a function of resolution for the AcNiR dataset. (a) Signal-to-noise ratio (SNR), (b) split-half R-factor (R_{split}), and (c) Pearson correlation coefficient (CC) are plotted against resolution (nm^{-1}). The trajectories compare MCDPS-SFX (dark teal, hexagons) with other indexing algorithms including pinkIndexer (dark orange, left-pointing triangles), XGANDALF (magenta, right-pointing triangles), and others. Across the low-to-mid resolution range (up to ~ 4.0 nm^{-1}), MCDPS-SFX demonstrates leading performance with the highest SNR and CC values.