3 Scripts used during Analysis of Large Reciprocal Space Map Datasets of BSCCO Single Crystals. A Fourier transform of the symmetrized data set is calculated, which yields the 3D Pair Distribution Function; the convolution of the electron density with itself.

1. 3D\_PDF\_from\_Diffraction: Large reciprocal space maps of the BSCCO single crystal obtained at the QM2 beamline at CHESS are used to make 3D Pair Distribution Functions. Features such as Bragg peaks or diffuse scattering can be eliminated from the diffraction pattern before the 3D PDFs are made. Sharp features (like structural Bragg peaks) can be interpolated over while diffuse scattering features below a certain intensity may be replaced with a fixed value. Since the data is obtained at low incidence angle, the diffraction map must be symmetrized before the Fourier transform yielding the 3D PDF is calculated
2. Visualize\_3D\_PDF: Use imshow to plot slices of the 3D Pair Distribution Function. The unit cell and Incommensurate Lattice Modulations in BSCCO are observed.
3. 3D\_PDF\_from\_structure: Use the CIF structure file to calculate the theoretical 3D PDF for the unit cell. First, the structure factor for a set of Bragg reflections are calculated using x-ray utilities. Second, the real space 3 PDF is calculated via Eqn 14.15 in the VESTA manual.