Supporting information for article:
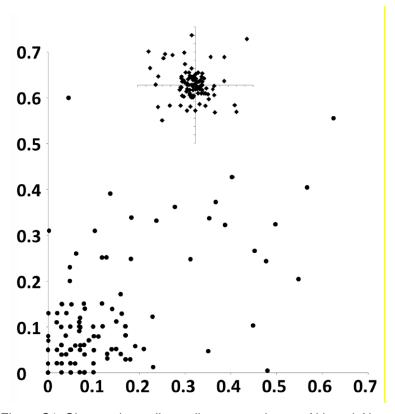
The use of haptic interfaces and web-based information in crystallography: an application for a `screen to beam' interface

Andrew E. Bruno, Alexei S. Soares, Robin L. Owen and Edward H. Snell

Supplementary Figure S1. Observed coordinate discrepancy in mm. Although X-ray diffraction data were obtained from only 10 crystals (Fig. 5), each of the 137 crystals in the lysozyme screening plate (§3¶3) was centered at the X-ray position using the G-rob robot. The observed coordinates for each crystal were recorded and compared to the coordinates that accompanied each annotated plate. The average discrepancy between the crystal coordinates that were observed when the plate was annotated and the coordinates that were observed at the beamline was 175 (median 130) μm. The distribution of observed coordinate discrepancies is shown in this figure. The inset shows the same data but preserving the sign of each discrepancy, showing that the discrepancy distribution was radially symmetric. A statistical analysis of these data shows that they fit well against an error model consisting of two components. The first component (accounting for 69% of the observed discrepancy) consists of a random error with a Gaussian distribution around the expected value. The second component (accounting for 31% of the observed discrepancy) consists of the pair distribution for two random points on a disk. This combined error model is consistent with the observation that most crystals remained at their recorded position (the discrepancy for these crystals consisted of measurement error, most likely caused by the mechanical precision of the G-rob system). Convoluted with this, a small number of crystals (20%) become dislodged and were randomly distributed within the crystallization drop when they were centered at the beamline.