Twinning

Samples that are twinned by non-merohedry are usually very difficult to index as a single crystal or have unusually long cell axes. However, indexing these samples can be usually be done by the CELL_NOW program as described in the Collect_Data-Photon document. The data is integrated with two or orientation matrices and then processed by TWINABS. Handling the data set has been described in the Reduce_Data document.

There are a few samples that are later shown be twins by non-merohedry that form that appear to be from a single crystal. The structure from these samples are difficult / impossible to solve and usually have odd reflection conditions (systematic absences). Hopefully the absences will point to the two twin domains in the data.

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Samples that are twinned by merohedry are identified near the end of refinement when the *R* does not drop to the values expected for the data quality. The twin law is usually some symmetry of the Laue group but not of the space group. The twin law(s) can be determined by the TwinRotMat routine in the PLATON program. To refine a twin be merohedry, include the twin law(s) using TWIN commands, and add a BASF command with enough variables to handle your problem.