

[Example Story]

Title: The Only Crystal, the Last Question

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During one beamtime, a user collected a diffraction dataset from the only available crystal that was expected to contain a bound ligand. The data collection went smoothly, and the user, still excited by the promising diffraction results, immediately started preliminary structure analysis at the beamline.

The result looked excellent. In COOT, the electron density map clearly showed the ligand exactly where it was expected to be. It was one of those moments when everyone feels that the experiment has worked beautifully.

Because the user wanted a student to perform the structure analysis from the beginning as a training exercise, he decided to remove the temporary analysis results. The idea was simple: delete the preliminary files, let the student start fresh, and allow them to experience the full process from data processing to model building.

Unfortunately, the deletion was a little too successful.

Not only the temporary analysis directory, but also the raw data, the data-processing directory, and the working directory containing the structure analysis were all deleted. Everything was gone.

Well, almost everything.

The only remaining evidence of the successful experiment was the electron density map and model still displayed on the COOT screen.

A phone call came shortly afterward. After carefully explaining what had happened, the user asked me one final question:

“Can this be converted back into an MTZ file?”

[What we learned]

Be extremely careful when deleting experimental data.

Before removing any directory after beamtime, check what it contains, check it again, and preferably make a backup first.