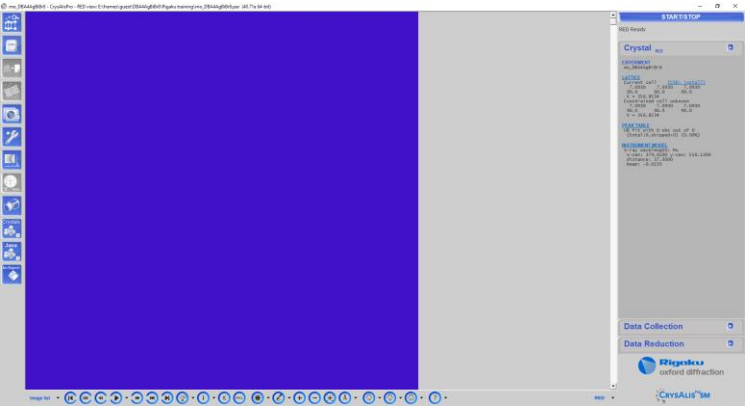
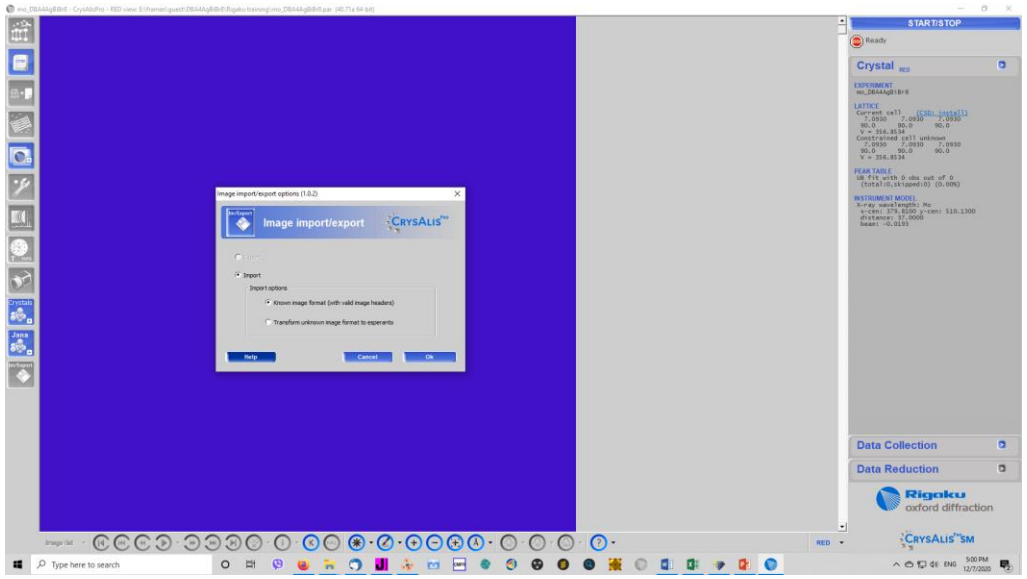
Single-Crystal X-ray Diffraction

I) Data Reduction
II) Structural Analysis

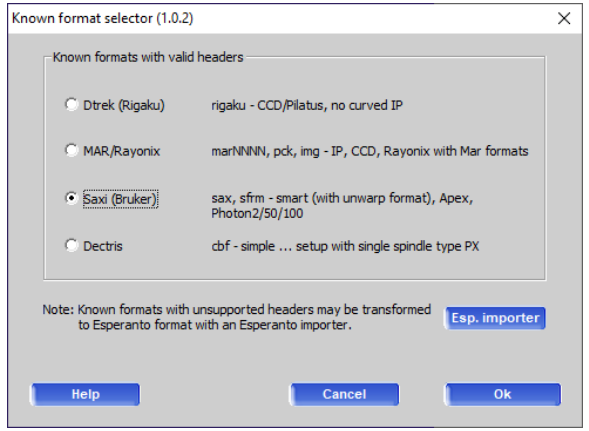
Open the .par file



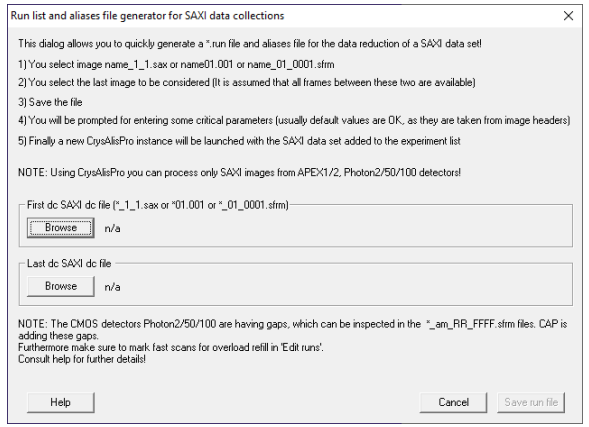
Import your data



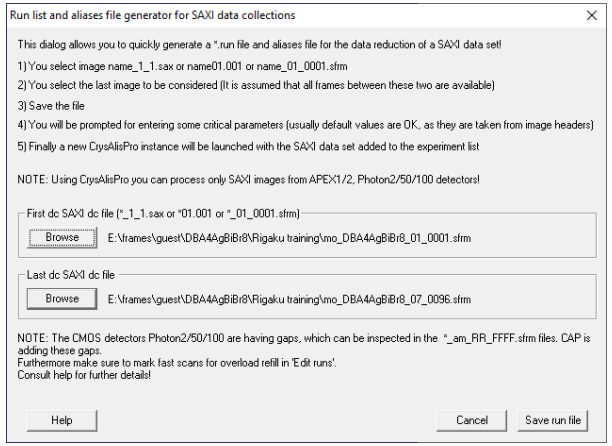
1



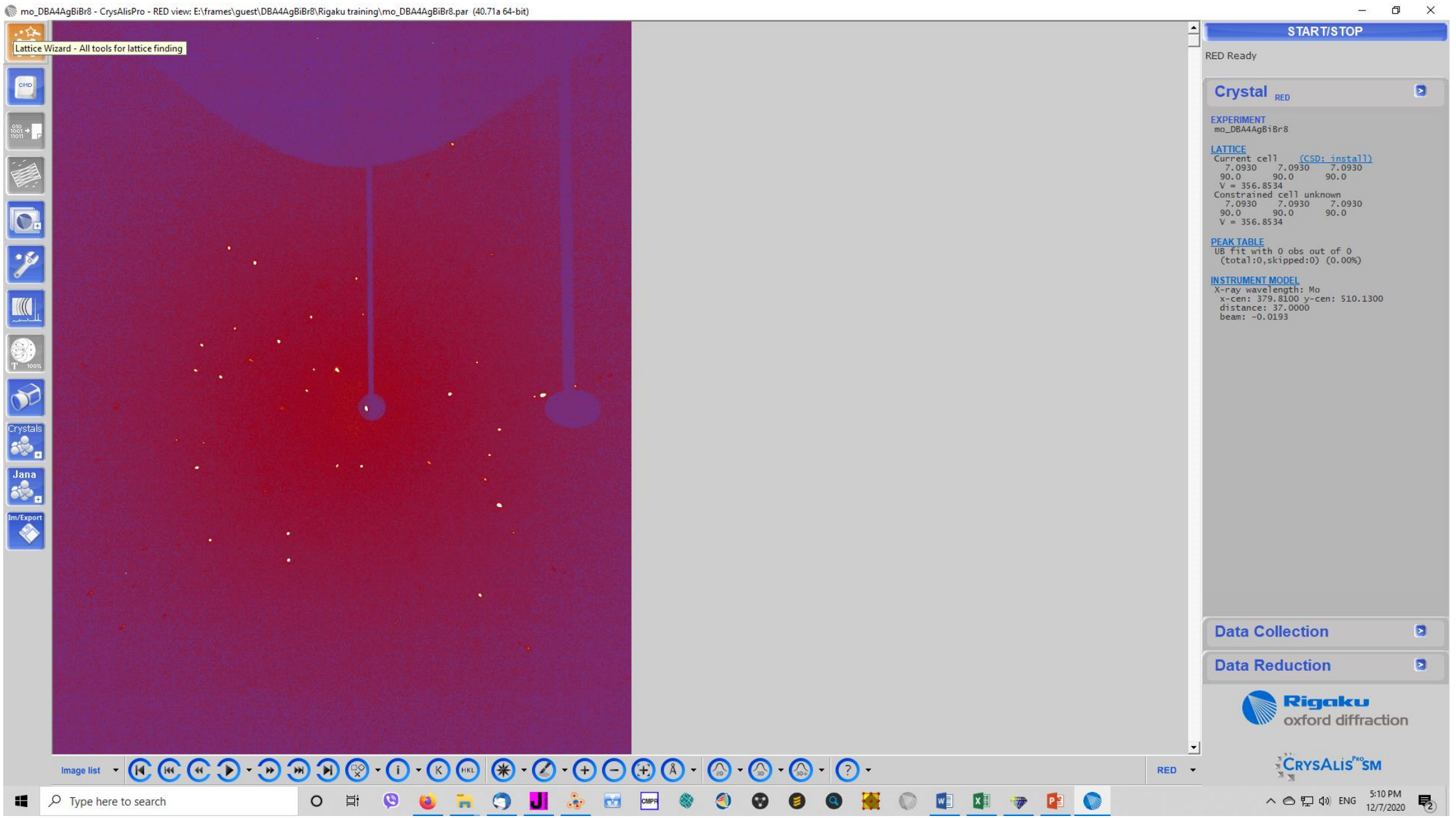
2



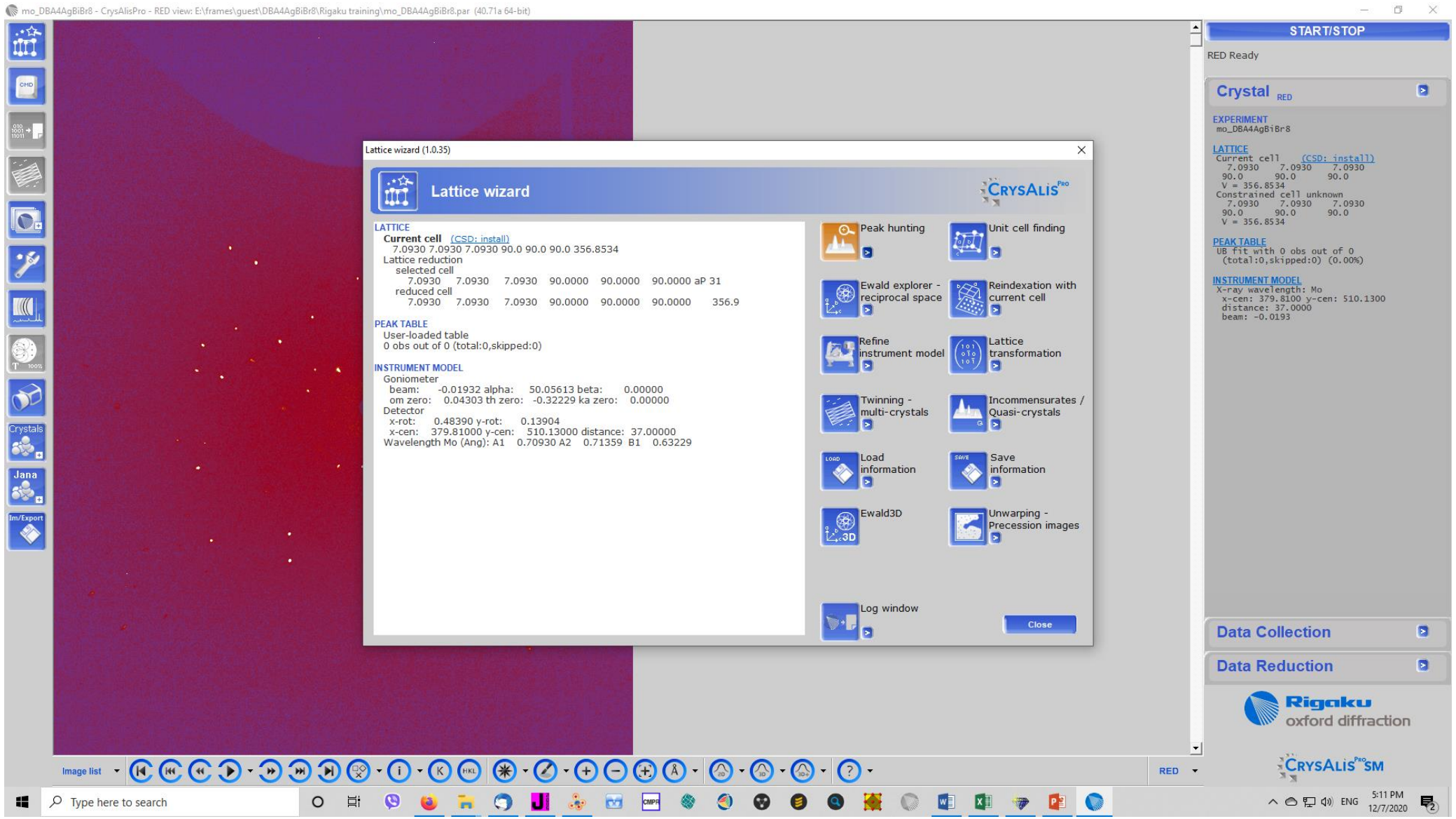
3



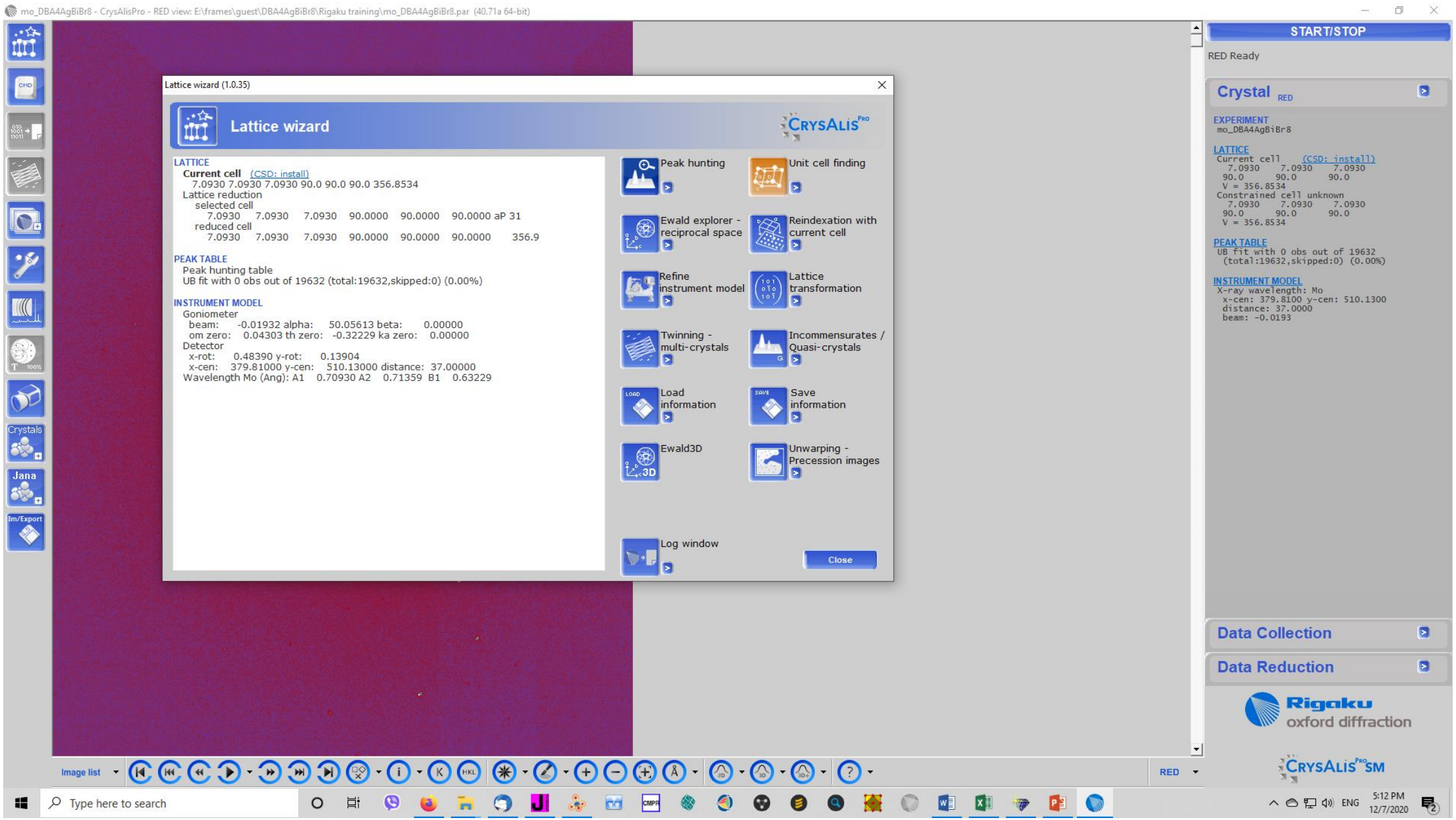
Once you have the data in (click ok through the questions, defaults seem to be ok)



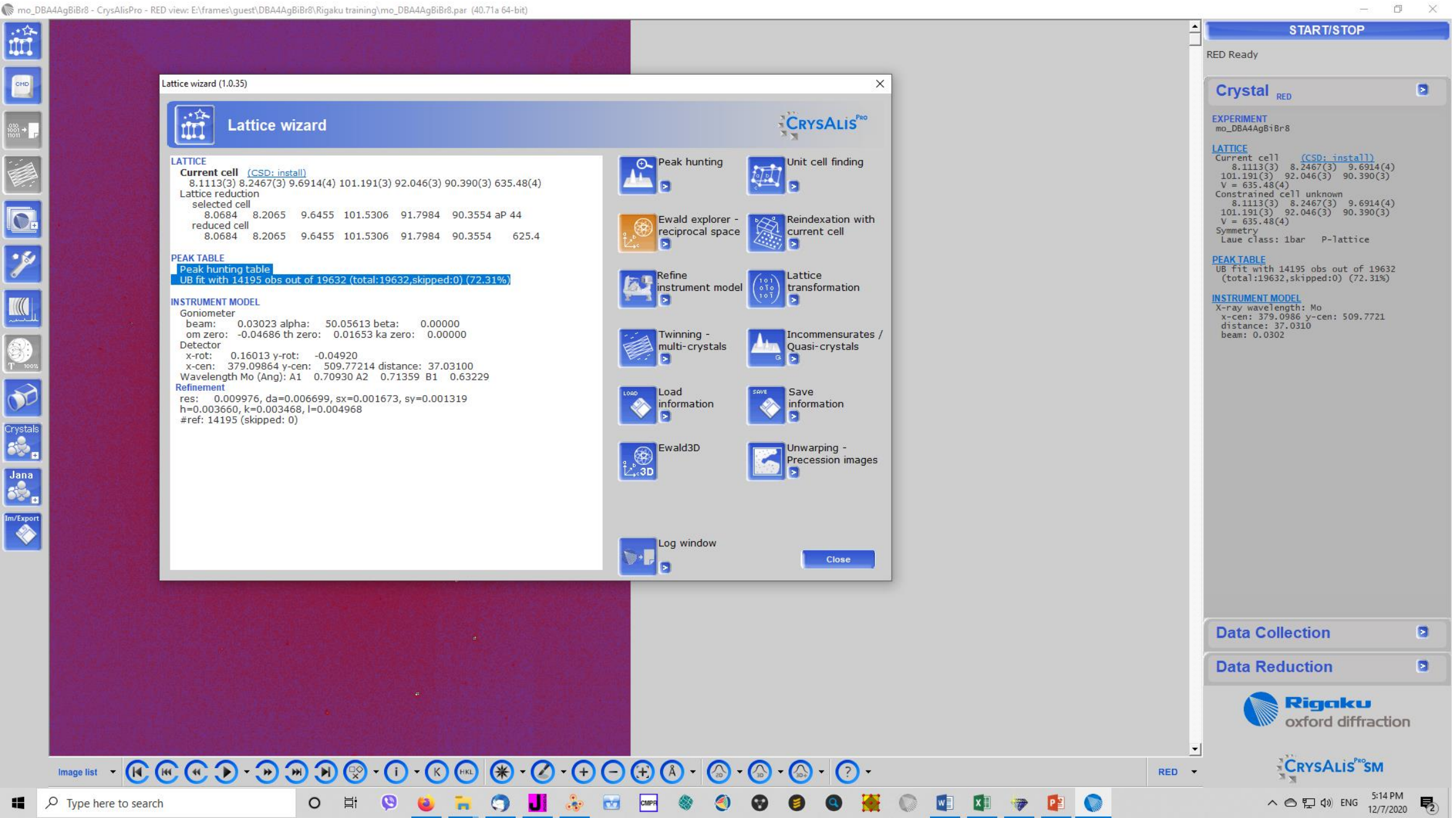
Find the peaks and index them



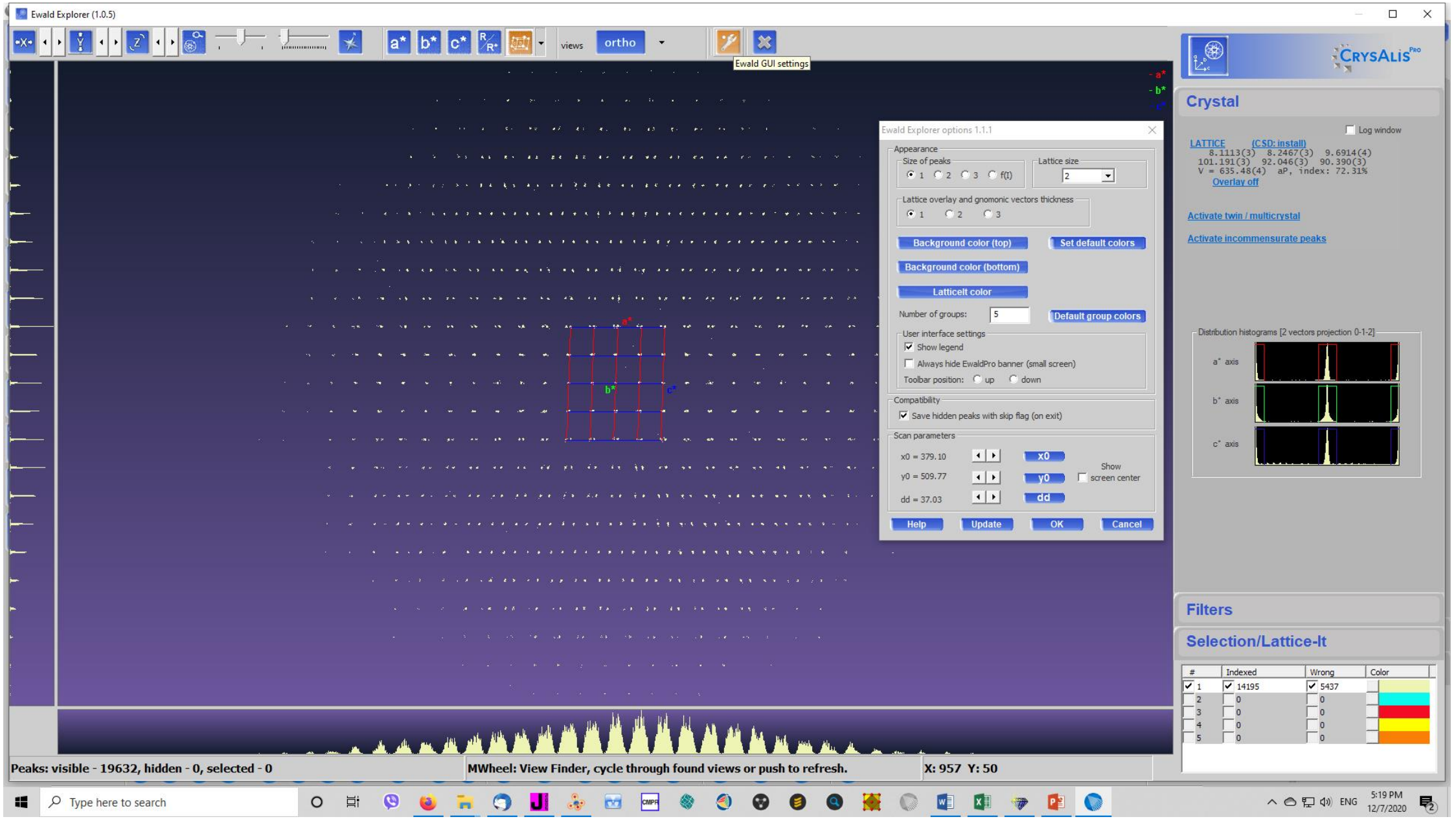
Find your unit cell



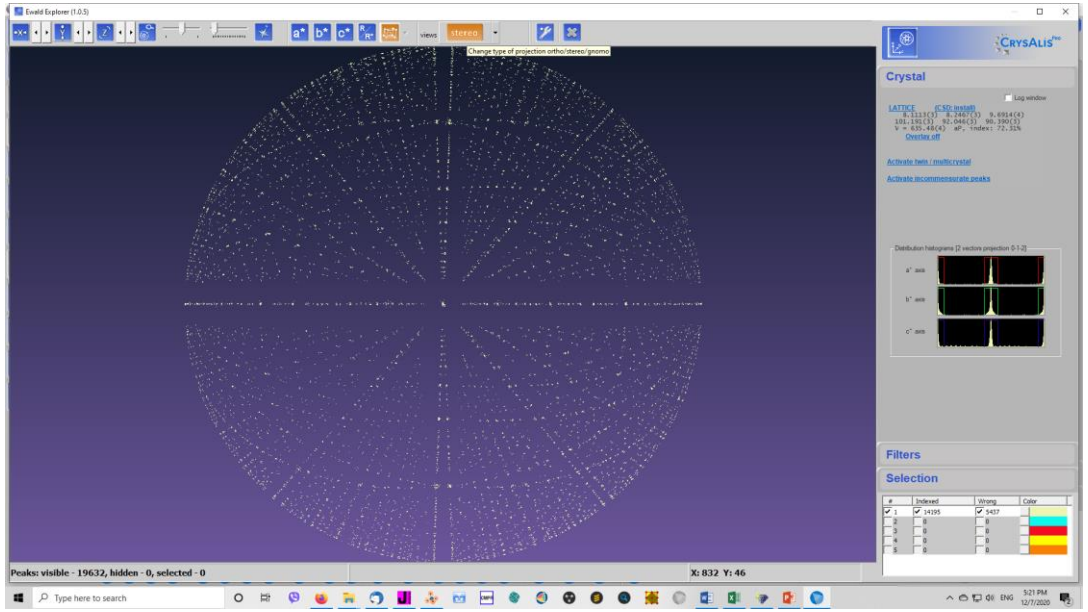
Look at your indexed reflections. Do you index most of them? Refine instrument model (if needed)

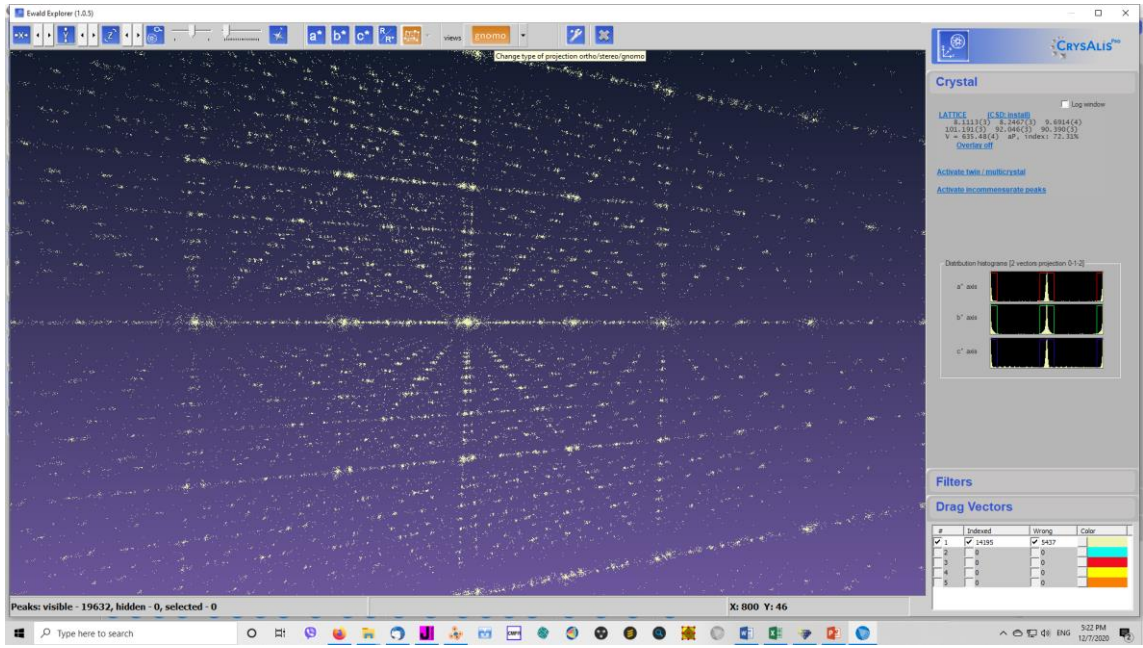


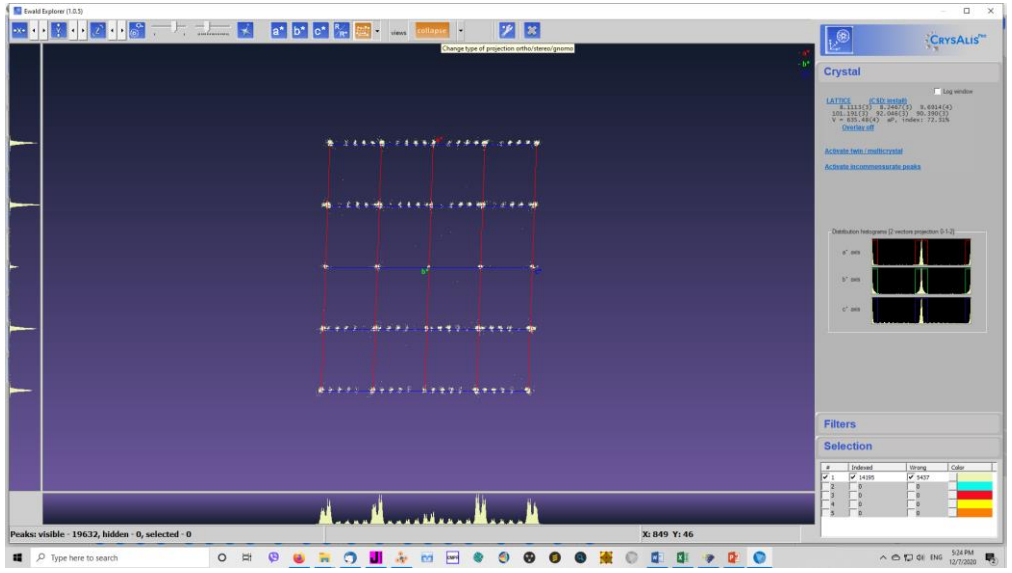
These are your indexed peaks. Play around by rotating and using the GUI settings menu



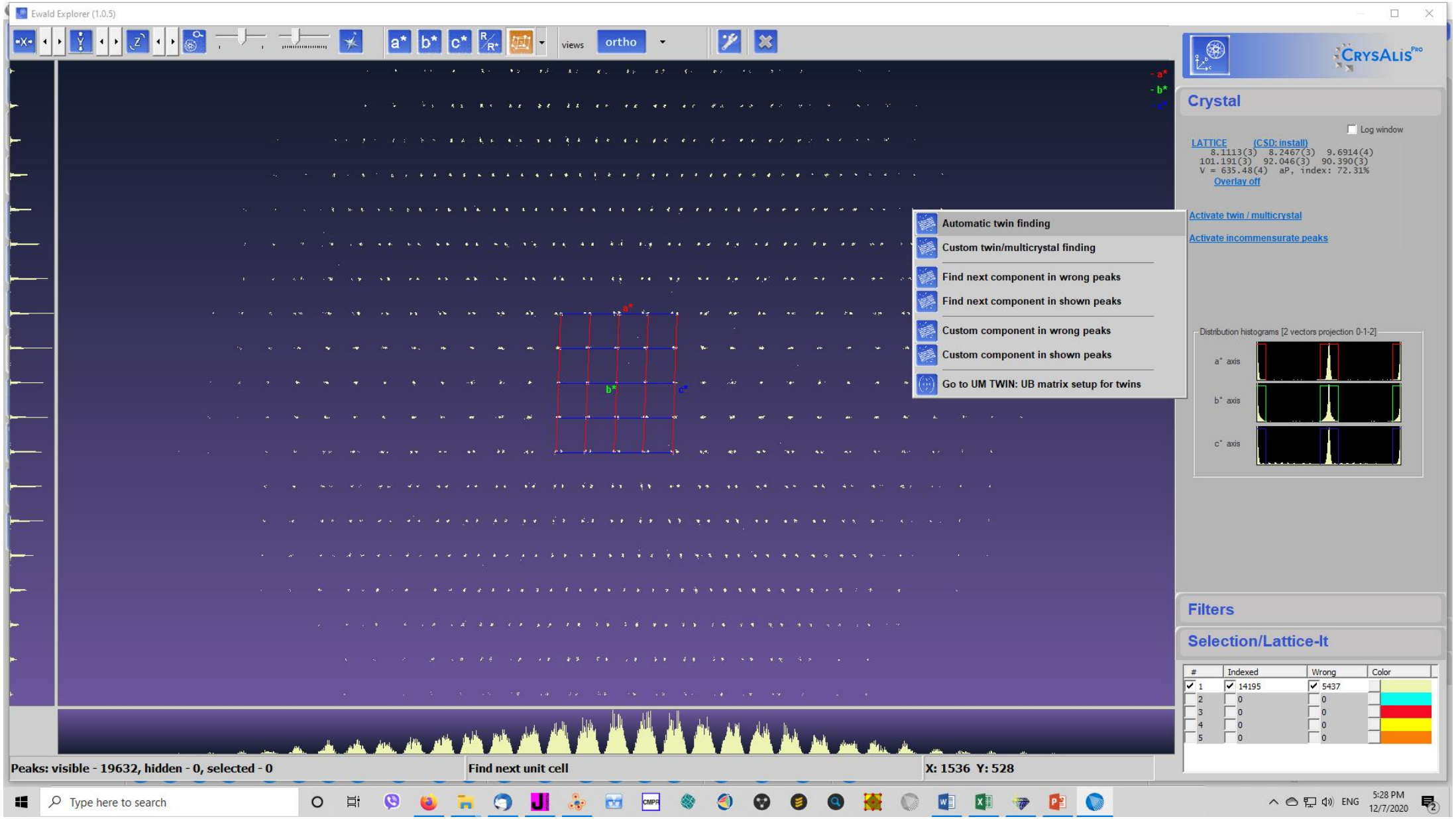
Don’t forget to look at the other aspects of projections (stereo and gnomonic are quite instructive)



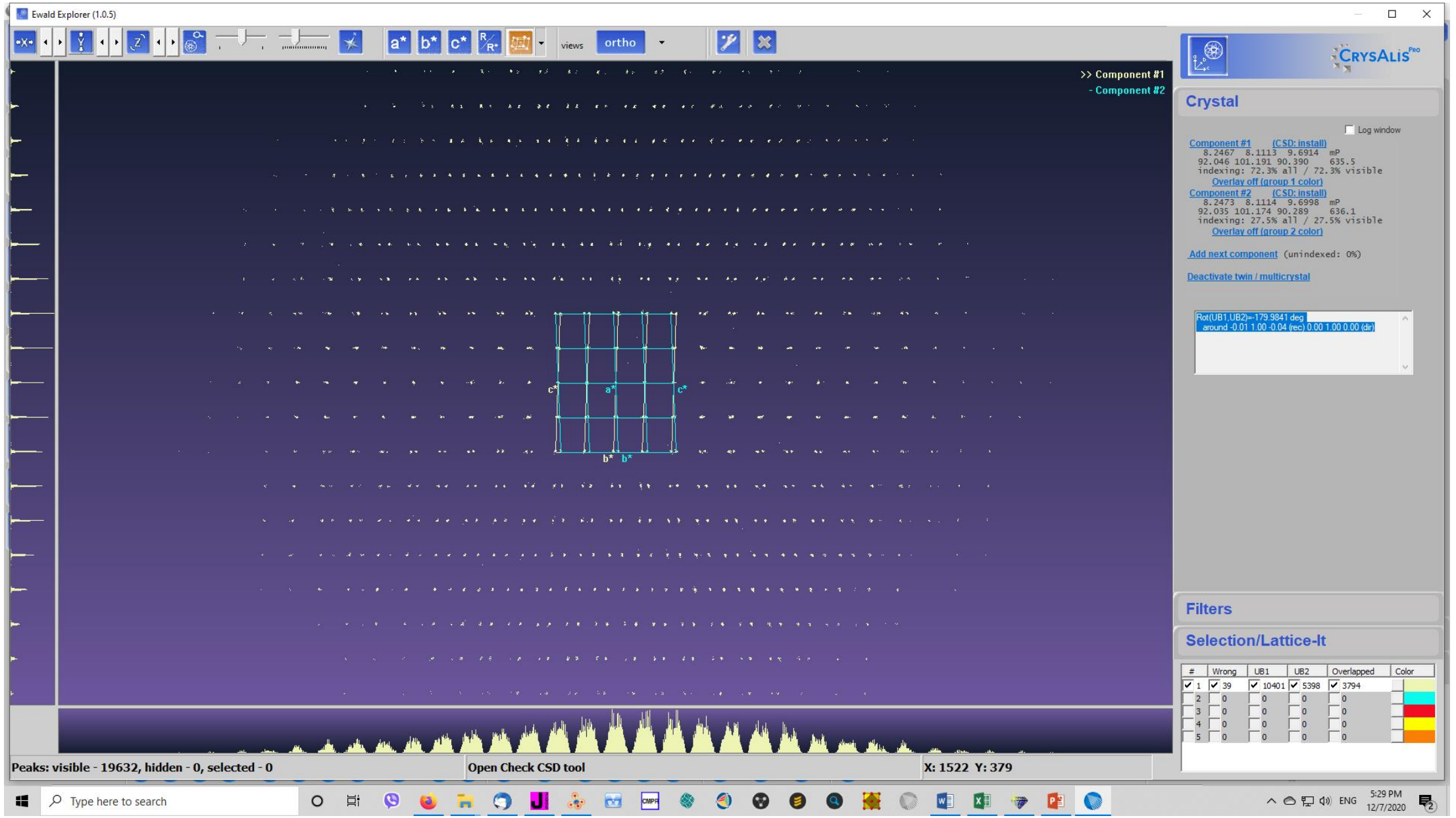




Probably a twin (or wrong indexing, less likely). Activate the menu for twinning on the right hand side

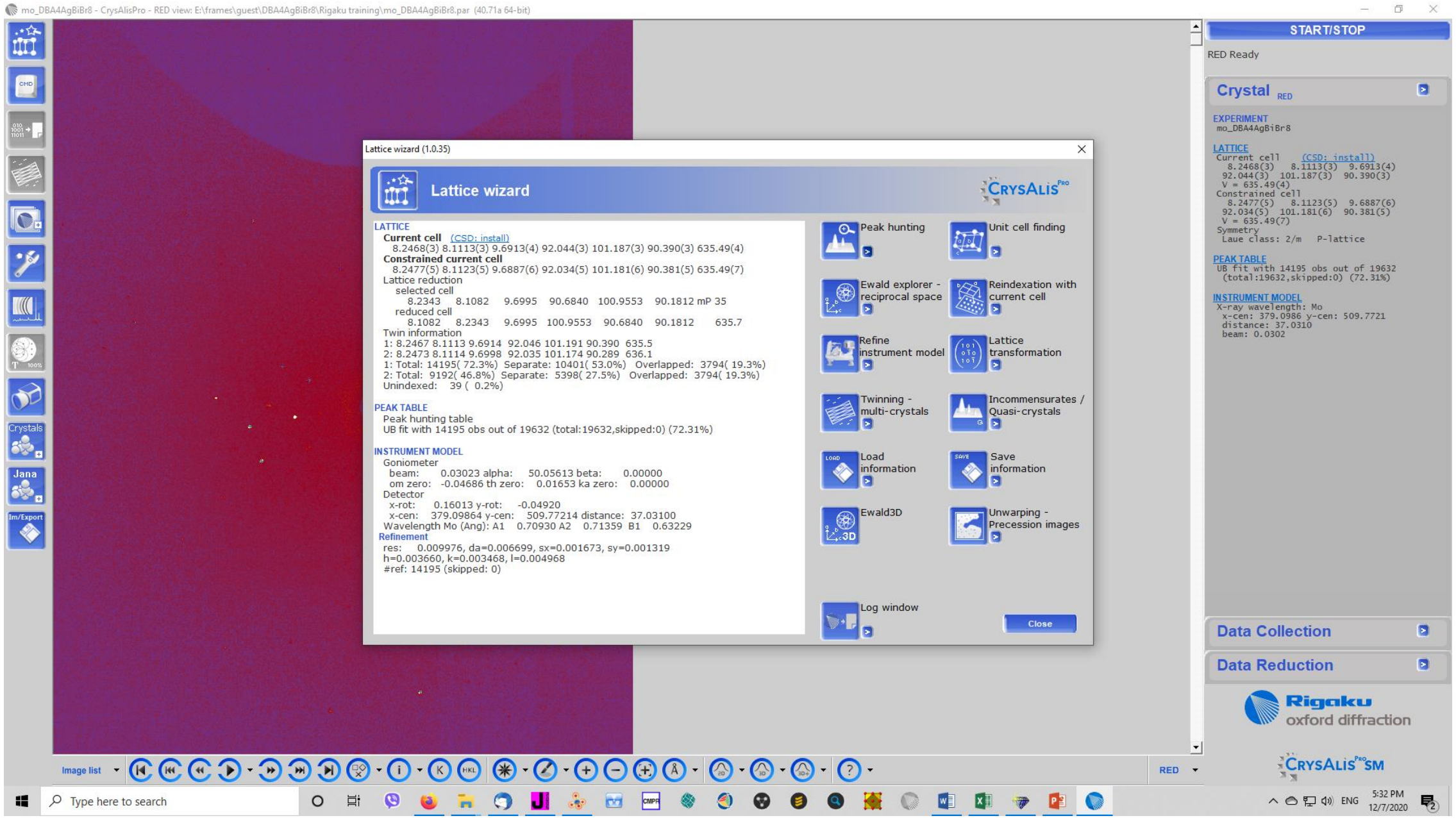


Second lattice found (lucky!). Most of the missing peaks found. The are due to a 180 degree rotations along b-axis



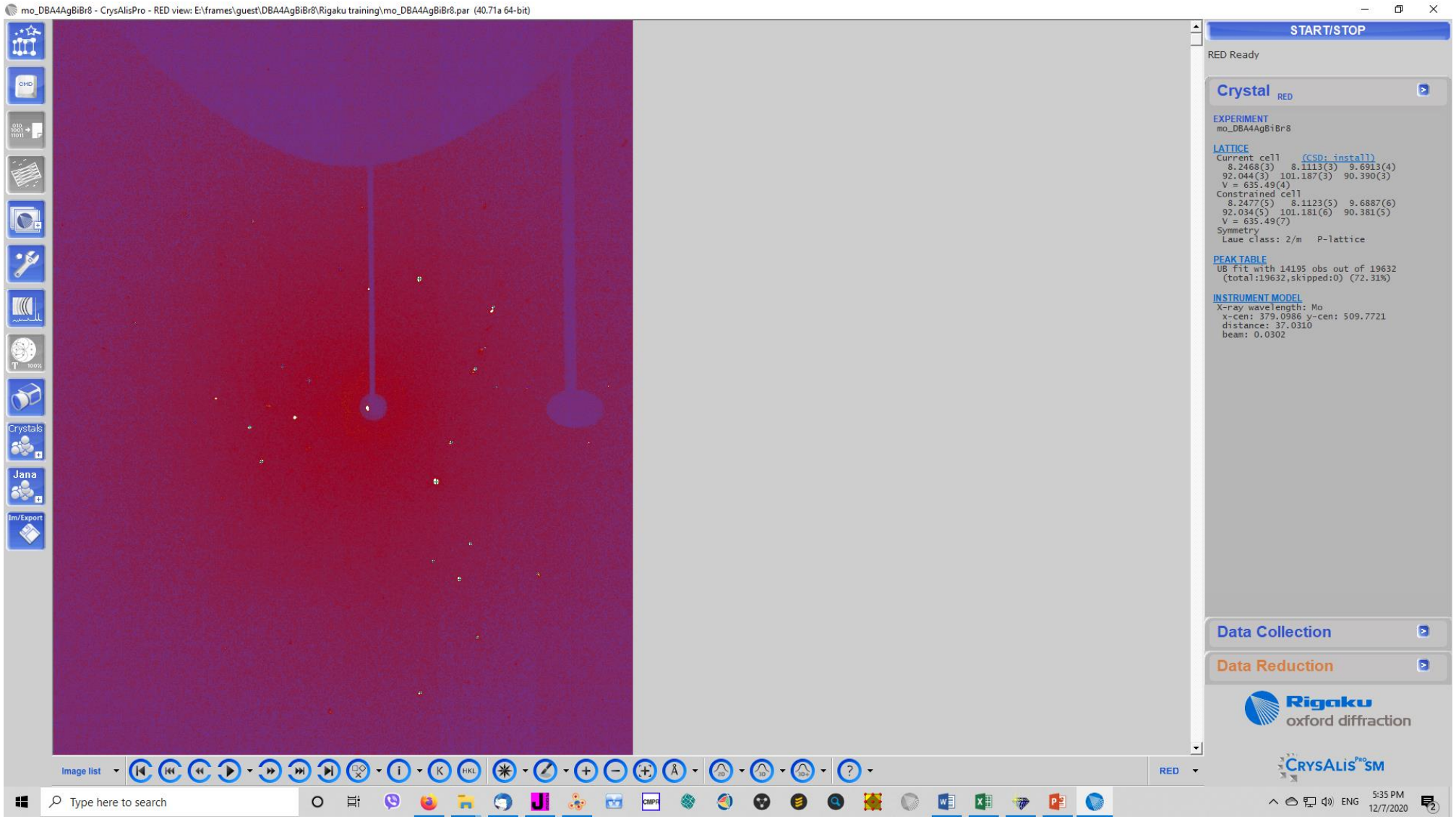
Close the Ewald menu.

A new “domain was found. The main domain is ~50% the second 25% and ~20% of reflections overlap



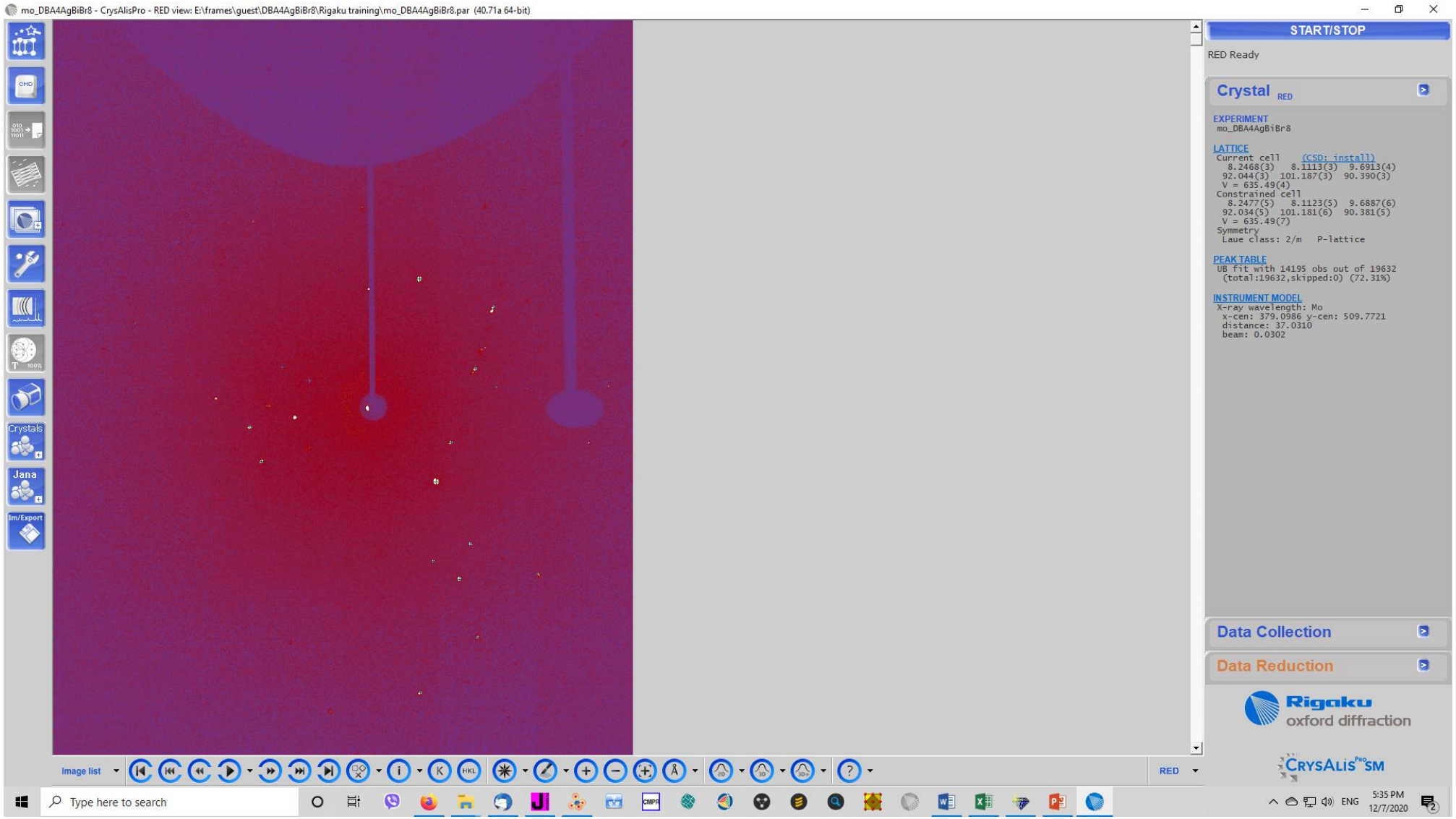
Save information and exit.

Menus are populated now with the correct parameters. You are ready for data reduction



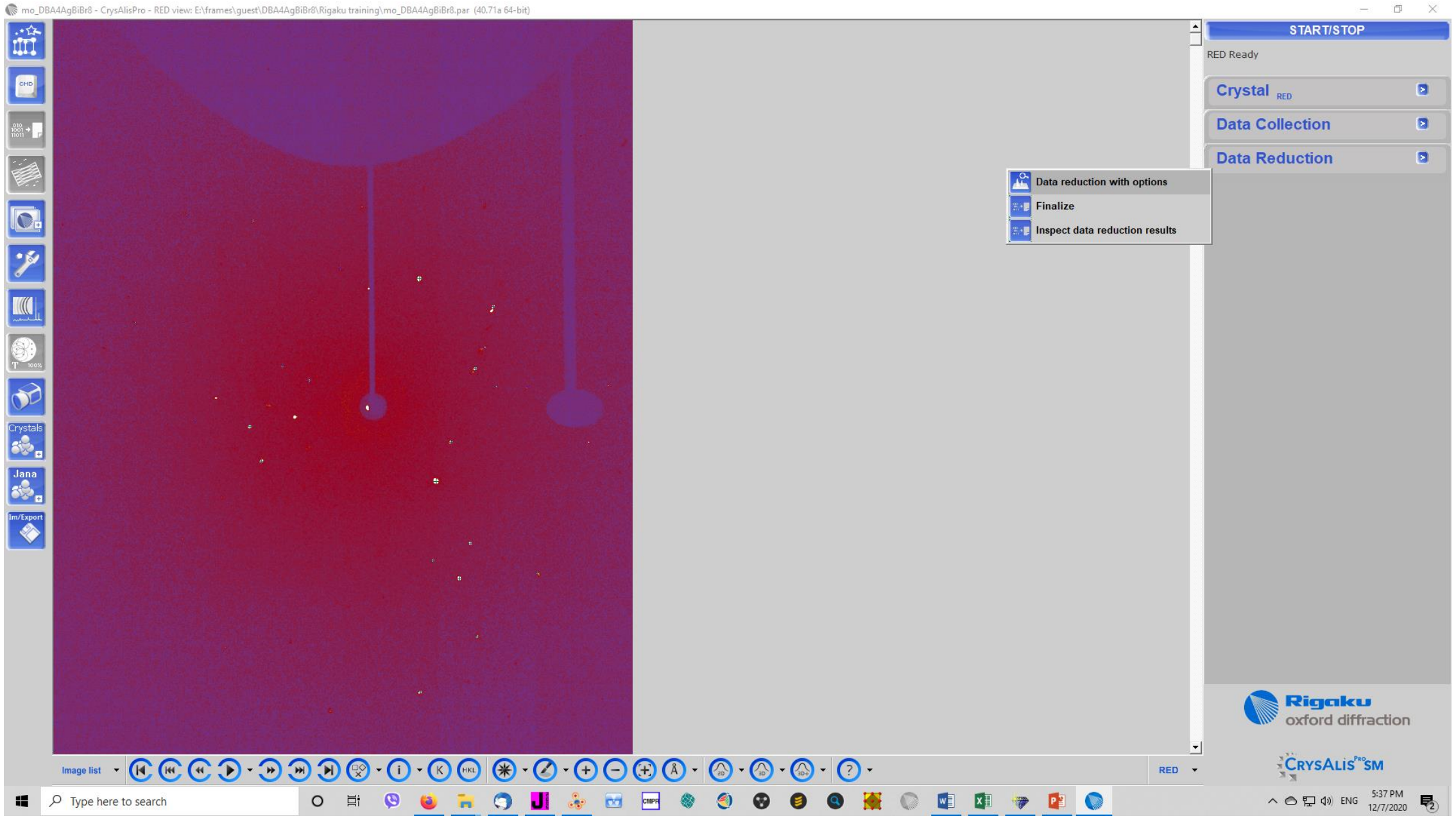
Save information and exit.

Menus are populated now with the correct parameters. You are ready for data reduction

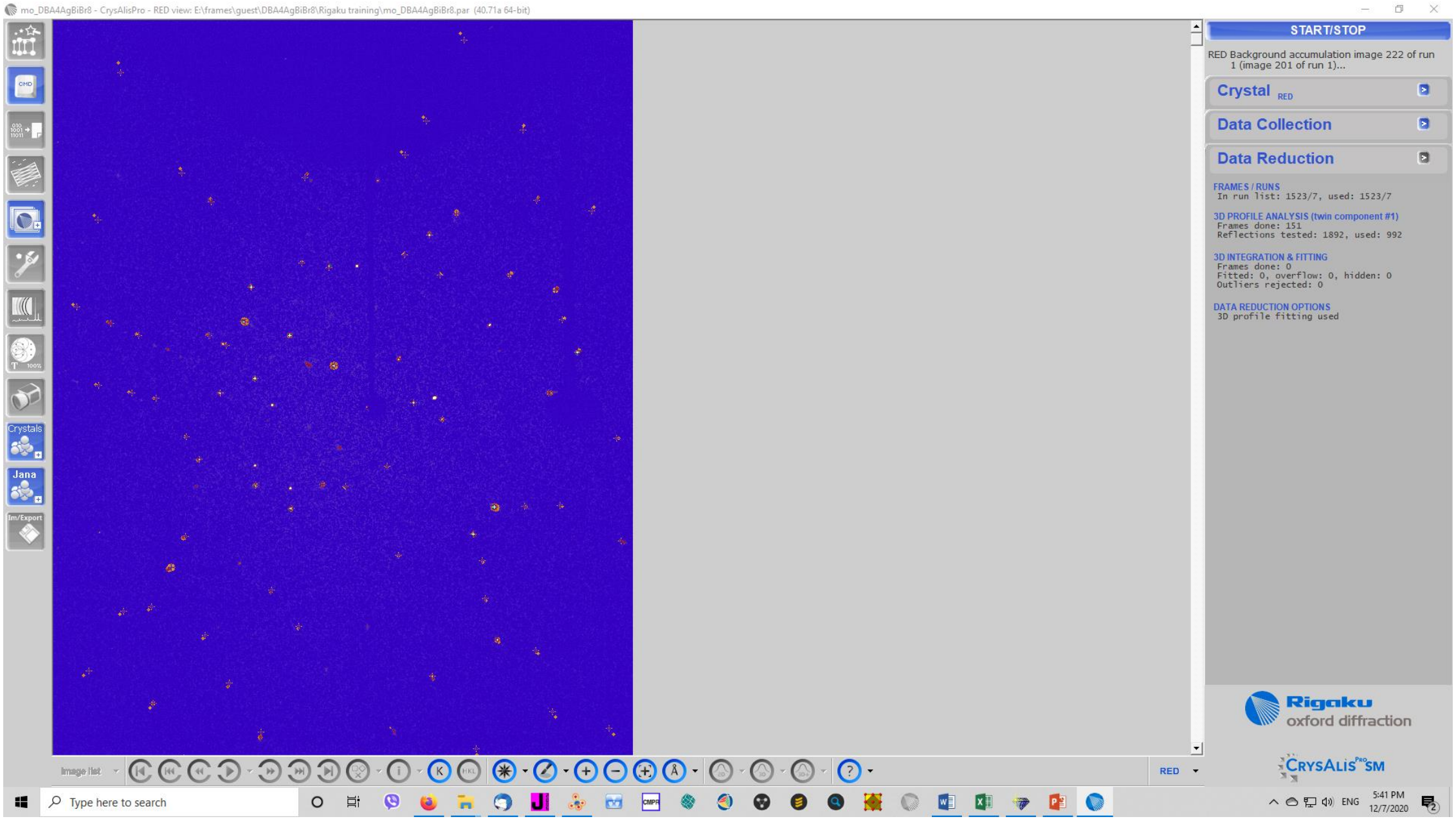


Data reduction

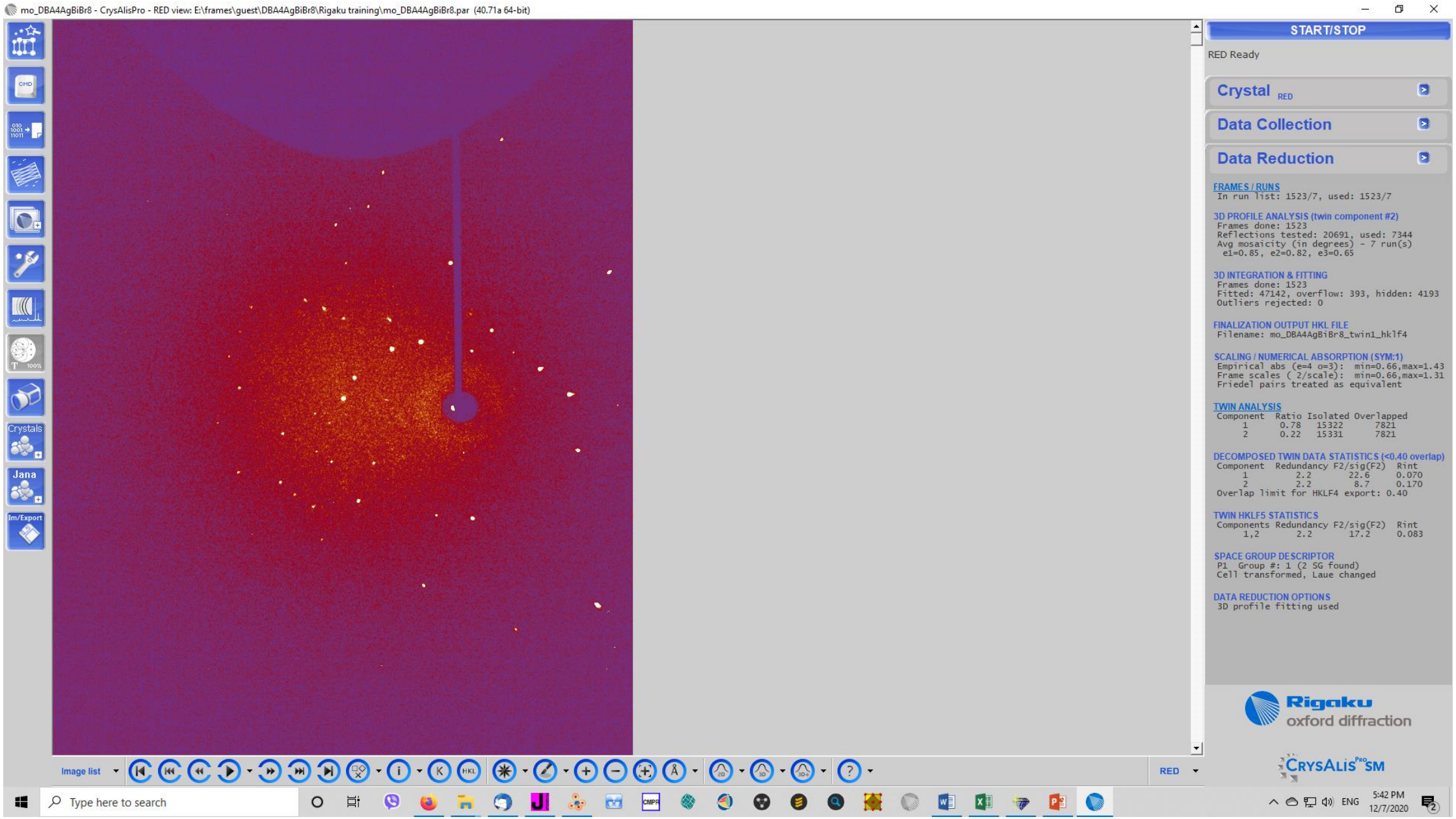
Press the option to start. This part can also be done automatically. Browse through the options and accept the defaults



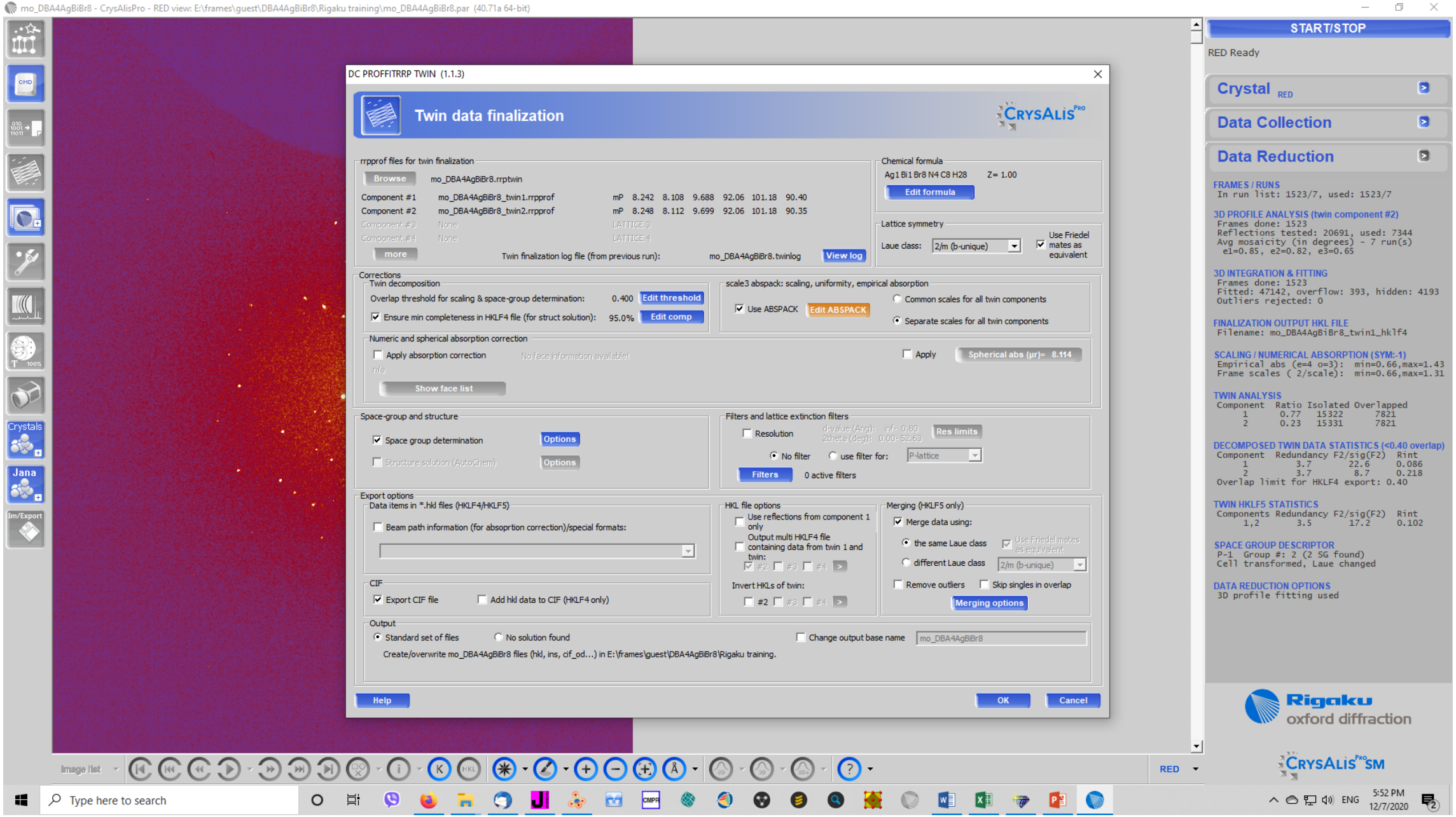
Integration on the indexed peaks starts. An .hkl file will be generated



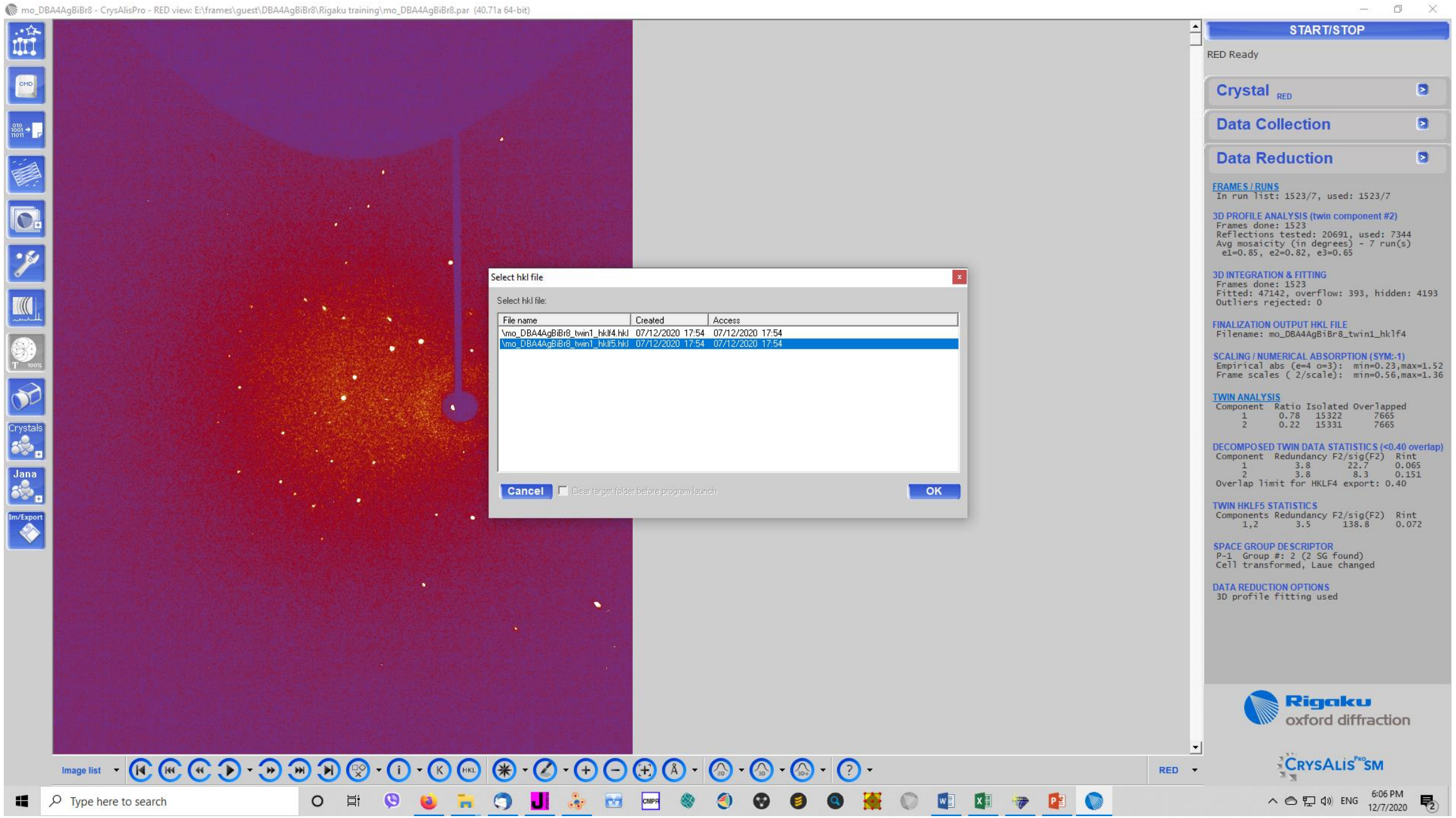
Once finished menu is populated. Go for the twin analysis to review it and finalize the data.



This is where you finalize data reduction to produce your files (corrected hkl and the instruction files)
Make all edits here (chemical formula, symmetry preferences, etc)



Choose the correct dataset and finish



Select the appropriate software for data solution and refinement
(Should appear on the left column as long as Jana2006, Olex2, etc. is already installed in C:\)