

Work Directory

The work directory is written out as a sub-directory of the folder which contains the diffraction images. It contains data, log and information files created during the data reduction process. Here is a list of the PROTEUM plugins for data reduction and some of the more commonly accessed output files.

Integrate Images (SAINT)

Output Files	Extension	Description
Raw intensity	*.raw	Contains the raw unscaled, unmerged intensities. A separate file is created for each scan which has the filename prefix plus the scan number (<i>prefix_#.raw</i>). A merged file is also created containing all the reflections from each scan (<i>prefix_0m.raw</i>).
Log	*._ls	Contains the output from integration. A separate file is created for each scan which has the filename prefix plus the scan number (<i>prefix_#._ls</i>). A merged file is also created containing all the reflections from each scan (<i>prefix_0m._ls</i>).
Matrix	*.p4p	This file contains unit cell information. When the integration is finished, a file called <i>prefix_0m.p4p</i> is created which contains the updated cell information. There is also a file written, <i>prefix_0u.p4p</i> which contains the unconstrained cell constants. This file can be manually created in PROTEUM by selecting "export>p4p" file from the "Sample" menu in the upper right corner. The p4p file also contains the table for the detector spatial correction. If you're creating a new database entry to work with old data, be sure to read in a p4p file before continuing after opening the entry by selecting "Import>p4p" from the "Sample" menu.
Active Mask	*.sfrm	This is an image file which contains the mask for the beamstop shadow. The filename contains the frame prefix, run number and frame number (0001). For example, <i>prefix_am_01_0001.sfrm</i> . You can view this file in PROTEUM as you would any image file to verify that SAINT is properly masking out the shadow.
Charting	*.cht	This file contains all the charts that were displayed in PROTEUM during the integration. The file can be re-opened in PROTEUM by clicking on the "Integrate Images" plugin and selecting "Open Chart File" from the Chart menu in the upper right corner of the GUI.

Scale (SADABS)

Output Files	Extension	Description
Scaled Intensities	*.hkl	File contains the scaled, unmerged intensities in SHELX HKLF4 format.
Log	*.abs	Scaling log file written out from SADABS.

XPREP

Output Files	Extension	Description
Log	*.prp	The file is actively updated as you navigate through XPREP or "Space Groups and Statistics" (PROTEUM's GUI interface for XPREP).
Different file formats		The intensity file output from SADABS (*.hkl) can be converted to other file formats using XPREP. Using the "W" option from the "Read, modify or merge DATASETS" ([D]) menu, you can output the intensities in Scalepack, CNS or X-PLOR formats. You can also output a Scalepack HKL file from "Space Groups and Statistics" by checking the "output .sca file" box.