

autoPROC reference card	
set up (probably already arranged by local IT)	
Set up for csh or tesh	<code>source /some/where/autoPROC/installed/setup.csh</code>
Set up for bash, ksh, zsh, or sh	<code>./some/where/autoPROC/installed/setup.sh</code>
autoPROC: most useful options	
Brief help message	<code>process -h</code>
Simple run (in directory containing images)	<code>process -d outputdir > log</code> - or - <code>process -d outputdir tee log</code>
Simple run (remote directory)	<code>process -d outputdir -I imagedir > log</code>
Read image header information	<code>imginfo test_0123.img</code>
Check beam centre conventions	<code>beam8.sh <beamX> <beamY> <sizeX> <sizeY></code>
Define direct beam transform	<code>process BeamCentreFrom="header:y,-x" -d outputdir > log</code>
Let autoPROC determine most likely direct beam transform [1]	<code>process BeamCentreFrom="getbeam:init" -d outputdir > log</code>
Define direct beam position [2]	<code>process beam="1556 1512" -d outputdir > log</code>
Identify image scans	<code>find_images -d imagedir -l</code>
Identify HDF5/Eiger scans	<code>find_images -d imagedir -l -h5</code>
Manual sweep definition	<code>process -Id "test,/where/ever/images,test_###.cbf,1,90" -d outputdir > log</code>
Manual sweep definition for HDF5/Eiger data	<code>process -Id "test,/where/ever,test_master.h5,1,900" -d outputdir > log</code>
Define cell dimensions and symmetry [3]	<code>process cell="a b c a l b e g a" symm="P21" -d outputdir > log</code>
Include "reference" file for symm, cell and test-set	<code>process -ref mtzfile -d outputdir > log</code>
List available "macros" [4]	<code>process -M list</code>
Settings that might help difficult diffraction data [5]	<code>process -M LowResOrTricky -d outputdir > log</code>
Process in "fast" mode [6]	<code>process -M fast -d outputdir > log</code>
Restrict number of "processors"	<code>process -nthreads <no> -d outputdir > log</code>
Restrict resolution range	<code>process -R 50.0 2.0 -d outputdir > log</code>
List known multi-axis goniostats	<code>x_kappa -list</code>
Process multi sweep data collected with different goniostat/2-theta settings	<code>process KapparovSite="siteID" -d outputdir > log</code>
Switch off detection/exclusion of ice-ring resolution ranges	<code>process XdsExcludeIceRingsAutomatically=no -d outputdir > log</code>
Exclude all known ice-ring resolution ranges from the start	<code>process XdsExcludeIceRingsAutomatically=all -d outputdir > log</code>
AIMLESS-only scaling path	<code>process -M ScalingA3 -d outputdir > log</code>
XSCALE-only scaling path	<code>process -M ScalingX -d outputdir > log</code>
Process Dectris/Eiger data (HDF5 format)	<code>process -h5 /where/ever/some_master.h5 -d outputdir > log</code>

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results	
Progress summary	summary.html (in output directory: open with browser) standard output (might give more details about problems)
Reflection data, traditional (isotropic) analysis	truncate-unique.mtz truncate_<wavelength>-unique.mtz (multi-wvl data)
Reflection data, anisotropic (STARANISO) analysis	staraniso_alldata-unique.mtz staraniso_<wavelength>_alldata-unique.mtz
PDF reports	report.pdf report_staraniso.pdf
XML (ISPyB compatible)	autoPROC.xml autoPROC_staraniso.xml
helper programs and options	
Scaling module: help message	aP_scale -h
Simple scaling of data set with 360 batches/images	aP_scale -mtz XDS_ASCII.mtz -P lyso test A -b 1-360 -id 01 > log
More detailed scaling of 'early' and 'late' batches	aP_scale -mtz XDS_ASCII.mtz -P lyso test early -b 1-180 -P lyso test late -b 181-360 -id 02 > log
Allowing different high-resolution limit for decaying crystal ("chunking")	aP_scale -mtz XDS_ASCII.mtz -P lyso test early -b 1-180,30 -P lyso test late -b 181-360,30 -id 03 > log
Use XSCALE for scaling	aP_scale -hkl XDS_ASCII.HKL ...
Compare indexing of datasets	check_indexing mtzfile1 mtzfile2 ... mtzfileN
Compare orientation matrices	cmpmat 01/XPARAM.XDS 02/XPARAM.XDS P21
Combine integrated intensities from several scans manually	combine_files -f 01/XDS_ASCII.mtz -P lyso test lowres \ -f 02/XDS_ASCII.HKL -P lyso test highres \ -o low-high.mtz
Calculate statistics on unmerged data	mrfana INTEGRATE.HKL - or - mrfana XDS_ASCII.mtz
further information	
autoPROC homepage	http://www.globalphasing.com/autoproc/
autoPROC manual	\$autoPROC_home/docs/autoproc/manual/autoPROC0.html - or - http://www.globalphasing.com/autoproc/manual/index.html
autoPROC wiki	http://www.globalphasing.com/autoproc/wiki/
beamline information	http://www.globalphasing.com/autoproc/wiki/index.cgi?BeamlineSettings

Notes:

- [1] This should only be attempted as a last resort – see also [2].
- [2] <http://www.globalphasing.com/autoproc/wiki/index.cgi?BeamlineSettings>
- [3] You could also only give the SG name (and let autoPROC decide on the most likely cell).
- [4] Using “show” instead of “list” gives details of each macro, ie. potential ideas for own macros.
- [5] Not all difficult crystals behave the same – please check diagnostics in summary.html carefully.
- [6] This involves various shortcuts that could impinge on data quality – use with care.