XDS procedure

```
>setxds
>xdsgui
```

Create a project in the xds subfolder Load the first frame of the dataset from /syno/frames/date_beamline/drop/... Generate XDS.INP Run XDS

- if the correct spacegroup and cell parameters were not identified by IDREF, provide them in XDS.INP
- if there is no anomalous signal to use, specify *FRIEDEL_LAW= TRUE*

Check the statistics and estimate the resolution limit at which CC(1/2)=0.1 (the last shell with a star) Re-run XDS with the specified resolution limit with only *JOB= CORRECT*

Item to check in XDS

- FRAME.cbf (last frame processed by INTEGRATE) for spot shape, splitting, multiple lattice, predicted/observed diffraction pattern, ice rings
- INTEGRATE.LP jumps or large changes in frame-wise parameters (sacle factors, mosaicity, beam divergence, cell, distance, ...)
- CORRECT.LP reports systematic errors (ISa) and precision of unmerged and merged intensities (Rmeas and CC(1/2))

Run XDSSTAT to analyze XDS_ASCII.HKL in XDSSTAT.LP