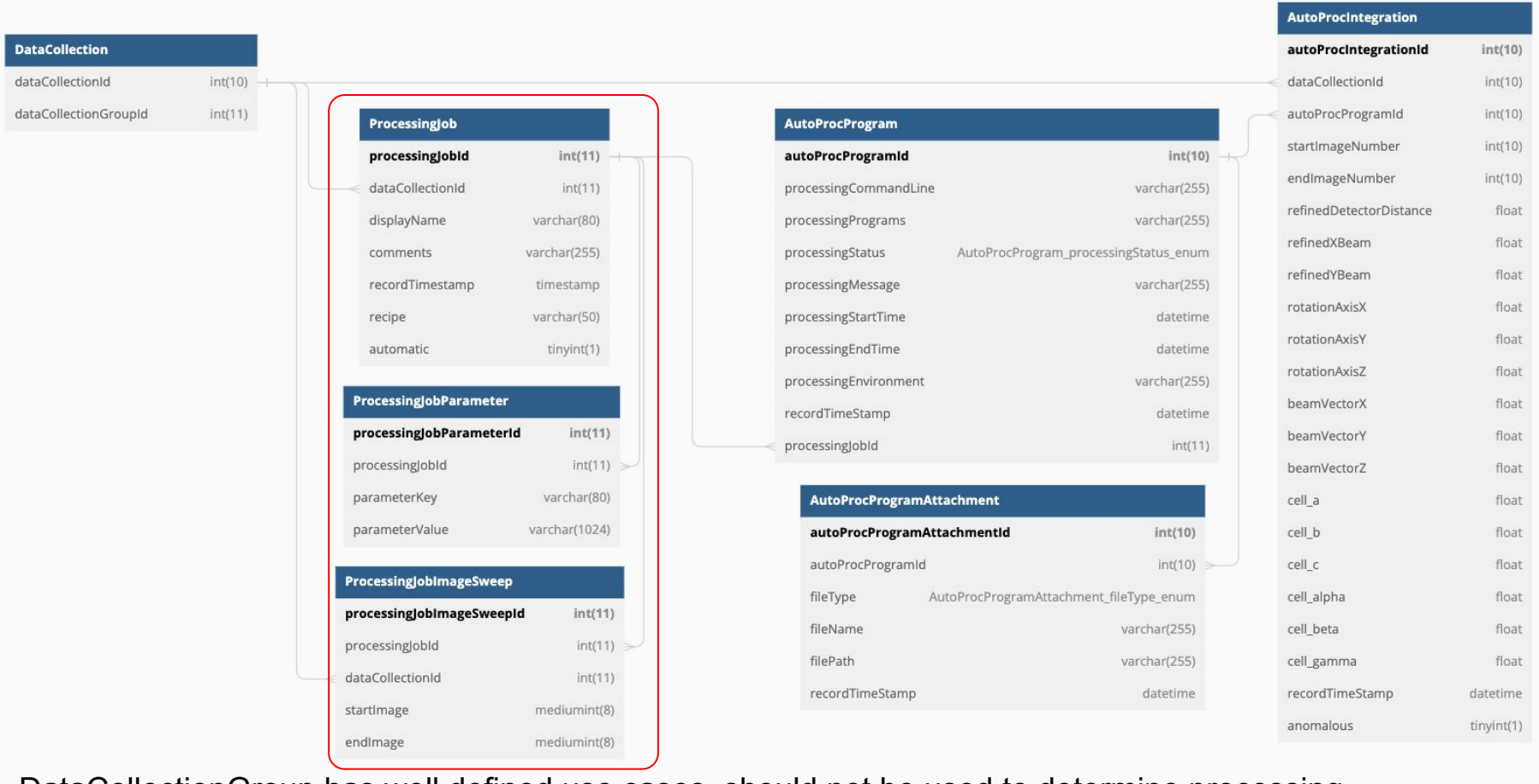

ESRF
The European Synchrotron

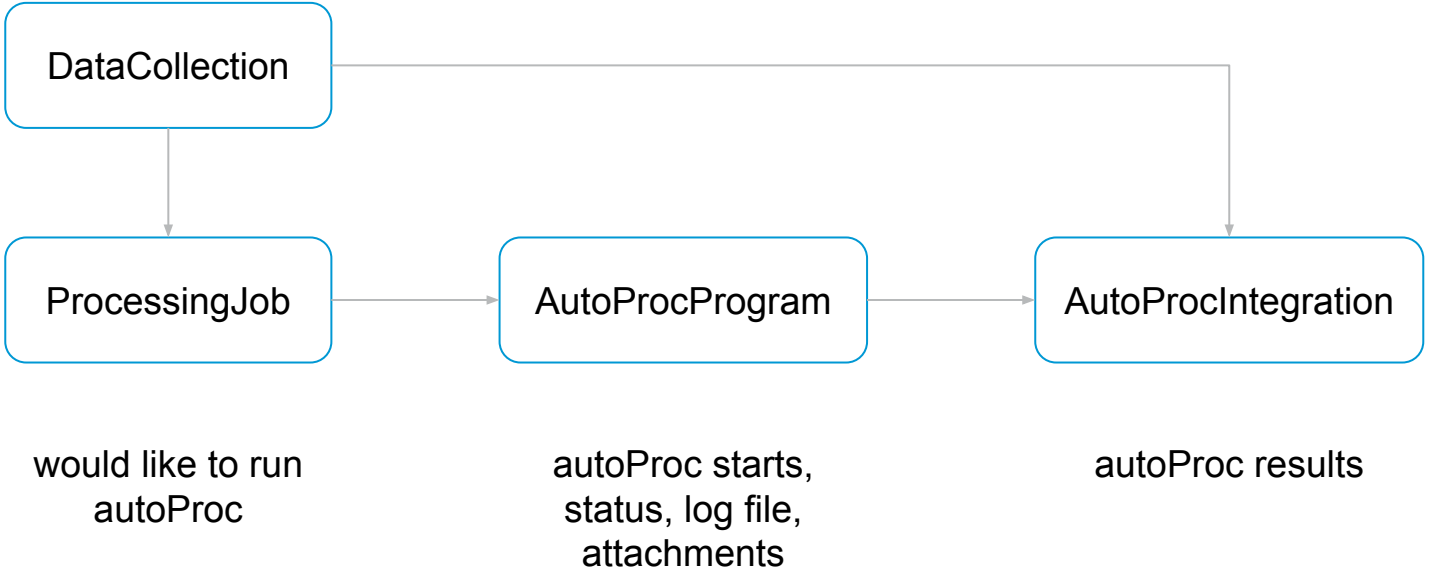
# ProcessingJob



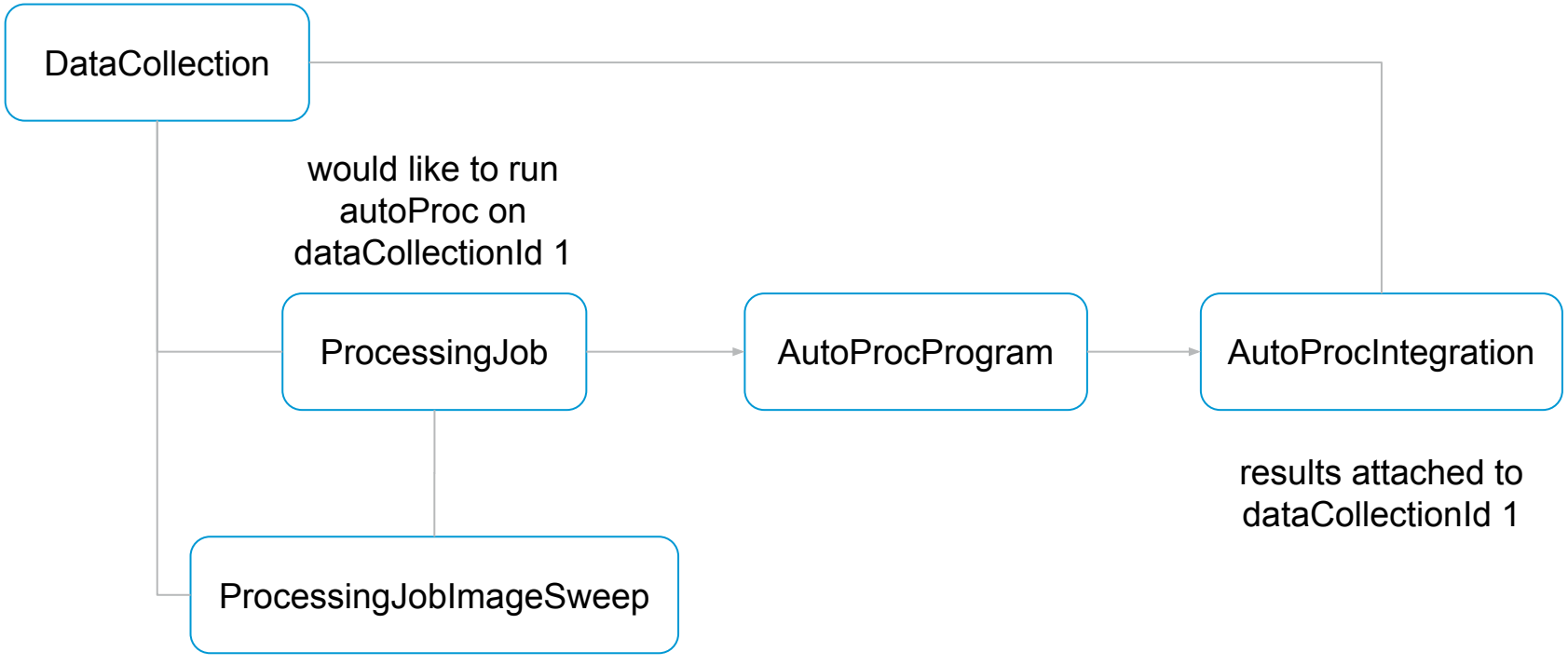

DataCollectionGroup has well defined use cases, should not be used to determine processing

# ProcessingJob

## Signals the intent to run some kind of processing on a DataCollection



# Multi sweep/sample integration



https://ispyb.diamond.ac.uk/dc/visit/nt31175-3/id/8472788

Auto Processing — fast_dp: ✔ | xia2 dials: 2x ✔ | autoPROC: 2x ✔ | xia2 3dii: 2x ✔ | xia2.multiplex: ✔ ✖ | autoPROC+STARANISO: 2x ✔

| Type | Resolution | Spacegroup | Mn<I/sig(I)> | Rmeas Inner | Rmeas Outer | Completeness | Cell | Status |
|---|---|---|---|---|---|---|---|---|
| fast_dp | 29.10 - 1.68 | P 4 2 2 | 47.0 | 0.019 | 0.066 | 69.4 | 67.86 67.86 102.65 90.00 90.00 90.00 | processing successful |
| xia2 dials | 40.95 - 1.67 | P 4 21 2 | 48.5 | 0.035 | 0.037 | 69.2 | 67.88 67.88 102.70 90.00 90.00 90.00 | processing successful |
| autoPROC | 43.47 - 1.68 | P 41 21 2 | 45.9 | 0.019 | 0.045 | 69.4 | 67.87 67.87 102.66 90.00 90.00 90.00 | processing successful |
| xia2 3dii | 43.47 - 1.68 | P 41 21 2 | 40.2 | 0.020 | 0.092 | 70.4 | 67.86 67.86 102.64 90.00 90.00 90.00 | processing successful |
| xia2 dials | 40.94 - 1.67 | P 43 21 2 | 51.2 | 0.033 | 0.043 | 69.3 | 67.86 67.86 102.68 90.00 90.00 90.00 | processing successful |
| xia2 3dii | 43.47 - 1.68 | P 43 21 2 | 40.2 | 0.020 | 0.092 | 70.4 | 67.86 67.86 102.64 90.00 90.00 90.00 | processing successful |
| autoPROC | 47.99 - 1.68 | P 43 21 2 | 45.9 | 0.020 | 0.041 | 69.4 | 67.87 67.87 102.66 90.00 90.00 90.00 | processing successful |
| xia2.multiplex | | | | | | | | processing failure |
| 199x xia2.multiplex | 102.70 - 1.00 | C 2 2 2 | 39.7 | 0.061 | 0.749 | 80.3 | 96.00 95.89 102.70 90.00 90.00 90.00 | processing successful |
| autoPROC+STARANISO | 47.99 - 1.67 | P 43 21 2 | 40.0 | 0.019 | 0.055 | 73.5 | 67.87 67.87 102.66 90.00 90.00 90.00 | processing successful |
| autoPROC+STARANISO | 47.99 - 1.67 | P 41 21 2 | 39.7 | 0.019 | 0.055 | 73.6 | 67.87 67.87 102.66 90.00 90.00 90.00 | processing successful |

fast_dp ! | xia2 dials ! | autoPROC | xia2 3dii ! | xia2 dials ! | xia2 3dii ! | autoPROC | xia2.multiplex | 199x xia2.multiplex ⚠ | autoPROC+STARANISO | autoPROC+STARANISO

8 check(s) passed

2 alert(s)

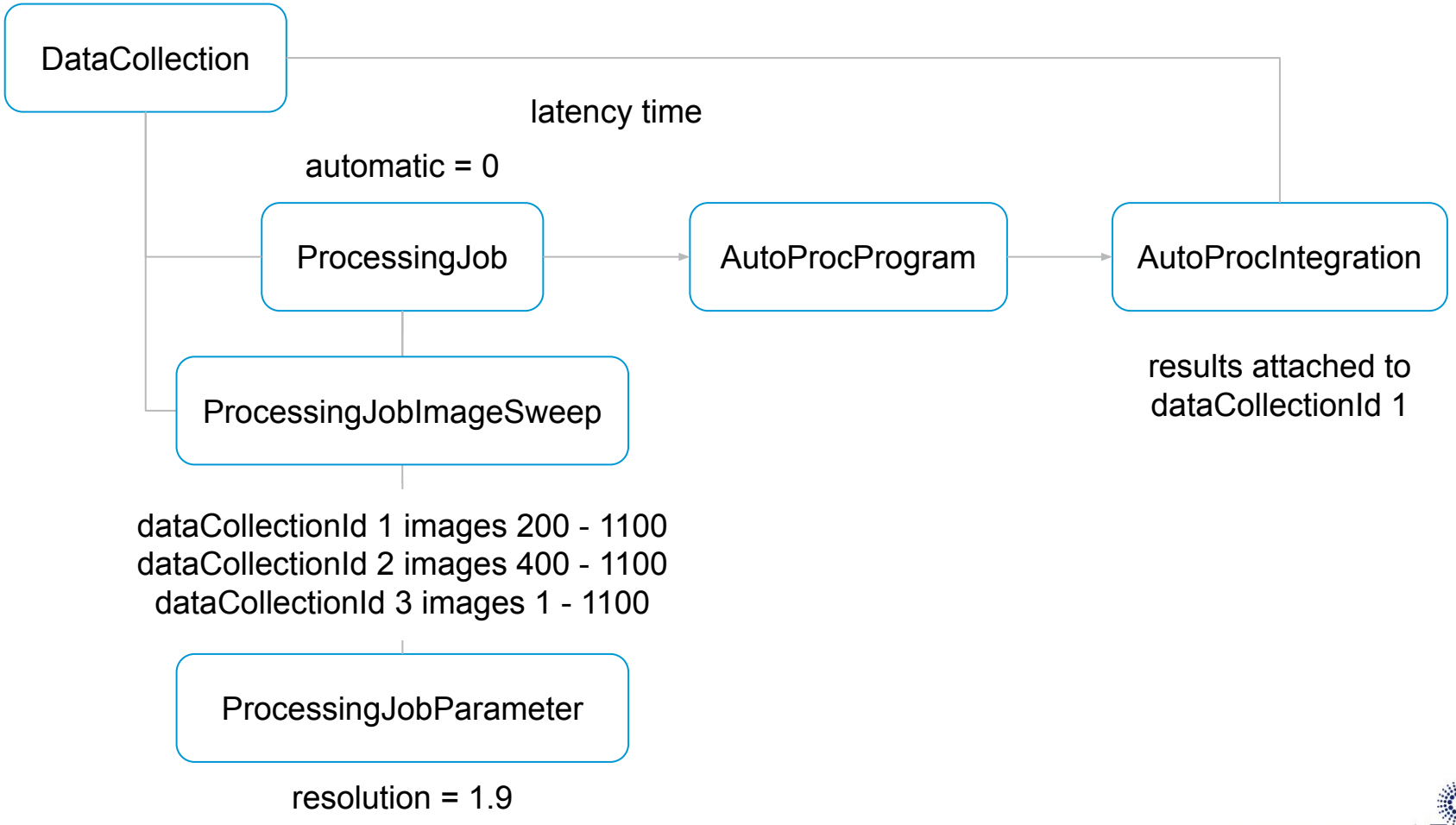
| Beam Centre | X | Y |
|---|---|---|
| Start | 157.66 | 165.77 |
| Refined | -- | -- |
| Δ | -- | -- |

| Space Group | A | B | C | α | β | γ |
|---|---|---|---|---|---|---|
| C 2 2 2 | 96.00 | 95.89 | 102.70 | 90.00 | 90.00 | 90.00 |

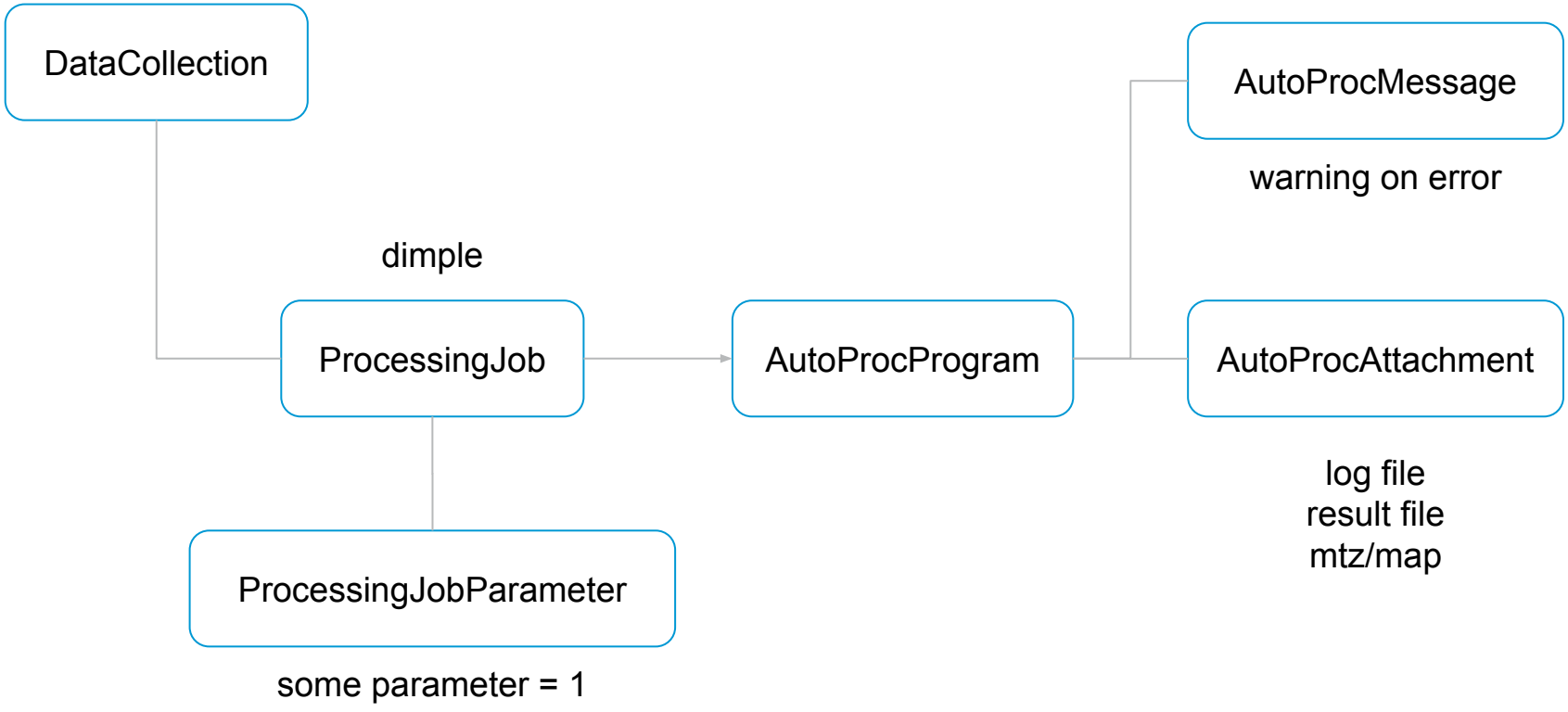
199 Data Sets | Plots | Archive | Logs & Files | Lookup Cell

| Shell | Observations | Unique | Resolution | Rmeas | I/sig(I) | CC Half | Completeness | Multiplicity | Anom Completeness | Anom Multiplicity | CC Anom |
|---|---|---|---|---|---|---|---|---|---|---|---|
| outerShell | 2385 | 1635 | 1.00 - 1.02 | 0.749 | 0.2 | 0.6 | 13.0 | 1.5 | 0.0 | 1.5 | 0.3 |
| innerShell | 7101245 | 13156 | 2.71 - 103.24 | 0.061 | 259.4 | 1.0 | 100.0 | 539.8 | 0.0 | 539.8 | 0.6 |
| overall | 20706129 | 203256 | 1.00 - 102.70 | 0.071 | 39.7 | 1.0 | 80.3 | 101.9 | 0.0 | 101.9 | 0.6 |

# Reprocessing



# Downstream Processing



Downstream Processing

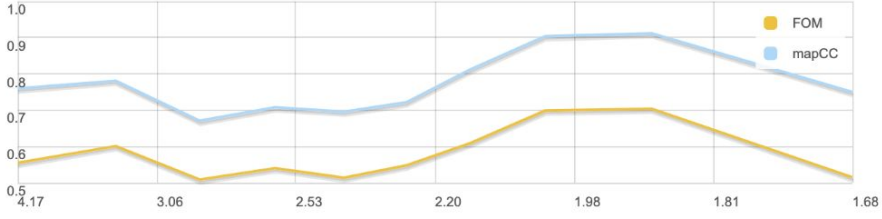
fast_ep: ✔ | dimple: ✔ 5x ✖ | MrBUMP: ⚙ 9x ✔ | autoSHARP: ✔ | AutoBuild: ✖ | Crank2: ✖

Fast EP | MrBUMP | Dimple | AutoSHARP | Autobuild | Crank2

Map / Model Viewer | Archive | Logs & Files

Figure of Merit: 0.58
Pseudo-free CC: 56.75

| # | X | Y | Z | Occ |
|---|---|---|---|---|
| 1 | 1.367 | 66.493 | 0.000 | 0.500 |
| 2 | 5.502 | 67.860 | 0.000 | 0.161 |
| 3 | 0.000 | 67.860 | 6.079 | 0.064 |
| 4 | 7.410 | 71.665 | -0.011 | 0.218 |
| 5 | 0.000 | 67.860 | 9.620 | 0.054 |

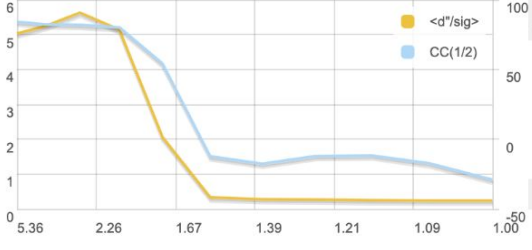



Fast EP | MrBUMP | Dimple | AutoSHARP | Autobuild | Crank2

xia2.multiplex

Map / Model Viewer | Archive | Logs & Files

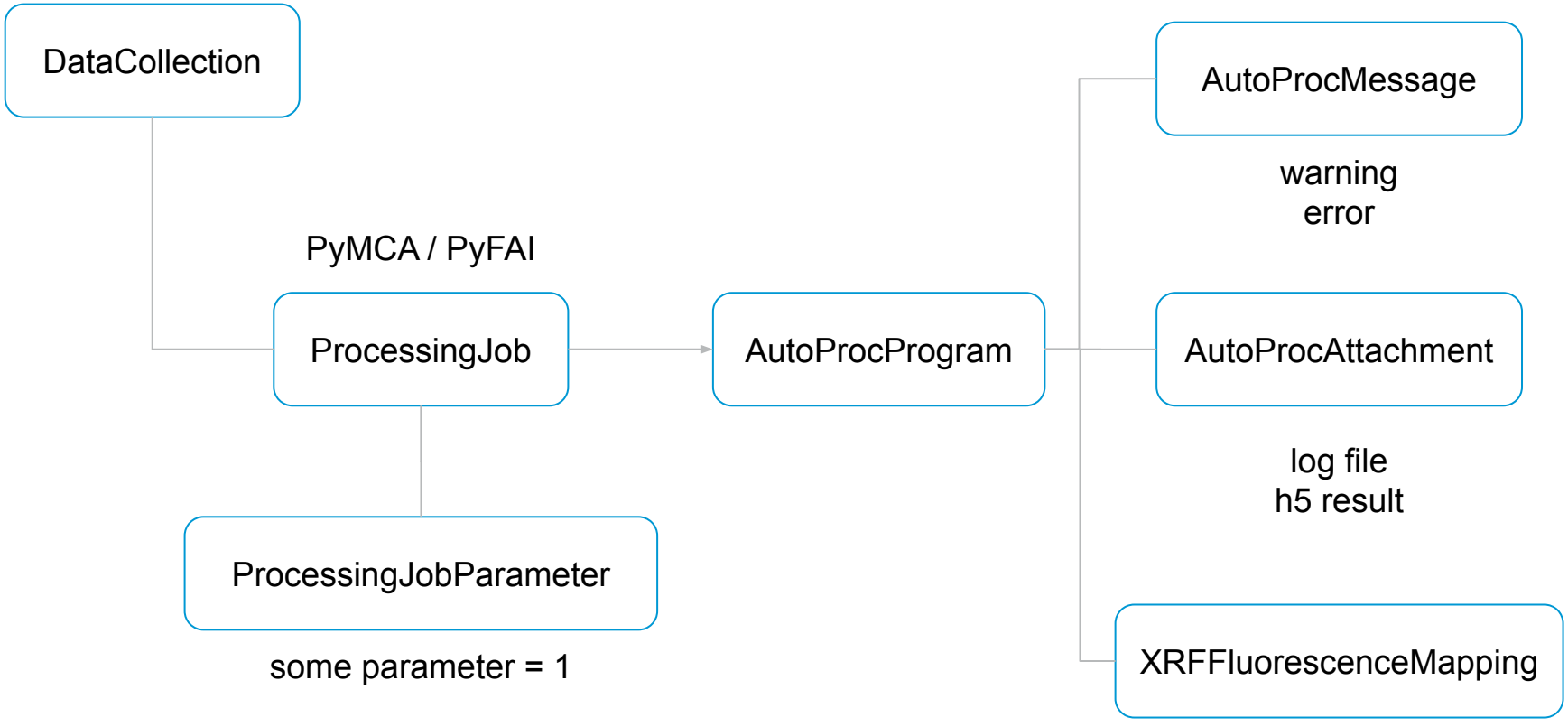
No Image




| Anom. scatterer | Space group | Num. scatterers | Dataset type | Compound | Sequence |
|---|---|---|---|---|---|
| S | C222 | 20 | peak | Protein | MRLSVLLSLLPLALGAPAVEQRSEAAPLIEARGEMVANKYIVKFKEGSALSALDAAMEKI SGKPDHVYKNVFSGFAATLDENMVRVLRAHPDVEYIEQDAVVTINAAQTNAPWGLARISS TSPGTSTYYYDESAGQGSCVYVIDTGIEASHPEFEGRAQMVKTYYYSSRDGNGHGTHCAG TVGSRTYGVAKKTQLFGVKVLDDNGSGQYSTIIAGMDFVASDKNNRNCPKGVVASLSLGG GYSSSVNSAAARLQSSGVMVAVAAGNNNADARNYSPASEPSVCTVGASDRYDRRSSFSNY GSVLDIFGPGTSILSTWIGGSTRSISGTSMATPHVAGLAAYLMTLGKTTAASACRYIADT ANKGDLSNIPFGTVNLLAYNNYQA |

| Resid. / Frag / Max. Frag. | Best MapCC (Resol.) |
|---|---|
| 12 / 3 / 6 | 0.05 (1.00) |

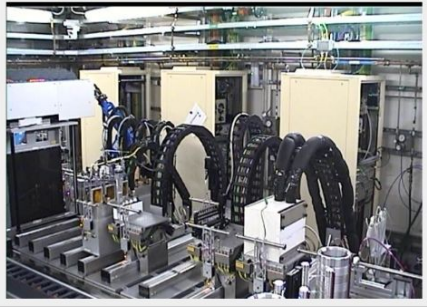
# Non-MX

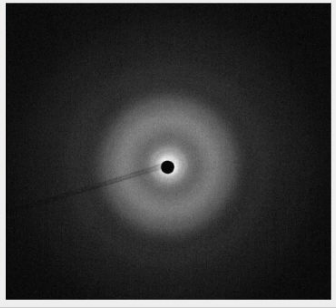

DataCollection
ProcessingJob
PyMCA / PyFAI
ProcessingJobParameter
some parameter = 1
AutoProcProgram
AutoProcMessage
warning
error
AutoProcAttachment
log file
h5 result
XRFFluorescenceMapping

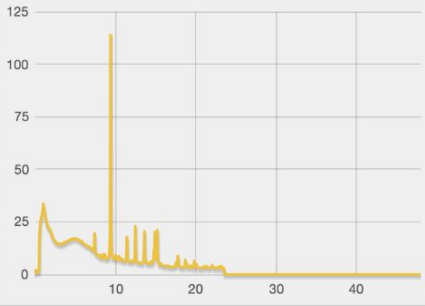
Download Data

10-10-2022 17:03:43 - /dls/i11-1/data/2022/cm31130-4/i11-1-64451.nxs

| | |
|---|---|
| Group: 1 Data Collections | Beam Centre: NaN x NaN |
| Wavelength: 0.0000Å | Detector Distance: 670.0mm |
| Exposure: 1.0000s | Beamsize: 0x0µm |
| No. Images: | Detector: |
| Comment: Undefined | |
| Scan Parameters: | |








Data Files — Download

Auto Processing — Jupyter (Papermill) Autoprocessing:

jupyter (papermill) autoprocessing

Archive | Logs & Files

| Processing Programs | Comments | Message | Start Time | End Time |
|---|---|---|---|---|
| Jupyter (Papermill) Autoprocessing | Running calibration on/dls/i11-1/data/2022/cm31130-4/i11-1-64451.nxs | Processing Successful | 2022-10-10 17:08:01 | 2022-10-10 17:10:48 |

# Implementation

## MR ready in ispyb-database

https://github.com/ispyb/ispyb-database/pull/35

https://github.com/ispyb/ispyb-database/pull/36

## Already supported in pyISPyB

https://github.com/ispyb/py-ispyb/compare/beamline-groups-permissions...stats-and-processing

## Could provide webservices for population

## In production > 5 years

https://github.com/ispyb/ispyb-database-modeling/issues/19