



| The European Synchrotron

# ProcessingJob

DataCollection	
dataCollectionId	int(10)
dataCollectionGroupId	int(11)

ProcessingJob	
processingJobId	int(11)
dataCollectionId	int(11)
displayName	varchar(80)
comments	varchar(255)
recordTimestamp	timestamp
recipe	varchar(50)
automatic	tinyint(1)

ProcessingJobParameter	
processingJobParameterId	int(11)
processingJobId	int(11)
parameterKey	varchar(80)
parameterValue	varchar(1024)

ProcessingJobImageSweep	
processingJobImageSweepId	int(11)
processingJobId	int(11)
dataCollectionId	int(11)
startImage	mediumint(8)
endImage	mediumint(8)

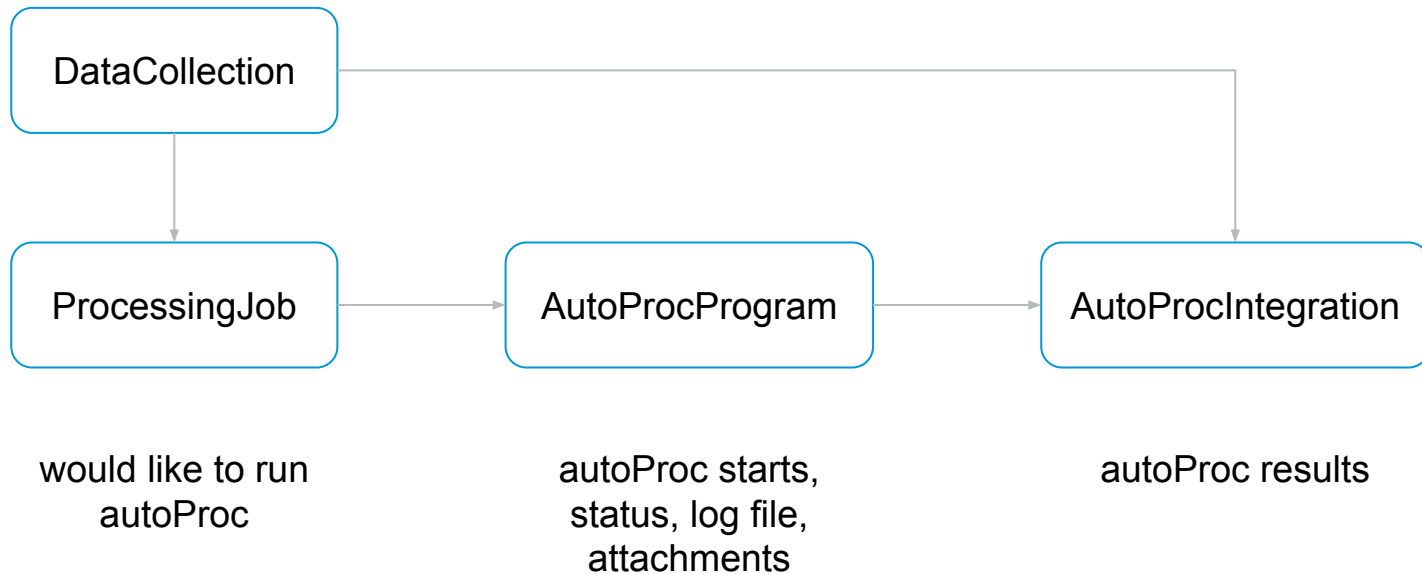
AutoProcProgram	
autoProcProgramId	int(10)
processingCommandLine	varchar(255)
processingPrograms	varchar(255)
processingStatus	AutoProcProgram_processingStatus_enum
processingMessage	varchar(255)
processingStartTime	datetime
processingEndTime	datetime
processingEnvironment	varchar(255)
recordTimeStamp	datetime
processingJobId	int(11)

AutoProcProgramAttachment	
autoProcProgramAttachmentId	int(10)
autoProcProgramId	int(10)
fileType	AutoProcProgramAttachment_fileType_enum
fileName	varchar(255)
filePath	varchar(255)
recordTimeStamp	datetime

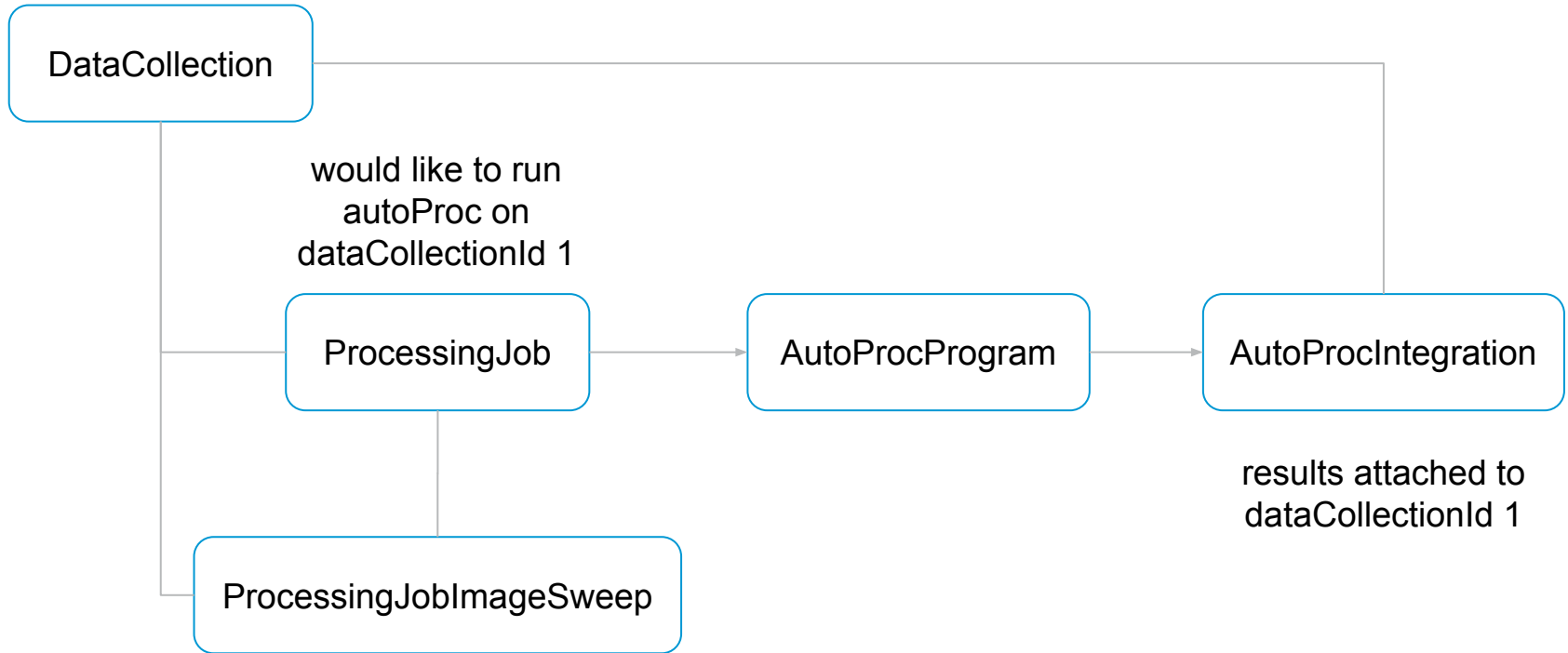
AutoProcIntegration	
autoProcIntegrationId	int(10)
dataCollectionId	int(10)
autoProcProgramId	int(10)
startImageNumber	int(10)
endImageNumber	int(10)
refinedDetectorDistance	float
refinedXBeam	float
refinedYBeam	float
rotationAxisX	float
rotationAxisY	float
rotationAxisZ	float
beamVectorX	float
beamVectorY	float
beamVectorZ	float
cell_a	float
cell_b	float
cell_c	float
cell_alpha	float
cell_beta	float
cell_gamma	float
recordTimeStamp	datetime
anomalous	tinyint(1)

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

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



# Multi sweep/sample integration



dataCollectionId 1 images 1 - 1100  
dataCollectionId 2 images 1 - 1100  
dataCollectionId 3 images 1 - 1100

dataCollectionId 4 images 1 - 1100 (sample 2)

Auto Processing fast\_dp: xia2 dials: 2x autoPROC: 2x xia2 3dii: 2x xia2.multiplex: autoPROC+STARANISO: 2x

Type	Resolution	Spacegroup	Mn</sig(l)>	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

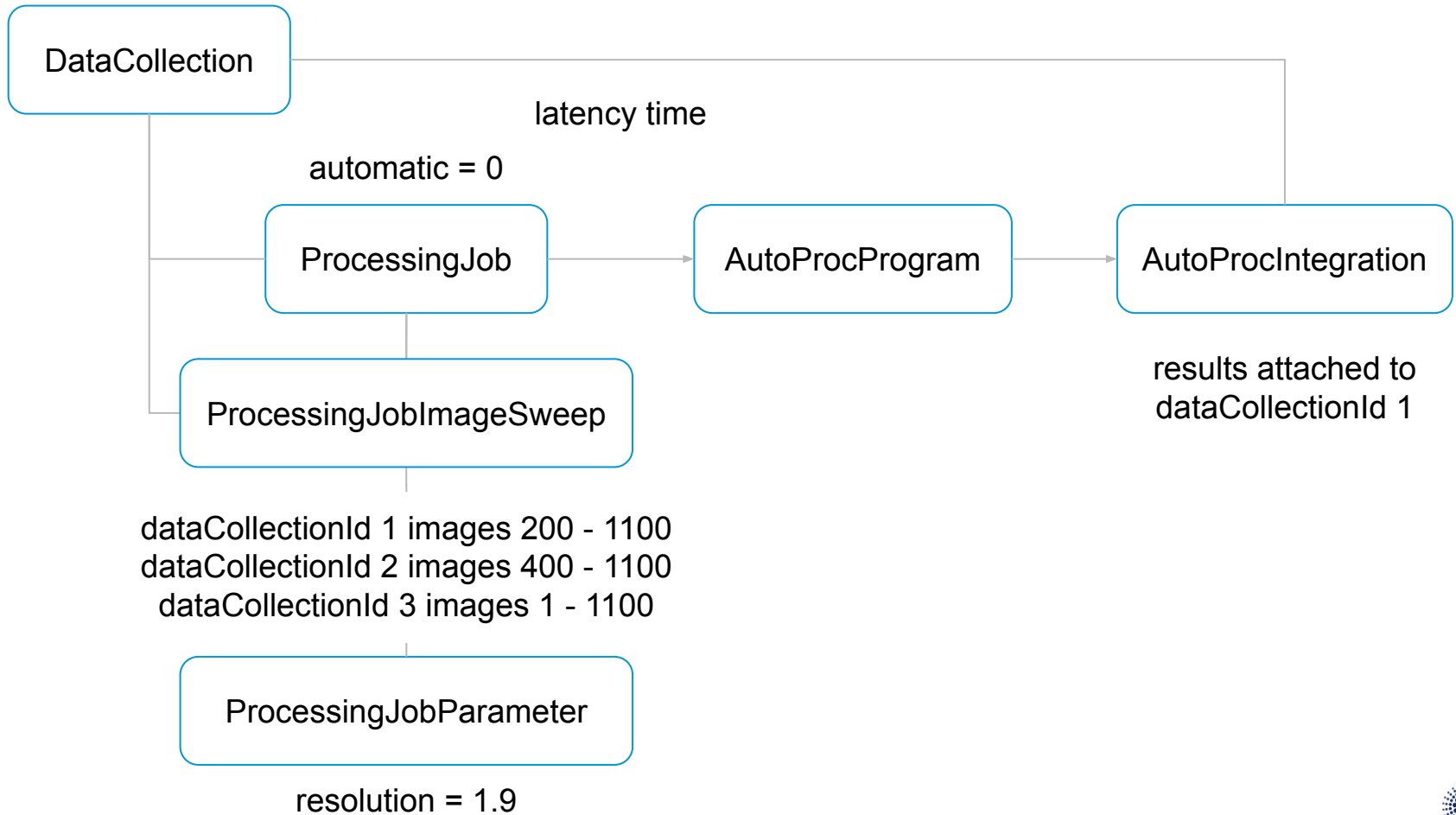
Archive

Logs & Files

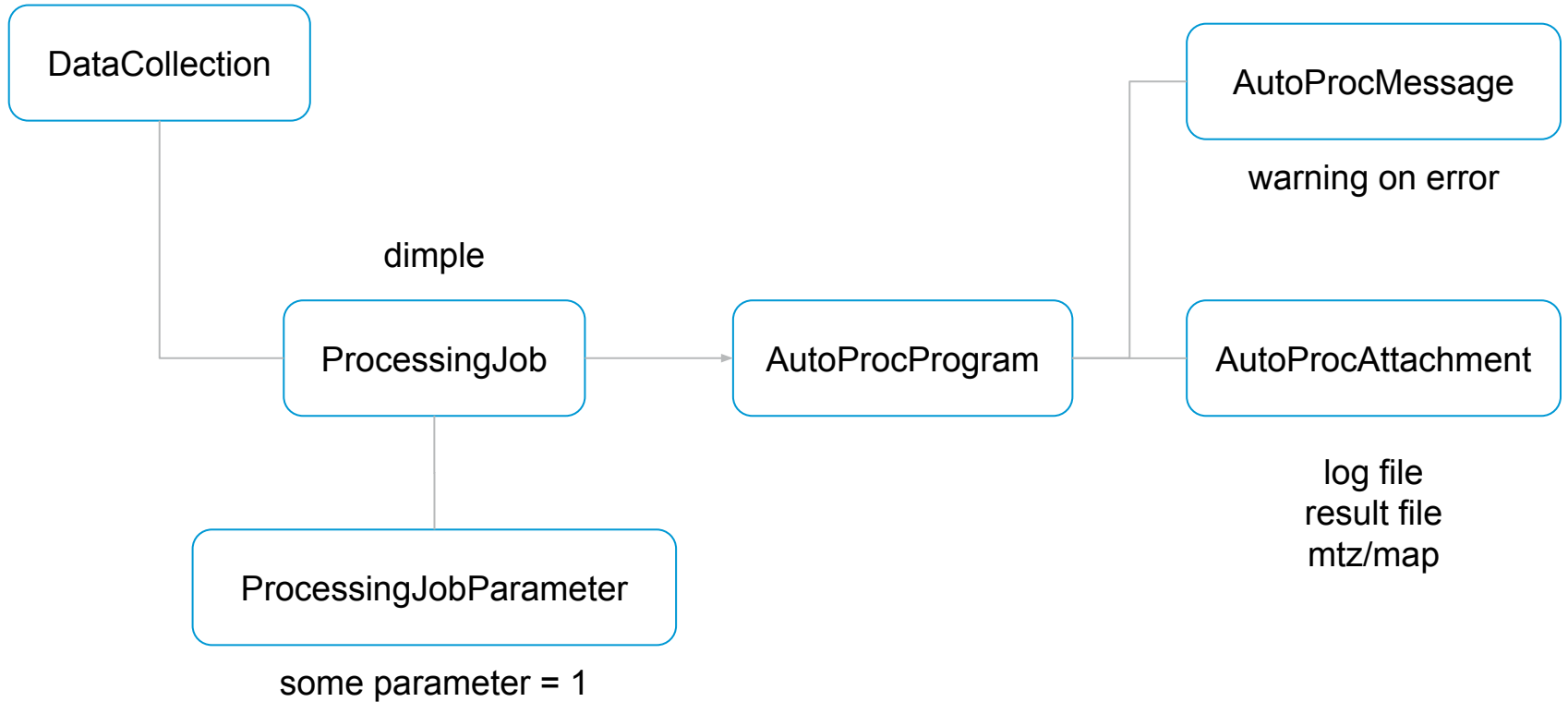
Lookup Cell

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



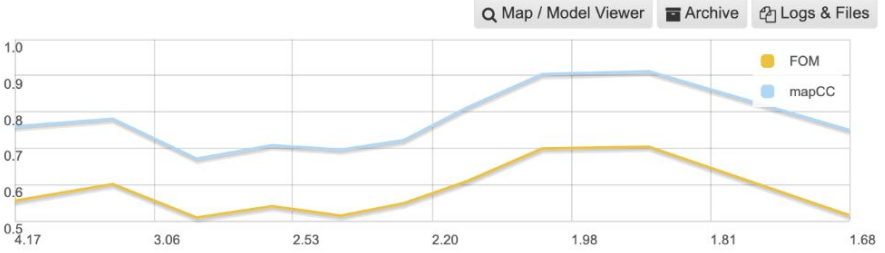
Downstream Processing

fast\_ep: ✔ | dimple: ✔ 5x ✖ | MrBUMP: ⚙️ 9x ✔ | autoSHARP: ✔ | AutoBuild: ✖ | Crank2: ✖

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

Figure of Merit: 0.58  
Pseudo-free CC: 56.75

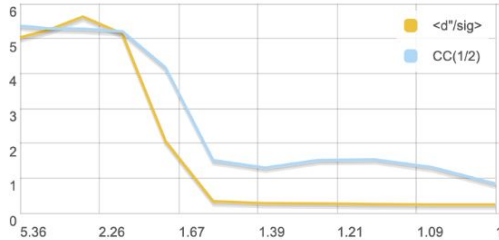
#	X	Y	Z	Occ
1	1.367	66.493	0.000	0.500
2	5.502	67.860	0.000	0.161
3	0.000	67.860	6.079	0.064
4	7.410	71.665	-0.011	0.218
5	0.000	67.860	9.620	0.054



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

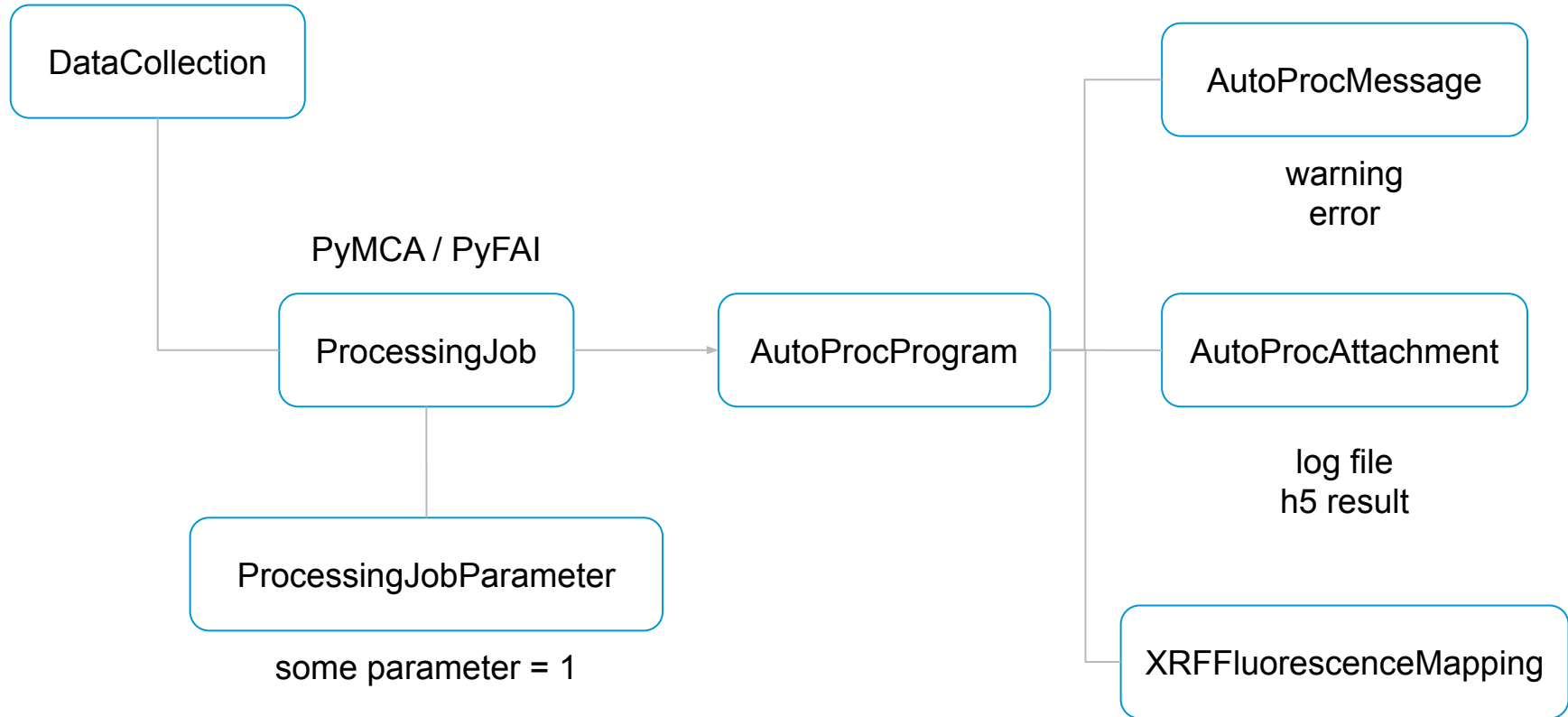
xia2.multiplex

Q Map / Model Viewer | Archive | Logs & Files



Anom. scatterer	Space group	Num. scatterers	Dataset type	Compound	Sequence
S	C222	20	peak	Protein	MRLSVLLSLLPLALGAPAVEQRSEAAPLIEARGEMVANKYIVKFKESALSALDAAMEKI SGKPDHVVYKNVFSGFAATLDENMVRVLRHPDVEYIEQDAVVTINAAQTNPWGLARISS TSPGTSYYVDESAGQGSQVYVIDTGLIEASHPEFEGRQAMVKTYYYSSRDNGHGHTCAG TVGSRITYGAKKTQLFGVKVLDNDGSGQYSTIIAGMDFVASDKNNRNCPKGVVASLSLGG GYSSSVNSAAARLQSSGVMMVAAGNNNADARNYSPASEPSVCTVGASDRYDRSSPSNY GSVLDIFGPOTSILSTWIGGSTSISCTSMATHVAGLAAYLMTLGKTTAASACRYIADT ANKGDLSNIPFGTVNLLAYNNYQA
Resid. / Frag / Max. Frag.					Best MapCC (Resol.)
12 / 3 / 6					0.05 (1.00)





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

Group: 1 Data Collections

Wavelength: 0.0000Å

Exposure: 1.0000s

No. Images:

Comment: Undefined

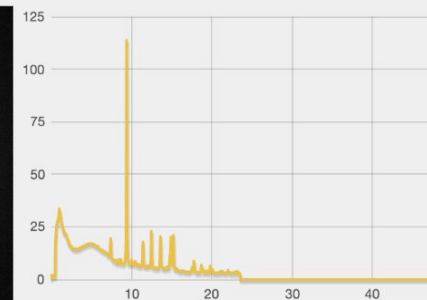
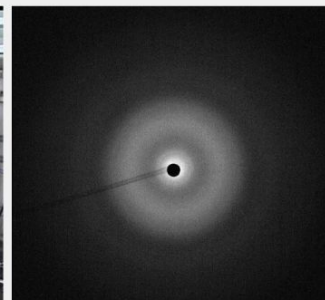
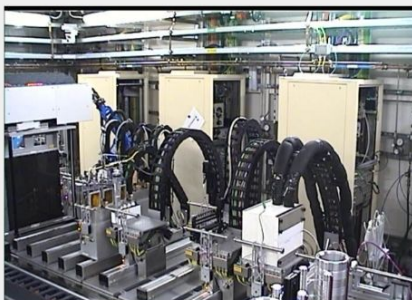
Scan Parameters:

Beam Centre: NaN x NaN

Detector Distance: 670.0mm

Beamsize: 0x0µm

Detector:



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

### 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 webservice for population

### In production > 5 years

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