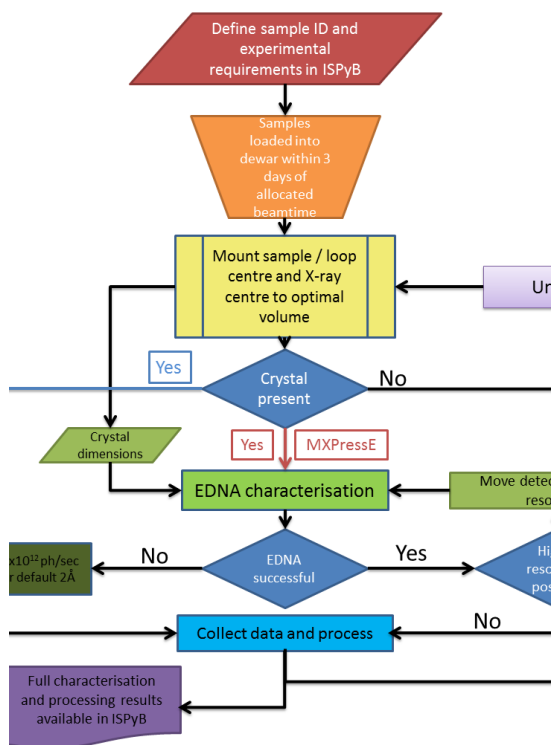


Automating complex data collection using workflows

Olof Svensson
Data Analysis Unit
ISDD / ESRF

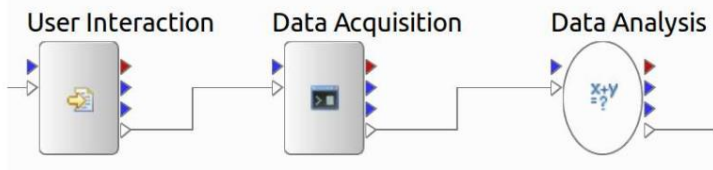


- **Automation of complex data collection**
 - Examples
 - Motivation and short history
- **The Beamline Expert System / Passerelle EDM**
 - Overview
 - Why Passerelle EDM?
 - Screenshots
 - Statistics
- **Interfaces to mxCuBE and ISPyB**
- **Implementation**
- **Future developments**

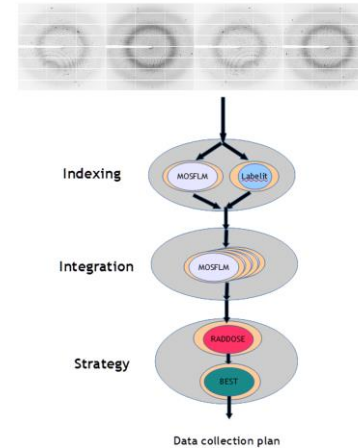
EXAMPLES OF COMPLEX DATA COLLECTION

• Combination of:

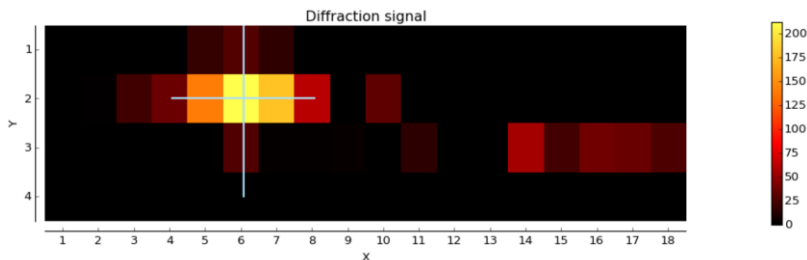
- Data collection
- Data processing
- [User interaction]



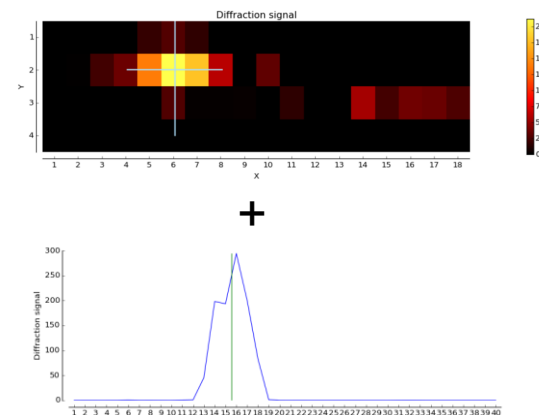
Characterisation (~64000)



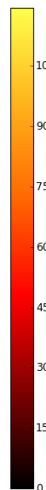
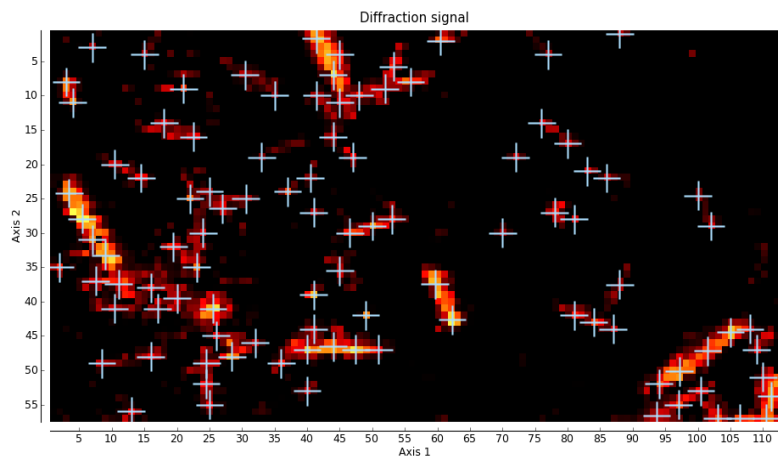
MeshScan (~2700)



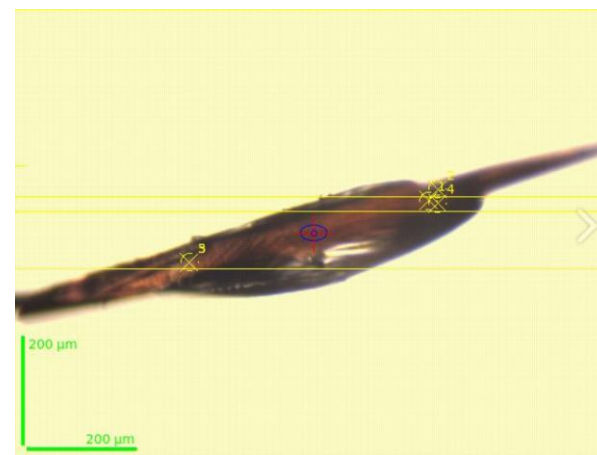
X-ray centring (~5900)



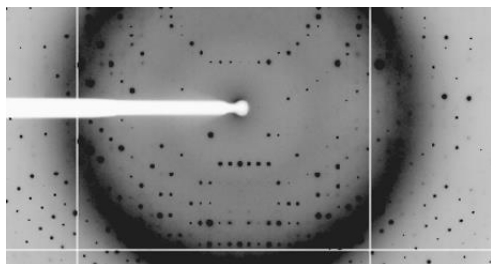
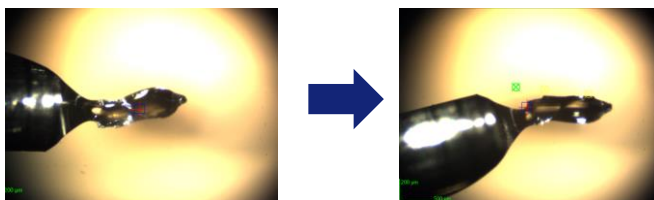
Mesh and collect (~600)



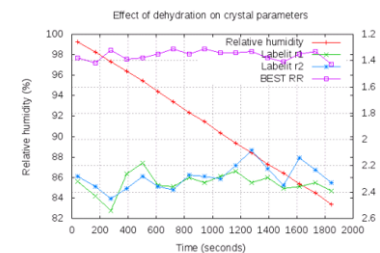
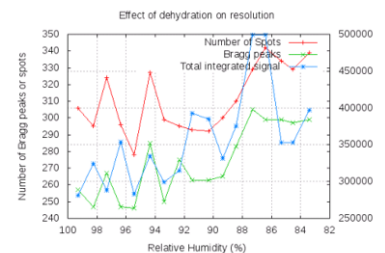
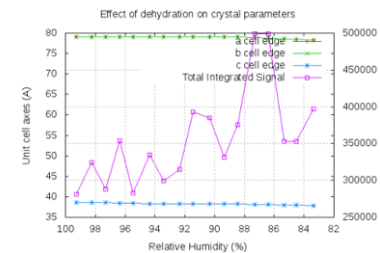
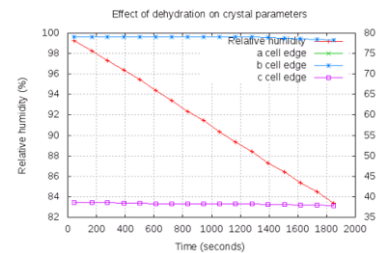
Helical characterisation (~370)



Visual + cell re-orientation (~360)

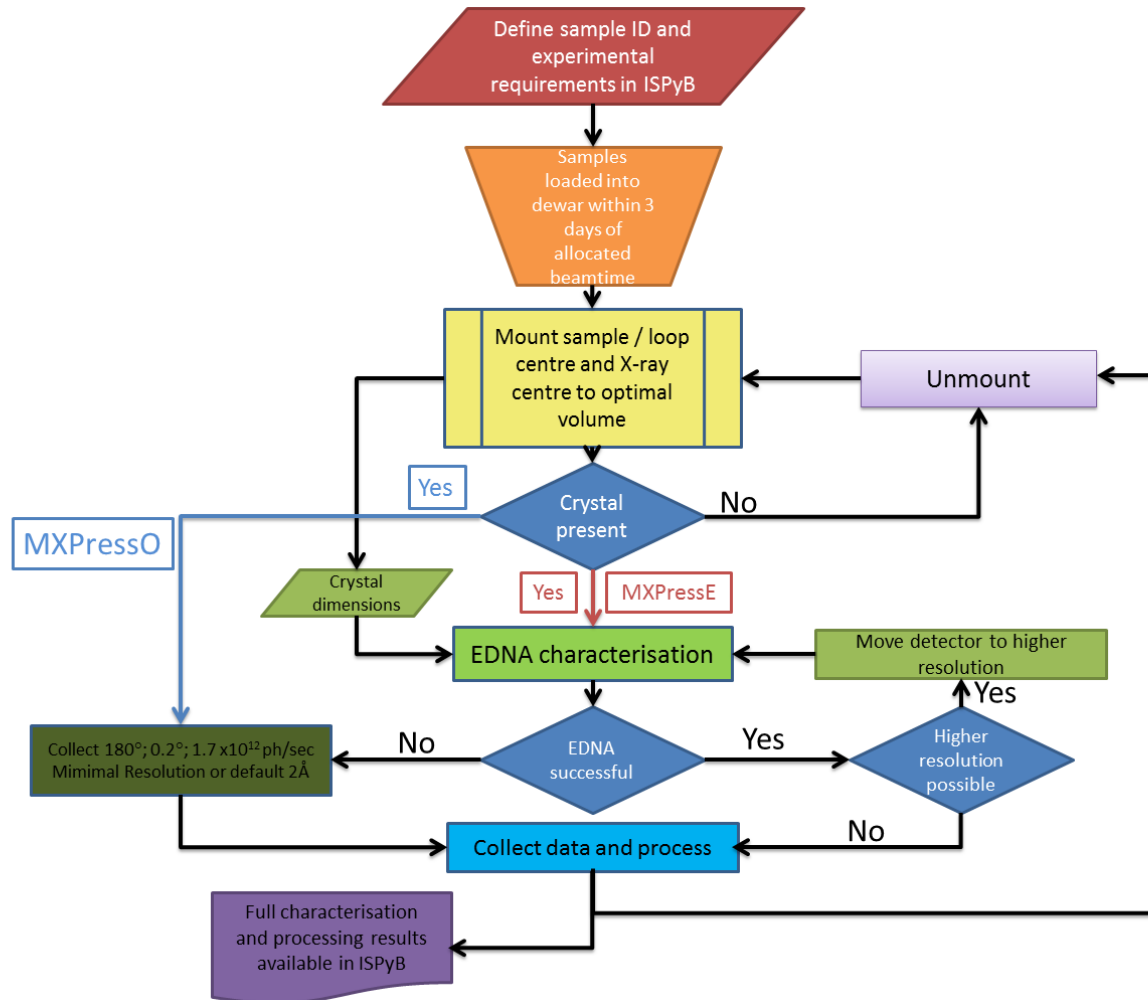


Dehydration (~80)



THE MOST COMPLEX DATA COLLECTION: MXPRESSA

MXPressA (~10000)



- **Interleaved MAD**
- **Burn strategy**
 - Carefully kills the crystal and measures the radiation damage
- **Spectroscopy**

- **Why automation?**

- Complex data collection is often tedious and time-consuming
- Avoid human errors
- Increase speed
- “Hands-off” data collections

- **Short history:**

- 2003 -> 2007 : DNA – automateD collectionN of datA. Dedicated to MX crystal characterization, dedicated GUI
- 2007 -> : EDNA – Enhanced DNA. Framework based on data models, plugins and testing facilities. Today used in MX for thumbnail generation, characterisation, automatic data processing and many other processing tasks.
- 2012 -> 2014 : Passerelle workflow tool (design and execution) in DAWN (open source)
- 2015 -> : Passerelle EDM (Entreprise Decision Manager, not open source)

- **The BES (Beamline Expert System)**
 - A customized version of Passerelle EDM for the ESRF
 - Similar to the SES (Soleil Expert System)
- **Passerelle EDM:**
 - Based on the open-source passerelle workflow engine, which is based on the Ptolemy II workflow engine (written in Java)
 - Combines the passerelle workflow engine with a workflow design tool
 - Both the engine and the design tool are connected to a data base
 - Accessed via a web GUI (Jboss Application Server 7)
- **Passerelle EDM is a commercial product:**
 - Initial one-off purchase followed by one-year maintenance contracts
 - ESRF license costs shared between the ESRF and EMBL Grenoble
 - Contact person: Erwin de Ley (erwin.de.ley@isencia.be)

The screenshot displays the BES Design Tool interface. At the top, the browser address bar shows the URL `mxhpc2-1705:8090/BES/bridge/app/`. The header includes the ESRF and EMBL logos, the text "BES 3.2.0", and navigation links for "Design", "Configuration", "Testing", "Support", and "Admin". The user name "Olof Svensson" is visible in the top right.

Below the header is a toolbar with buttons for "Commit", "Save", "Lock", "General", "Validate", "Flow", "Run", and "Customize". A dropdown menu is open, showing "ired Submodel MXPressDataCollection (2.1)" and "Original layout".

The main workspace is divided into two panes. On the left is the "Palette" containing various actors and submodels, including "Throttling Delay", "Error Observer", "Error Catcher", "Router", "Transform", "I/O", "Expert", "Cluster", "Events", "Monitoring", "Continuation", "ESRF actors", and "Shared Submodels". On the right is the "MXPressDataCollection" workflow diagram. The diagram shows a sequence of actors connected by arrows, representing a data collection process. Key actors include "Select aperture", "Do characterisation", "Prepare automatic characterisation and data collection", "CollectReferenceImages", "EDNAStrategy", "Check results", "New data collection", "Do data collect_2", "Only EDNA resolution", "Load mcCUBE queue", "Collection with", "Do data collect_1", "Retrieve flux from SPyB", "Prepare collect without strategy", "Load and execute mcCUBE queue", and "No data collection".

- **Advantages of using a workflow design tool:**
 - Modularity by design
 - Easy to get global overview – documentation “built in”
 - Easier discussions with non-programmers
 - Of course if “spaghetti”-like workflows avoided
- **Further advantages of using Passerelle EDM:**
 - Built-in revision handling of workflows
 - Workflow and actor execution details in database
- **Disadvantages:**
 - Proprietary software which needs an annual budget
 - Hence collaborations difficult

SCREENSHOTS BES – PASSERELLE EDM

The screenshot displays the BES 3.2.0 web interface. The top navigation bar includes 'Design', 'Configuration', 'Testing', 'Support', and 'Admin'. The user 'Olof Svensson' is logged in. The main content area shows a table of 'Beamline production workflows' with columns for Rev, Type, Name, Status, Last Updated By, Modify date, and Comment. The table lists various workflows such as 'BurnStrategy', 'Characterisation', 'CollectAndSpectra', etc., with their respective statuses and update dates.

Rev	Type	Name	Status	Last Updated By	Modify date	Comment
4.1	Flow	BurnStrategy	Done	MASTER	2015-01-28 10:21:39	message_text
2.1	Flow	Characterisation	Done	SVENSSON	2015-09-09 08:21:46	Changed status to "Done".
1.0	Flow	CollectAndSpectra	New	SVENSSON	2015-11-23 11:06:22	Added sampleInfo to do collect input
1.2	Flow	CreateLucidBackgroundImage	Done	SVENSSON	2015-09-09 08:21:59	Changed status to "Done".
3.1	Flow	CreateThumbnails	Done	SVENSSON	2015-09-09 08:22:12	Changed status to "Done".
2.3	Flow	Dehydration	Done	SVENSSON	2015-02-03 11:25:45	Renamed to Dehydration
1.7	Flow	EDNA_dp	Done	SVENSSON	2015-09-09 08:22:24	Changed status to "Done".
1.1	Flow	EDNA_proc	Done	SVENSSON	2016-05-03 09:44:18	Renamed from EDNA_dp
2.0	Flow	EDNA_proc_OAR	New	SVENSSON	2016-10-12 16:28:03	Added wait for first and last image
1.1	Flow	EnergyInterleavedMAD	Done	SVENSSON	2016-04-14 11:15:48	First version
3.1	Flow	EnhancedCharacterisation	Done	SVENSSON	2015-02-03 11:26:13	Renamed to EnhancedCharacterisation
2.2	Flow	HelicalCharacterisation	Done	SVENSSON	2015-12-03 14:05:43	Changed user input python script path
5.1	Flow	KappaReorientation	Done	MASTER	2015-01-28 10:22:32	message_text
2.1	Flow	LowDoseDC	In Progress	SVENSSON	2015-11-24 09:23:38	Renamed redo low dose DC input python script
6.0	Flow	MXPressA	Done	SVENSSON	2015-11-17 10:00:38	Removed stop actor.
1.1	Flow	MXPressA_aperture_100um	Done	SVENSSON	2015-12-01 14:17:48	First revision
1.1	Flow	MXPressA_aperture_10um	Done	SVENSSON	2015-12-01 14:18:14	First revision
1.1	Flow	MXPressA_aperture_15um	Done	SVENSSON	2015-12-01 14:18:43	First revision
1.1	Flow	MXPressA_aperture_30um	In Progress	SVENSSON	2015-12-01 14:11:58	First revision

BES EXECUTION LOG

Beamline Expert System x

mxhpc2-1705:8090/BES/bridge/app/

ESRF | EMBL | BES 3.2.0

Design Configuration Testing Support Admin

Olof Svensson

Requests
My settings

↑ ? CreateThumbNails 🔍 ⚙️

Reference: Id: Correlation Id:

Type: External Reference:

Initiator: bm14 id23eh1 id23eh2 id29 id30a1 id30a2 id30a3 id30b

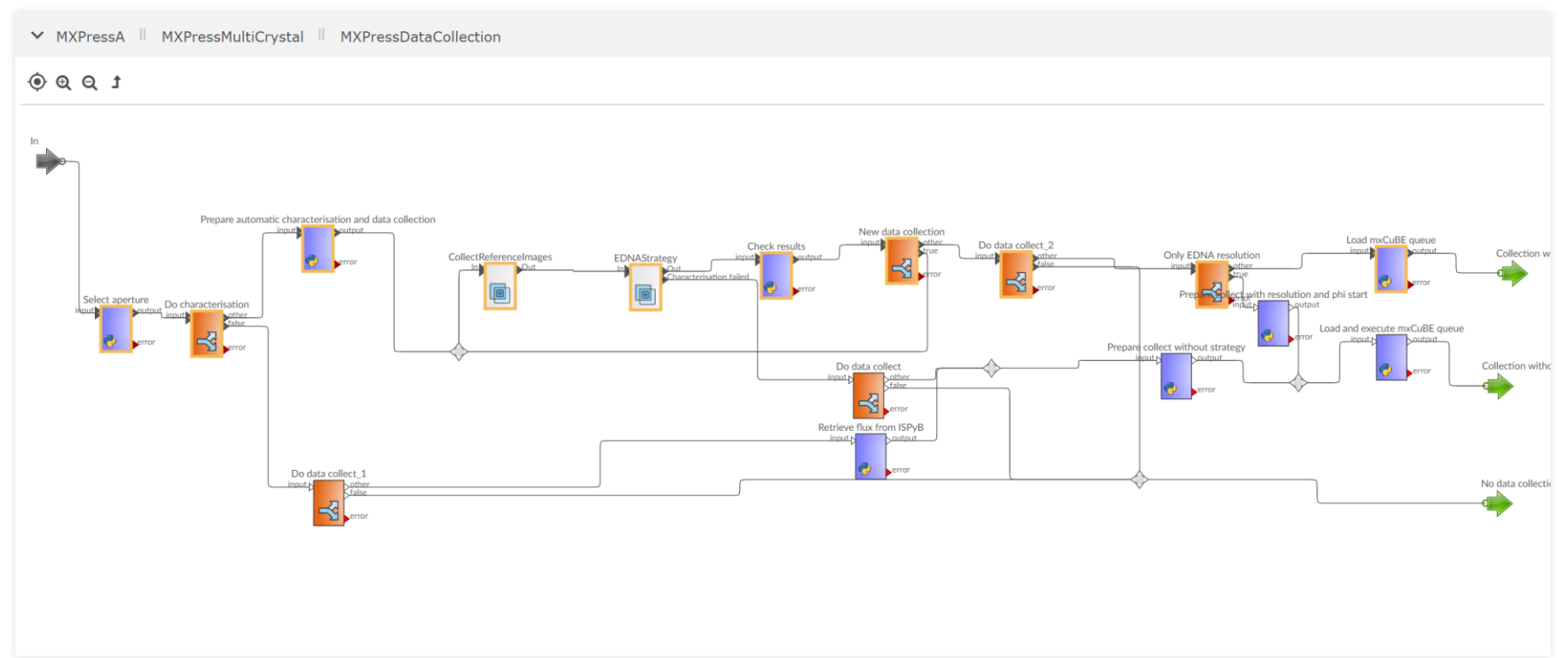
Status: Created Error Finished Cancelled Started Timeout

Creation Date: 2016-12-08 📅 00:00:00 ⏱ To 2016-12-09 📅 16:04:59 ⏱

🔍 View 📄 Export ⋮

⏪ < 1-200 of ? rows > ⏩ 200 🔄

<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Reference	Id	Type	Creation Date	Initiator	External Reference	Status	Duration(ms)	+
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	3841	4734310	EDNA_proc_OAR	2016-12-09 16:03:06	id23eh1	mx1777	Finished	200,355	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	3841	4734303	dozor_OAR	2016-12-09 16:03:04	id23eh1	mx1777	Finished	131,912	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	3841	4734302	XIA2_DIALS_OAR	2016-12-09 16:03:04	id23eh1	mx1777	Finished	3,707,707	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	3841	4734301	autoPROC_OAR	2016-12-09 16:03:04	id23eh1	mx1777	Finished	2,219,649	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	9070	4734179	MXPressA	2016-12-09 16:02:31	id30a1	fx57	Finished	1,010,921	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	4191	4734243	Characterisation	2016-12-09 16:01:47	id29	mx1833	Finished	26,202	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	4191	4734254	dozor_OAR	2016-12-09 16:01:22	id29	mx1833	Finished	49,588	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	4191	4733359	Characterisation	2016-12-09 15:57:41	id29	mx1833	Finished	33,214	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	4191	4733650	dozor_OAR	2016-12-09 15:57:14	id29	mx1833	Finished	46,688	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	3661	4734186	EDNA_proc_OAR	2016-12-09 15:56:50	id30a1	fx57	Finished	389,262	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	3661	4734181	XIA2_DIALS_OAR	2016-12-09 15:56:48	id30a1	fx57	Finished	661,905	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	3661	4734130	dozor_OAR	2016-12-09 15:56:48	id30a1	fx57	Finished	221,346	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	1523	4734147	EDNA_proc_OAR	2016-12-09 15:56:19	id30a2	mx415	Finished	52,785	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	1523	4734135	XIA2_DIALS_OAR	2016-12-09 15:56:17	id30a2	mx415	Finished	478,871	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	1523	4734134	autoPROC_OAR	2016-12-09 15:56:17	id30a2	mx415	Finished	568,424	
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	1523	4734141	XDSAPP_OAR	2016-12-09 15:56:17	id30a2	mx415	Finished	467,971	



BES – WORKFLOW EXECUTION LOG

Beamline Expert System

mxhpc2-1705:8090/BES/bridge/app/

ESRF | EMBL | BES 3.2.0

Design Configuration Testing Support Admin

Olof Svensson

Request details
Request (id= 4734179, type = MXPressA)

Reference: 9070
Id: 4734179
Type: MXPressA
Creation Date: 2016-12-09 16:02:31
Status: Finished
External Reference: fx57
Correlation Id:
Initiator: id30a1
Executor:

Name	Value	Data Type
collection_software	mxCuBE_-_2.0	STRING
directory	/data/visitor/fx57/id30a1/20161209/RAW_DATA/BIPDE1/BIPDE1-CD014403_H04-3_DI01318464	STRING
modelpath	MXPressA	STRING
prefix	BIPDE1-CD014403_H04-3_DI01318464	STRING
run_number	1	STRING
sample_lims_id	575403	STRING
sample_node_id	119	STRING

Task Result Item Event

Enter search string here

Id: Status: Created Error Finished Cancelled Started Timeout
Type: Discriminator: Initiator:

View 101 rows 400

Id	Creation Date	Duration(ms)	Status	Type	Initiator
4734180	2016-12-09 16:02:31	8	Finished	Start	actor:/MXPressA.Start
4734291	2016-12-09 16:02:31	632	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.Beamline%20setup
4734292	2016-12-09 16:02:32	576	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.Prepare%20MXPressA
4734293	2016-12-09 16:02:32	1850	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.CommonPrepareExperiment.Init%20workflow
4734294	2016-12-09 16:02:34	768	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.CommonPrepareExperiment.Read%20motor%20positions
4734295	2016-12-09 16:02:35	299	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.CommonPrepareExperiment.Default%20parameters
4734296	2016-12-09 16:02:35	2295	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.MXPressMultiCrystal.Interpretation%20of%20diffraction%20p
4734297	2016-12-09 16:02:37	315	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.MXPressMultiCrystal.Contact%20user%20if%20first%20acro

BES – ACTOR EXECUTION LOG

Beamline Expert System x

mxhpc2-1705:8090/BES/bridge/app/

ESRF | EMBL | BES 3.2.0

Design Configuration Testing Support Admin

Olof Svensson



Task details

Request (id= 4734179, type = MXPressA)

Id: 4734296
Creation Date: 2016-12-09 16:02:35
Status: Finished
Type: eu.esrf.services.python.v2.6
Initiator: actor:/MXPressA.MXPressMultiCrystal.Interpretation%20of%20diffraction%20plan
Executor:

1-2 of 10 rows 2

Name	Value	Data Type	+
beamline	id30a1	STRING	
Case ID	9070	STRING	

1-2 of 10 rows 2

- Resultitems
- Resultblocks
- Event
- Task

Enter search string here

Result Block Type: Name:

Value: Colour:

View 14 rows 30

Colour	Name	Value	Discriminator	+
▼	Resultblock [id=3809818, type=python]			
<input type="checkbox"/>	aimedCompleteness		NULL_RESULT	
<input type="checkbox"/>	aimedMultiplicity		NULL_RESULT	
<input type="checkbox"/>	anomalousData	false	STRING_RESULT	
<input type="checkbox"/>	dataCollectionGroupComment	Number of positions: 2.	STRING_RESULT	
<input type="checkbox"/>	do2DMeshOnly	false	STRING_RESULT	
<input type="checkbox"/>	doCharacterisation	true	STRING_RESULT	
<input type="checkbox"/>	doOnlyEDNAResolution	false	STRING_RESULT	
<input type="checkbox"/>	do_data_collect	true	STRING_RESULT	
<input type="checkbox"/>	findLargestMesh	false	STRING_RESULT	
<input type="checkbox"/>	minOscWidth		NULL_RESULT	

- Shipped with Passerelle EDM:

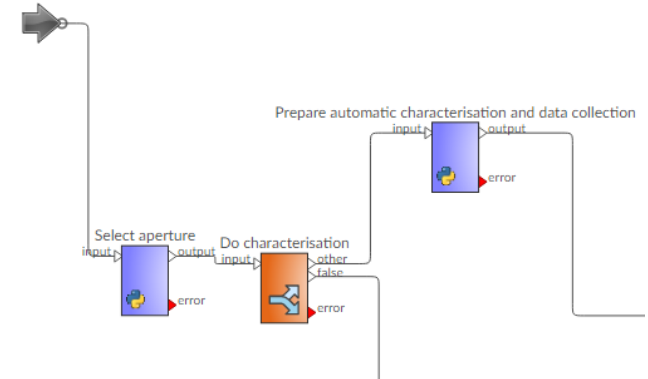
Enter search string here

Type: Day(Creation Day): 01/12/2016 To 07/12/2016

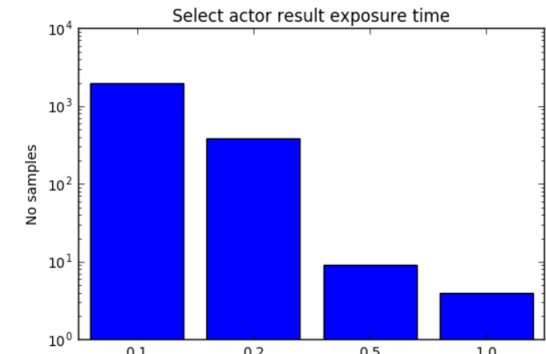
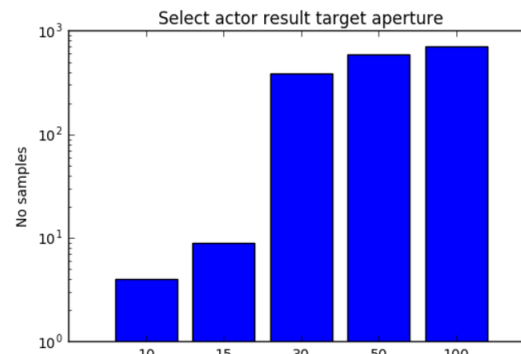
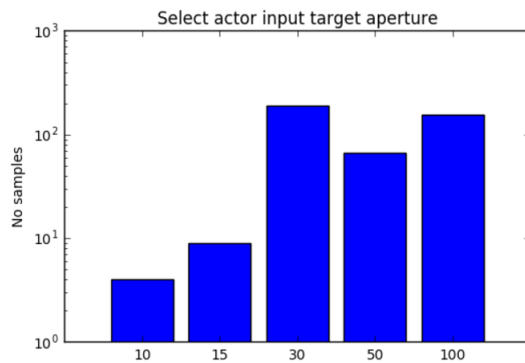
Initiator: bm14 id23eh1 id23eh2 id29 id30a1 id30a2 id30a3 id30b

71 rows

Creation Date/Day	dozor_OAR	autorPROC_OAR	Xray_Centring	XIA2_DIALS_OAR	XDSAPP_OAR	VisualReorientation	TroubleShooting	MeshScan	MeshAndCollect	MyPressA_aperture_30um	MyPressA	KappaReorientation	HelicalCharacterisation	EDNA_proc_OAR	CreateThumbnails	Characterisation	Sum
01/12/2016	303	113	1	139		2	91		29			139	2565	154		3,536	
02/12/2016	408	107	17	107		1	93		40	2	107	3371	300			4,553	
03/12/2016	253	127	18	140		2			94			140	2787	117		3,678	
04/12/2016	406	81	1	81				29	11			80	1974	325		2,988	
05/12/2016	580	108	2	108		10	1	28	9			108	1799	463		3,221	
06/12/2016	162	49		49	6			5				42	518	111		942	
07/12/2016	276	66	38	71		1	11		8	6	1	68	1821	203		2,570	
Sum	2,388	651	77	695	6	10	7	228	9	29	187	6	3	684	14,835	1,673	21,488



- Custom statistics with Python script accessing BES database:



WORKFLOW ERROR STATISTICS

^ ? Enter search string here Q

Type: Day(Creation Day): 10/12/2016 To 10/12/2016

Initiator: bm14 id23eh1 id23eh2 id29 id30a1 id30a2 id30a3 id30b

⋮ 9 rows

Type	Error	Finished	Started	Sum
dozor_OAR		35		35
autoPROC_OAR		24		24
XIA2_DIALS_OAR		35		35
MXPressA	4	34	1	39
EDNA_proc_OAR		35		35
CreateThumbnails	6	923		929
Sum	10	1,086	1	1,097

WORKFLOW TROUBLESHOOTING

Enter search string here 🔍

Reference: Id: Correlation Id:

Type: External Reference:

Initiator: bm14 id23eh1 id23eh2 id29 id30a1 id30a2 id30a3 id30b

Status: Created Error Finished Cancelled Started Timeout

Creation Date: 2016-12-10 08:00:00 To 2016-12-10 08:30:00

View Export

	Reference	Id	Type	Creation Date	Initiator	External Reference	Status	Duration(ms)	+
<input type="checkbox"/>	2832	4756048	CreateThumbnails	2016-12-10 08:29:50	id30a1	fx1	Finished	6,055	
<input type="checkbox"/>	2832	4756044	CreateThumbnails	2016-12-10 08:29:36	id30a1	fx1	Finished	6,913	
<input type="checkbox"/>	2832	4756020	CreateThumbnails	2016-12-10 08:28:56	id30a1	fx1	Finished	5,674	
<input type="checkbox"/>	2832	4756016	CreateThumbnails	2016-12-10 08:28:42	id30a1	fx1	Finished	6,801	
<input type="checkbox"/>	2832	4756012	CreateThumbnails	2016-12-10 08:28:08	id30a1	fx1	Finished	5,684	
<input type="checkbox"/>	2832	4756008	CreateThumbnails	2016-12-10 08:28:01	id30a1	fx1	Finished	7,557	
<input type="checkbox"/>	2832	4756003	CreateThumbnails	2016-12-10 08:27:44	id30a1	fx1	Finished	5,580	
<input type="checkbox"/>	2832	4755999	CreateThumbnails	2016-12-10 08:27:37	id30a1	fx1	Finished	6,588	
<input type="checkbox"/>	2832	4755995	CreateThumbnails	2016-12-10 08:27:22	id30a1	fx1	Finished	5,578	
<input type="checkbox"/>	2832	4755991	CreateThumbnails	2016-12-10 08:27:15	id30a1	fx1	Finished	6,844	
<input type="checkbox"/>	2832	4755987	CreateThumbnails	2016-12-10 08:26:59	id30a1	fx1	Finished	5,631	
<input type="checkbox"/>	2832	4755983	CreateThumbnails	2016-12-10 08:26:49	id30a1	fx1	Finished	8,640	
<input type="checkbox"/>	2832	4755979	CreateThumbnails	2016-12-10 08:26:32	id30a1	fx1	Finished	5,601	
<input type="checkbox"/>	2832	4755975	CreateThumbnails	2016-12-10 08:26:23	id30a1	fx1	Finished	9,346	
<input type="checkbox"/>	2832	4755971	CreateThumbnails	2016-12-10 08:26:06	id30a1	fx1	Finished	5,777	
<input type="checkbox"/>	2832	4755967	CreateThumbnails	2016-12-10 08:25:56	id30a1	fx1	Finished	8,553	
<input type="checkbox"/>	2832	4755963	CreateThumbnails	2016-12-10 08:25:39	id30a1	fx1	Finished	5,596	
<input type="checkbox"/>	2832	4755959	CreateThumbnails	2016-12-10 08:25:30	id30a1	fx1	Finished	9,293	
<input type="checkbox"/>	2832	4755954	CreateThumbnails	2016-12-10 08:25:15	id30a1	fx1	Finished	5,657	
<input type="checkbox"/>	2832	4755951	CreateThumbnails	2016-12-10 08:25:06	id30a1	fx1	Finished	9,592	
<input type="checkbox"/>	2832	4755947	CreateThumbnails	2016-12-10 08:24:49	id30a1	fx1	Finished	6,195	
<input type="checkbox"/>	2832	4755943	CreateThumbnails	2016-12-10 08:24:42	id30a1	fx1	Finished	6,608	
<input type="checkbox"/>	2832	4755938	CreateThumbnails	2016-12-10 08:24:25	id30a1	fx1	Finished	5,727	
<input type="checkbox"/>	2832	4755935	CreateThumbnails	2016-12-10 08:24:18	id30a1	fx1	Finished	7,336	
<input type="checkbox"/>	2832	4755931	CreateThumbnails	2016-12-10 08:24:00	id30a1	fx1	Finished	5,805	
<input type="checkbox"/>	2832	4755917	CreateThumbnails	2016-12-10 08:23:51	id30a1	fx1	Finished	7,809	
<input type="checkbox"/>	9100	4755877	MXPressA	2016-12-10 08:22:41	id30a1	fx1	Error	490,444	
<input type="checkbox"/>	2832	4755904	CreateThumbnails	2016-12-10 08:20:03	id30a1	fx1	Finished	6,632	
<input type="checkbox"/>	2832	4755890	CreateThumbnails	2016-12-10 08:18:28	id30a1	fx1	Finished	5,944	
<input type="checkbox"/>	2832	4755887	EDNA_proc_OAR	2016-12-10 08:18:28	id30a1	fx1	Finished	139,347	
<input type="checkbox"/>	2832	4755870	XIA2_DIALS_OAR	2016-12-10 08:18:26	id30a1	fx1	Finished	282,136	
<input type="checkbox"/>	2832	4755869	dozor_OAR	2016-12-10 08:18:26	id30a1	fx1	Finished	131,598	
<input type="checkbox"/>	2832	4755868	autoPROC_OAR	2016-12-10 08:18:26	id30a1	fx1	Finished	562,360	
<input type="checkbox"/>	2832	4755863	CreateThumbnails	2016-12-10 08:17:42	id30a1	fx1	Finished	6,305	
<input type="checkbox"/>	2832	4755849	CreateThumbnails	2016-12-10 08:17:37	id30a1	fx1	Finished	5,634	

External Reference:fx1	modelpath	MXPressA	STRING
Correlation Id:	prefix	AV147-D_679_1	STRING
Initiator:Id30a1	run_number	1	STRING
Executor:	sample_line_id	575875	STRING
	sample node id	136	STRING

Task Result Item Event

Enter search string here

Id: Status: Created Error Finished Cancelled Started Timeout

Type: Discriminator: Initiator:

Q View	Id	Creation Date	Duration(ms)	Status	Type	Initiator
<input type="checkbox"/>	4755878	2016-12-10 08:22:41	9	Finished	Start	actor:MXPressA.Start
<input type="checkbox"/>	4755879	2016-12-10 08:22:41	692	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.Beamline%20Setup
<input type="checkbox"/>	4755880	2016-12-10 08:22:42	586	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.Prepare%20MXPressA
<input type="checkbox"/>	4755921	2016-12-10 08:22:43	2904	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.CommonPrepareExperiment.Init%20workflow
<input type="checkbox"/>	4755922	2016-12-10 08:22:46	772	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.CommonPrepareExperiment.Read%20motor%20positions
<input type="checkbox"/>	4755923	2016-12-10 08:22:46	290	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.CommonPrepareExperiment.Default%20parameters
<input type="checkbox"/>	4755924	2016-12-10 08:22:47	1461	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.Interpretation%20of%20diffraction%20plan
<input type="checkbox"/>	4755925	2016-12-10 08:22:48	310	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.Contact%20user%20of%20first%20acronym%20collection
<input type="checkbox"/>	4755926	2016-12-10 08:22:48	40139	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.PrepareAutoMesh.Auto%20Mesh
<input type="checkbox"/>	4755927	2016-12-10 08:23:29	1434	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.PrepareAutoMesh.Get%20grid%20positions
<input type="checkbox"/>	4755928	2016-12-10 08:23:30	280245	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.ExecuteMesh2D.Collect%20and%20process%20data
<input type="checkbox"/>	4755929	2016-12-10 08:28:10	29	Finished	Check if meshPositionsAcquired	actor:MXPressA.MXPressMultiCrystal.ExecuteMesh2D.Check%20if%20meshPositionsAcquired
<input type="checkbox"/>	4755930	2016-12-10 08:28:10	2212	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.ExecuteMesh2D.Find%20best%20position
<input type="checkbox"/>	4756021	2016-12-10 08:28:12	43961	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.ExecuteMesh2D.ISP%20upload
<input type="checkbox"/>	4756022	2016-12-10 08:28:13	13924	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.ExecuteMesh2D.Send%20results%20to%20mxCuBE
<input type="checkbox"/>	4756023	2016-12-10 08:28:13	62	Finished	Check if signal	actor:MXPressA.MXPressMultiCrystal.ExecuteMesh2D.Check%20if%20signal
<input type="checkbox"/>	4756024	2016-12-10 08:28:13	338	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.ExecuteMesh2D.Extract%20best%20position
<input type="checkbox"/>	4756025	2016-12-10 08:28:13	25	Finished	Check if 2d mesh only	actor:MXPressA.MXPressMultiCrystal.Check%20if%202D%20mesh%20only
<input type="checkbox"/>	4756026	2016-12-10 08:28:13	7661	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.Move%20to%20new%20sample%20position
<input type="checkbox"/>	4756027	2016-12-10 08:28:21	594	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.Correct%20for%20old30a1%20phy
<input type="checkbox"/>	4756028	2016-12-10 08:28:21	28	Finished	Extra vertical scan	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.Extra%20vertical%20scan
<input type="checkbox"/>	4756029	2016-12-10 08:28:21	17	Finished	Check if center rotation axis	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.Check%20if%20center%20rotation%20axis
<input type="checkbox"/>	4756030	2016-12-10 08:28:21	1583	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.Prepare%20first%20time%20scan
<input type="checkbox"/>	4756031	2016-12-10 08:28:23	36506	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.Collect%20and%20process%20data
<input type="checkbox"/>	4756032	2016-12-10 08:29:00	27	Finished	Check if meshPositionsAcquired	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.Check%20if%20meshPositionsAcquired
<input type="checkbox"/>	4756033	2016-12-10 08:29:00	2611	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.Find%20best%20position
<input type="checkbox"/>	4756034	2016-12-10 08:29:02	47900	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.ISP%20upload
<input type="checkbox"/>	4756035	2016-12-10 08:29:02	17778	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.Send%20results%20to%20mxCuBE
<input type="checkbox"/>	4756036	2016-12-10 08:29:02	55	Finished	Check if signal	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.Check%20if%20signal
<input type="checkbox"/>	4756037	2016-12-10 08:29:02	383	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.Extract%20best%20position
<input type="checkbox"/>	4756038	2016-12-10 08:29:03	12415	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.Move%20Sample%20180%20degrees
<input type="checkbox"/>	4756039	2016-12-10 08:29:15	1679	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.Prepare%20second%20time%20scan
<input type="checkbox"/>	4756040	2016-12-10 08:29:17	36642	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.1.Collect%20and%20process%20data
<input type="checkbox"/>	4756051	2016-12-10 08:29:53	40	Finished	Check if meshPositionsAcquired	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.1.Check%20if%20meshPositionsAcquired
<input type="checkbox"/>	4756052	2016-12-10 08:29:54	2070	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.1.Find%20best%20position
<input type="checkbox"/>	4756053	2016-12-10 08:29:56	15513	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.1.ISP%20upload
<input type="checkbox"/>	4756054	2016-12-10 08:29:56	7929	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.1.Send%20results%20to%20mxCuBE
<input type="checkbox"/>	4756055	2016-12-10 08:29:56	31	Finished	Check if signal	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.1.Check%20if%20signal
<input type="checkbox"/>	4756056	2016-12-10 08:29:56	485	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.1.No%20diffraction%20signal%20error%20message
<input type="checkbox"/>	4756057	2016-12-10 08:29:56	31	Finished	Check if more positions to collect	actor:MXPressA.MXPressMultiCrystal.Check%20if%20more%20positions%20to%20collect
<input type="checkbox"/>	4756058	2016-12-10 08:29:56	6679	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.Move%20to%20next%20best%20position
<input type="checkbox"/>	4756059	2016-12-10 08:30:03	9326	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.Move%20to%20new%20sample%20position
<input type="checkbox"/>	4756060	2016-12-10 08:30:12	592	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.Correct%20for%20old30a1%20phy
<input type="checkbox"/>	4756071	2016-12-10 08:30:13	44	Finished	Extra vertical scan	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.Extra%20vertical%20scan
<input type="checkbox"/>	4756072	2016-12-10 08:30:13	17	Finished	Check if center rotation axis	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.Check%20if%20center%20rotation%20axis
<input type="checkbox"/>	4756073	2016-12-10 08:30:13	1508	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.Prepare%20first%20time%20scan
<input checked="" type="checkbox"/>	4756074	2016-12-10 08:30:14	34323	Error	eu.esrf.services.python.v2.6	actor:MXPressA.MXPressMultiCrystal.XrayCenteringVertical.CenterRotationAxis.ExecuteMesh1D.Collect%20and%20process%20data
<input type="checkbox"/>	4756075	2016-12-10 08:30:49	279	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.CommonErrorReporter.Log%20Error%20message
<input type="checkbox"/>	4756076	2016-12-10 08:30:49	1723	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.CommonErrorReporter.Set%20ISP%20status%20to%20failure.1
<input type="checkbox"/>	4756077	2016-12-10 08:30:51	749	Finished	eu.esrf.services.python.v2.6	actor:MXPressA.CommonErrorReporter.Display%20error%20message%20in%20mxCuBE

Id:4756074

Creation Date: 2016-12-10 08:30:14

Status: Error

Type: esrf.services.python.v2.6

Initiator: actor/MXPressA.MXPressMultiCrystal.XrayCentringVertical.CenterRotationAxis.ExecuteMesh1D.Collect%20and%20process%20data

Executor:

Name	Value
beamline	id30a1
Case ID	9100
Creator	.MXPressA@snp4755877.MXPressMultiCrystal.XrayCentringVertical.CenterRotationAxis.ExecuteMesh1D.Collect and process data
dataCollectionGroupComment	
directory	/data/visitor/xf1/id30a1/20161210/RAW DATA/AV147/AV147-D 679 1/MXPressA 01
expTypePrefix	line
firstImagePath	/data/visitor/xf1/id30a1/20161210/RAW DATA/AV147/AV147-D 679 1/MXPressA 01/line-AV147-D 679 1 3 0001.cbf
grid info	{'x1': 0.0, 'y1': -0.300, 'dx mm': 0.1, 'dy mm': 0.600, 'steps x': 1, 'steps y': 60, 'angle': 0.0}
meshPositionFile	/data/visitor/xf1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244/meshPositionsAxisCentring fu0vM.json
meshQueueListFile	/data/visitor/xf1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244/meshQueueListFileAxisCentring sHM9w.json
meshZigZag	false
motorPositions	{'sampx':-0.5485013623978202,'pshy':-0.377,'zomm':2.0,'chi':0.0,'pshz':0.37275833333333336,'kappa_ph':null,'kappa':null,'Focus':-0.6,'r':-0.075,'Y':-0.178,'phi':60.0,'sampy':0.016893732970027248}
prefix	AV147-D 679 1
pyarch_html_dir	/data/pyarch/id30a1/xf1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244/html
raw_directory	/data/visitor/xf1/id30a1/20161210/RAW DATA/AV147/AV147-D 679 1
Request ID	4755877
resolution	2.0
Result type	
run_number	2
sampleInfo	{'cellBeta':0.0,'nodeId':136,'lmsId':575875,'cellC':0.0,'numberOfPositions':2,'cellB':0.0,'experimentKind':'Default','crystalSpaceGroup':'Undefined','cellAlpha':0.0,'groupNodeId':346,'cellGamma':0.0,'cellA':0.0}
script_asset	
script_path	execute_mesh_startDataCollection.py
suffix	cbf
useFastMesh	false
workflowParameters	{'index':1,'stackTraceFile':/data/visitor/xf1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244/stackTrace tv c5', 'workflowWorkingDir':/data/visitor/xf1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244, 'logFile':/data/visitor/xf1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244/workflow_log.txt, 'copy': id'534398, 'type':MXPressA, 'pyarchLogFile':/data/pyarch/id30a1/xf1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244/workflow_log.txt, 'isSimulator':false, 'debugLogFile':/data/visitor/xf1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244/workflow_debug_log.txt, 'pyarch_html_dir':/data/pyarch/id30a1/xf1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244/html, 'workflowPyarchLogFile':/data/pyarch/id30a1/xf1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244/workflow_log.txt, 'title':MXPressA X-centre, 'eDNA + dc on id30a1', 'workflowLogFile':/data/visitor/xf1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244/workflow_log.txt, 'workingDir':/data/visitor/xf1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D 679 1/MXPressA 01/Workflow 20161210-082244}
workflow_id	63498

Result items Result blocks Event Task

Creation Date	Topic	Message
2016-12-10 08:30:14	CREATED	
2016-12-10 08:30:14	STARTED	
2016-12-10 08:30:14	ADD ATTRIBUTE	raw_directory
2016-12-10 08:30:14	ADD ATTRIBUTE	meshZigZag
2016-12-10 08:30:14	ADD ATTRIBUTE	resolution
2016-12-10 08:30:14	ADD ATTRIBUTE	pyarch_html_dir
2016-12-10 08:30:14	ADD ATTRIBUTE	run_number
2016-12-10 08:30:14	ADD ATTRIBUTE	workflow_id
2016-12-10 08:30:14	ADD ATTRIBUTE	sampleInfo
2016-12-10 08:30:14	ADD ATTRIBUTE	meshQueueListFile
2016-12-10 08:30:14	ADD ATTRIBUTE	grid_info
2016-12-10 08:30:14	ADD ATTRIBUTE	useFastMesh
2016-12-10 08:30:14	ADD ATTRIBUTE	meshPositionFile
2016-12-10 08:30:14	ADD ATTRIBUTE	firstImagePath
2016-12-10 08:30:14	ADD ATTRIBUTE	motorPositions
2016-12-10 08:30:14	ADD ATTRIBUTE	suffix
2016-12-10 08:30:14	ADD ATTRIBUTE	beamline
2016-12-10 08:30:14	ADD ATTRIBUTE	expTypePrefix
2016-12-10 08:30:14	ADD ATTRIBUTE	workflowParameters
2016-12-10 08:30:14	ADD ATTRIBUTE	dataCollectionGroupComment
2016-12-10 08:30:14	ADD ATTRIBUTE	directory
2016-12-10 08:30:14	ADD ATTRIBUTE	prefix
2016-12-10 08:30:14	com.isencia.passerfile.edm.request.service.ServiceException: TASK_ERROR - ERROR - [PASS_FUNC-5000] - Task processing error - Error from python script Traceback (most recent call last): File "/usr/local/SES/id30a1/workflow/pythonservices/scisoftpy/python/pyrpc.py", line 86, in xmrpcHandler.common ret = handler(*unflattened) File "/usr/local/SES/id30a1/workflow/pythonservices/python_service_runscript.py", line 77, in runScript result = vars(funcName)(*inputs)	

- **Start of workflows:**

- Hardware object “EdnaWorkflow”
- Corresponding XML file “ednaparameters.xml” contains host/port of BES and list of available workflows:

```
<object class = "EdnaWorkflow" role = "workflow">
  <bes_host>mxhpc2-1705</bes_host>
  <bes_port>38180</bes_port>
  <object href="/session" role="session"/>
  <workflow>
    <title>MXPressA</title>
    <path>MXPressA</path>
  </workflow>
  <workflow>
    <title>MXPressE</title>
    <path>MXPressE</path>
  </workflow>
  ...
</object>
```

- **Call-back from Workflows to mxCuBE:**

- Handled by the XMLRPCServer hardware object
- Almost all methods used (start_queue, log_message, shape_history_get_grid, open_dialog, workflow_end etc)

• Interface to mxCuBE v2:

The screenshot displays the mxCuBE v2 interface. On the left, a 'Workflow type' list includes options like 'MXPressA', 'X-ray Centring', 'Mesh Scan', and 'Dehydration' (which is selected). An 'Add to queue' button is at the bottom. A blue arrow points from this list to a 'Sample list' panel on the right. This panel shows 'Mode: Manually mounted' and 'Centring: Semi Automatic'. Below, a tree view shows 'manually-mounted' expanded to 'X-ray Centring - 1' and 'Workflow task - 0'. A second blue arrow points down to a configuration dialog box. This dialog has fields for 'Diffraction signal detection' (set to 'Dozor (macro-molecules)'), 'Use 'Mesh Best' for best position' (set to 'false'), 'Exposure time' (0.1), 'Total oscillation range' (1.0), and 'Transmission' (50.0). A 'Continue' button is at the bottom.

• Interface to mxCuBE v3:

- Better integrated, context driven
- Improved dialogs

MXCUBE WORKFLOW RESULT

mxCuBE (mx-415) (on ub1004)

File Instrumentation Help Expert mode

Collect | XRF spectrum | System | Feedback | Chat

User: mx-415 Group: Set Logout

Sample list

Mode: Manually mounted Show SC-details

Centring: Semi Automatic Synch ISPyB

- manually-mounted
 - X-ray Centring - 1
 - Workflow task - 0
 - XrayCentering - 1
 - mesh-t1_1 Collection done
 - mesh-t1_1 Collection done
 - mesh-t1_1 Collection done
 - mesh-t1_1 Collection done
 - line-t1_2 Collection done

Results

Sample centring | Data collection

Diffraction signal

Grid size

Machine current: -1.0 mA (unknown) 00:00

Flux: ? ph/s

Energy:

Wavelength:

Resolution:

Current:

Move to:

Transmission

Current:

Set to:

Current users

Selecting gives control

Allow timeout control

My name:

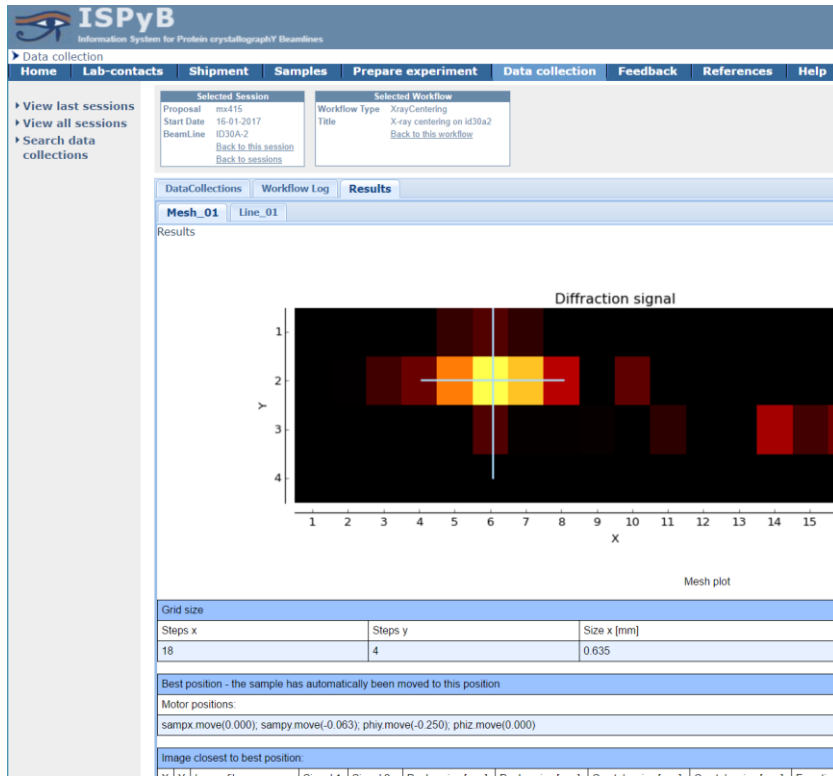
[2017-01-16 09:42:09] Workflow: Sending email

[2017-01-16 09:42:09] Workflow: Storing workflow mesh

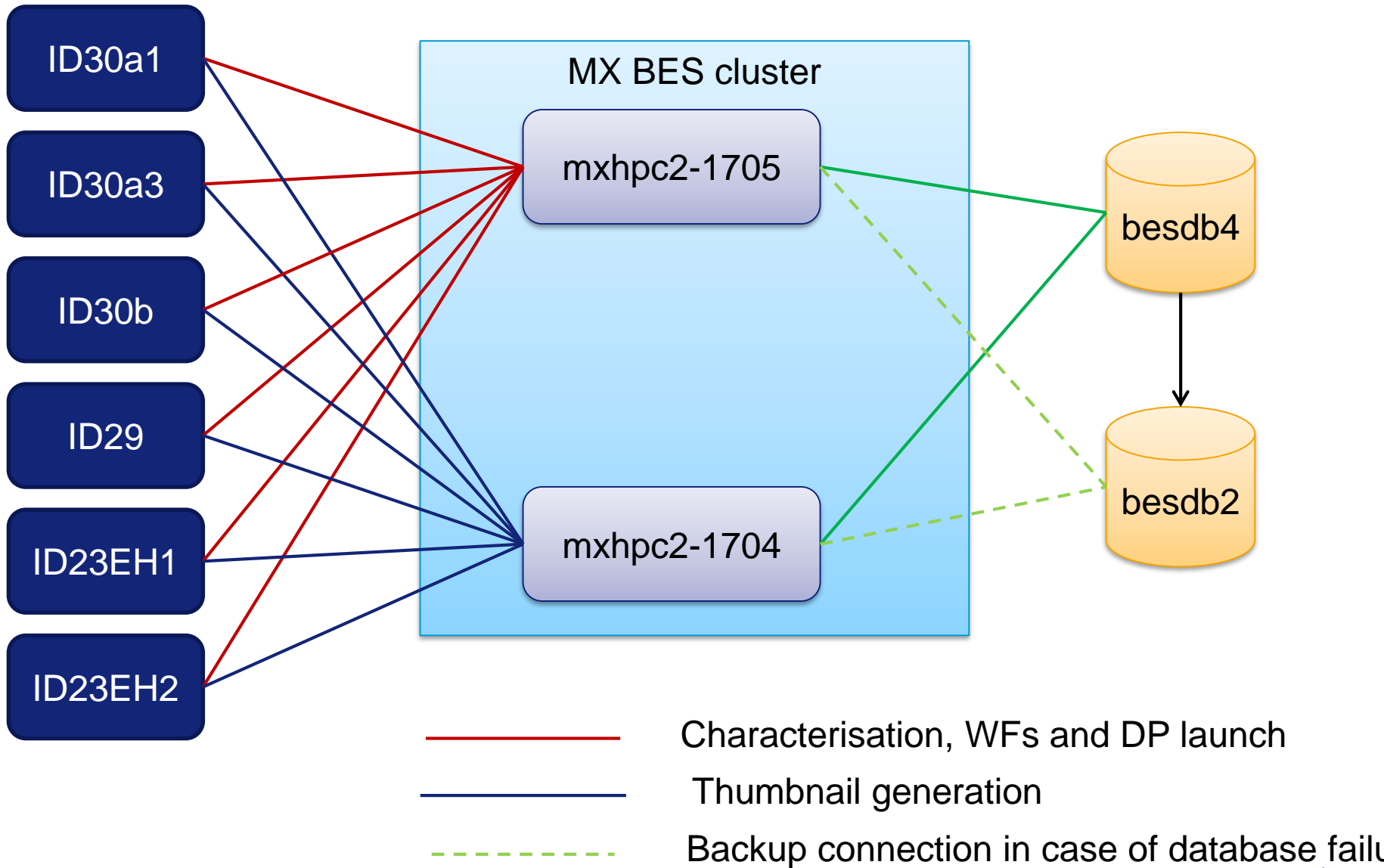
[2017-01-16 09:42:10] Workflow: ISPyB uploading finished.

INTERFACE TO ISPYB

- Same type of web services as mxCuBE for retrieving and uploading data
- (Old) ISPyB GUI and (new) EXI result pages:



CURRENT BES INSTALLATION



- David von Stetten, Max Nanao, Sasha Popov, Daniele de Sanctis, Stéphanie Monaco, Didier Nurizzo, Matias Guijarro, Solange Delagenière, Alejandro de Maria, Marcus Oskarsson (ESRF)
- Matthew Bowler (EMBL Grenoble)
- Erwin de Ley and Koen Heunick (Isencia, Belgium)
- The ESRF Data Analysis Unit, Beamline Control Unit and Structural Biology group

Further reading:

- **Fully automatic characterization and data collection from crystals of biological macromolecules**, Svensson, O., Malbet-Monaco, S., Popov, A., Nurizzo, D., & Bowler, M. W. (2015). *Acta Crystallographica Section D: Biological Crystallography*, 71(Pt 8), 1757–1767. <http://doi.org/10.1107/S1399004715011918>
- **MeshAndCollect: an automated multi-crystal data-collection workflow for synchrotron macromolecular crystallography beamlines**, Ulrich Zander · Gleb Bourenkov · Alexander N Popov · Daniele De Sanctis · Olof Svensson · Andrew A Mccarthy · Ekaterina Round · Valentin Gordeliy · Christoph Mueller-Dieckmann · Gordon A Leonard, *ACTA CRYSTALLOGRAPHICA SECTION D BIOLOGICAL CRYSTALLOGRAPHY* 71(11):2328-2343 · NOVEMBER 2015
- **Facilitating best practices in collecting anomalous scattering data for de novo structure solution at the ESRF Structural Biology Beamlines**, Daniele de Sanctis · Marcus Oscarsson · Alexander Popov · Olof Svensson · Gordon Leonard, *Acta Cryst.* (2016). D72, 413-420
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