Recent ISPyB Developments
@ESRF

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ESRF
Triestre 12/09/2018

MX

Shipments

Information | Transport history

Name	mx2082	Date	10-09-2018	Send shipment to the facility	Comments: Edit
Beamline	ID30A-3	Status	sent to User		

According to the A-form, you are allowed to have **2 parcels reimbursed by the ESRF**. Please use the Reimburse button to select/unselect the parcels to be reimbursed.

From	[redacted]	Courier company	[redacted]	Allowed Reimb. parcels	2
Return address	[redacted]	Billing Reference	[redacted]	Fedex Reference	MX-2082/ID30A-3/10-09-2018

Content (1 Parcels (1 reimbursed selected out of 2 allowed.) - 96 Samples - 38 Measured) Add Parcel | Import from CSV | Export PDF View

Content | Statistics

#1

Name:	ESRF0316001 (R)
Status:	sent to User
Location:	ID30A-3

Add container
Edit
Reimburse
Print labels

Shipments

Add a new field in BLSession table to handle nb of reimbursed dewars #21

Closed **delageniere** opened this issue on Feb 1 · 3 comments

delageniere commented on Feb 1 — Collaborator

At ESRF we are asked to track in ISPyB the number of reimbursed dewars authorized in the User Portal software.
Therefore we will need an extra field in BLSession table:
nbReimbursedDewars

This number will be defined in the User Portal according to the type of experiment, to the nb of reimbursed users and to a maximum possible. This number is linked to a session and can change between 2 sessions of the same proposal (currently between 0 and 4).

Shipments

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ISPyB Data Modeling

Retrieve the nb of reimbursed dewars from User Portal software and use it at the shipment/labels step. #230

Closed **delageniere** opened this issue on Feb 1 · 0 comments

delageniere commented on Feb 1 — Collaborator

This is linked to ispyb/ispyb-database-modeling/issues/21.
A dedicated fedex account is created at ESRF to be used by some users to send their dewars and to be paid by ESRF. The number of dewars/boxes is limited and is attached to the session info.

A special warning shall be displayed to users explaining if they use this account outside the number of authorized dewars, they would no more benefit from ESRF reimbursement for their sessions.

ISPyB

CSV Upload

Browse...

Do you need help? Click here. Examples can be found here: example.csv

Parcel Name should be unique for the whole shipment

Accepted values for container type are: SPINEpuck, Unipuck

Container name should be unique for this shipment

Protein + sample name should be unique for the whole proposal

Parcel Name	Container Name	Container Type	#	Protein Acronym	Sample Name	Pin Barcode	Space group	a	b	c	α	β	γ	Exp. Type	Aimed Resolution	Required Resolution	Beam Diameter	Number of positions	Aimed Multiplicity	Aimed Completeness	Forced SPG	

CSV Upload

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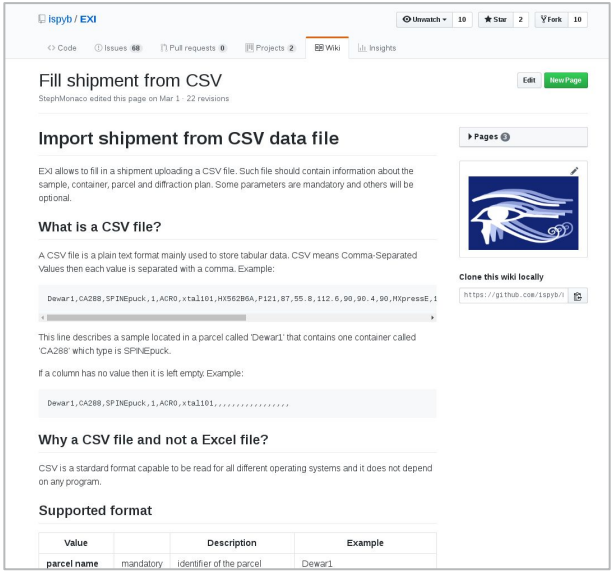
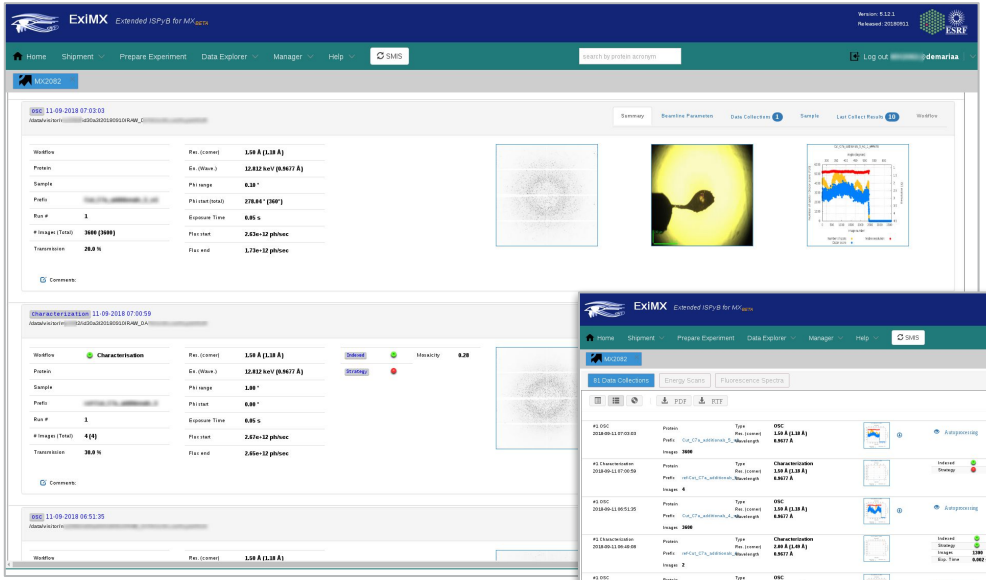
Parcel Name should be unique for the whole shipment | Accepted values for container type are: SPINEpuck, Unipuck | Container name should be unique for this shipment | Protein + sample name should be unique for the whole proposal

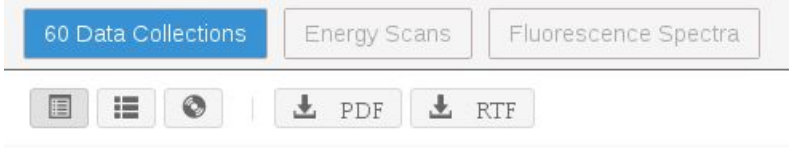
Parcel Name	Container Name	Container Type	#	Protein Acronym	Sample Name	Pin Barcode	Space group	a	b	c	α	β	γ	Exp. Type	Aimed Resolution	Required Resolution	Beam Diameter	Number of positions	Aimed Multiplicity	Aimed Completeness	Forced SPG

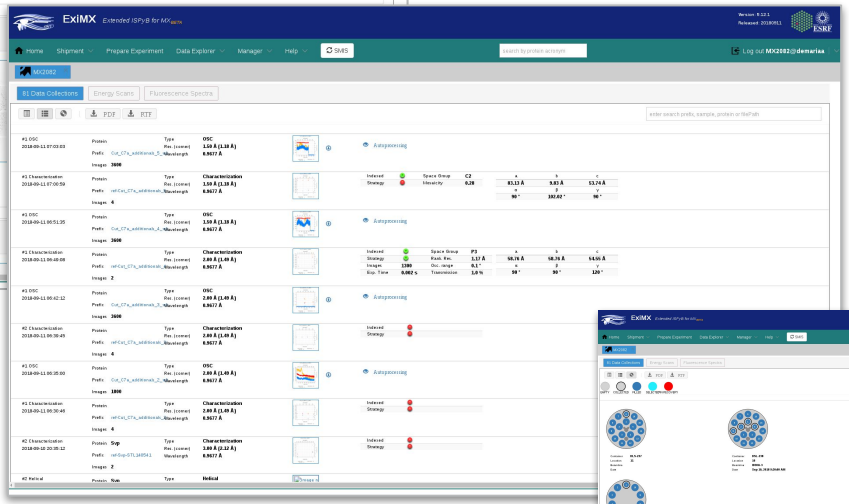


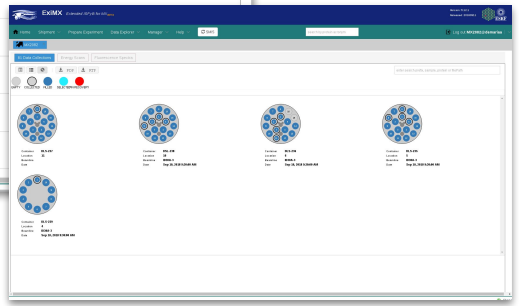
https://github.com/ispyb/EXI/wiki/Fill-shipment-from-CSV

Session view and Protein and crystals view









Session vs Protein view

therm Collected last time on Jul 20, 2016 4:26:36 PM

bsec_therm

Data Collections	
Energy Scans	
XRF	2
Samples	30
Tests (< 4 images)	28
Data Collections	160

Sessions (3)	
ID30A-1	14-11-2014
ID29	13-06-2016
ID30B	20-07-2016

Automatic SAD appears to have worked	
Space Group	P212121

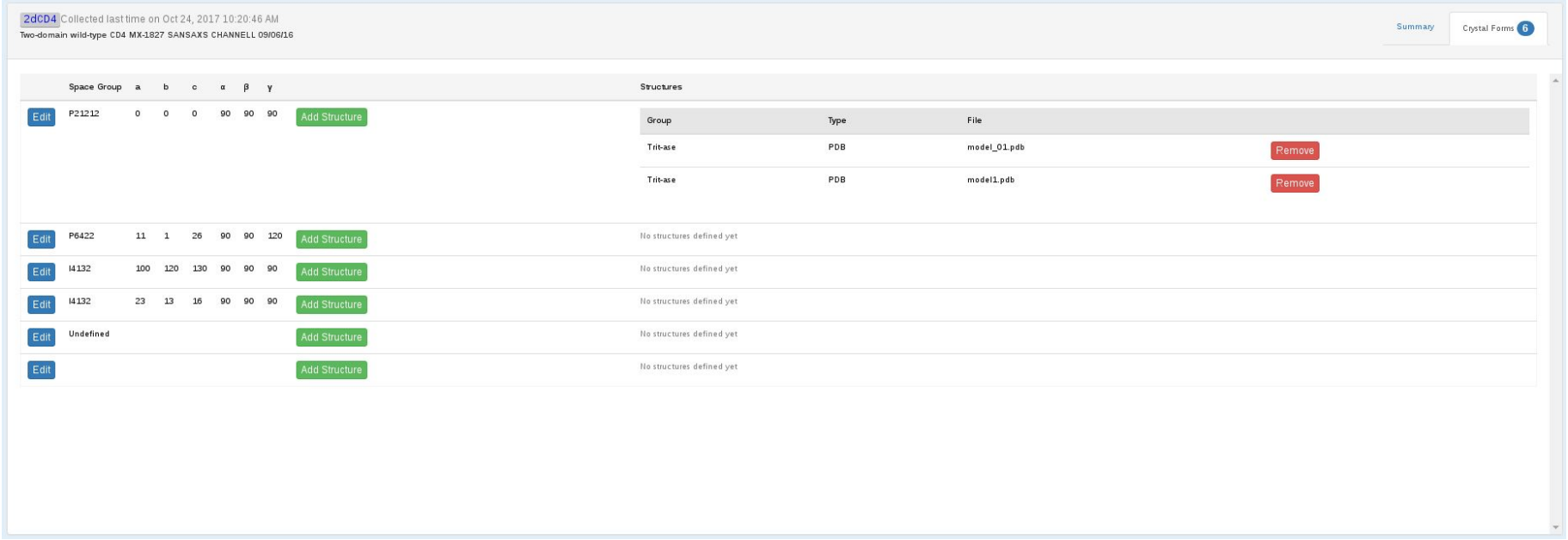
TIM Collected last time on May 19, 2008 5:07:17 PM

Triosephosphate isomerase

Data Collections	
Energy Scans	
XRF	
Samples	10
Tests (< 4 images)	20
Data Collections	1

Sessions (2)	
ID14-1	21-04-2008
ID14-1	19-05-2008

Ligands and PDBs



Ligands and PDBs

Adding fields for anisotropic diffraction data #29

Open **rhfogh** opened this issue on Jun 4 · 0 comments

rhfogh commented on Jun 4 • edited

Justification

The STARANISO program is providing a new approach to describing diffraction limits of reflection data, taking anisotropy into account. Apart from the general approach to anisotropy it also gives a simplified description of this anisotropy via an ellipsoid fitted to the anisotropic cut-off surface which in turn can be used to calculate well-known statistical data merging descriptors.

These data are not autoPROC-specific. Diffraction anisotropy is a general phenomenon, which by its nature makes traditional statistics like resolution and completeness difficult to apply consistently without modification, once diffraction anisotropy is present and accounted for. In order to consider these effects appropriately, and to make the data accessible to all programs that (will) wish to take them into account, the anisotropy-derived values for resolution and completeness should be stored in ISPyB as general data, and not quarantined to summary files or program-specific tables.

AutoProcScalingStatistics

Field	Type	Null	Default
completenessSpherical	float	YES	NULL
completenessEllipsoidal	float	YES	NULL
anomalousCompletenessSpherical	float	YES	NULL
anomalousCompletenessEllipsoidal	float	YES	NULL

AutoProcScaling

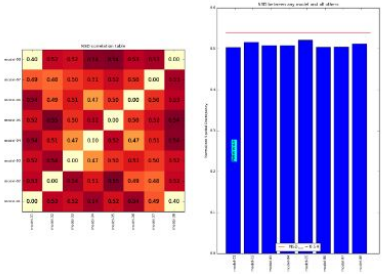
Field	Type	Null	Default
resolutionEllipsoidAxis11	float	YES	NULL
resolutionEllipsoidAxis12	float	YES	NULL
resolutionEllipsoidAxis13	float	YES	NULL
resolutionEllipsoidAxis21	float	YES	NULL
resolutionEllipsoidAxis22	float	YES	NULL
resolutionEllipsoidAxis23	float	YES	NULL
resolutionEllipsoidAxis31	float	YES	NULL
resolutionEllipsoidAxis32	float	YES	NULL
resolutionEllipsoidAxis33	float	YES	NULL
resolutionEllipsoidValue1	float	YES	NULL
resolutionEllipsoidValue2	float	YES	NULL
resolutionEllipsoidValue3	float	YES	NULL

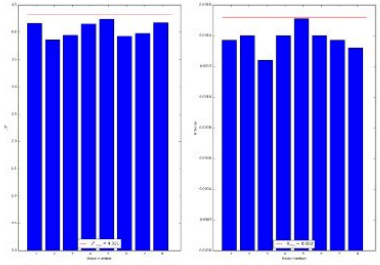
Ligands and PDBs

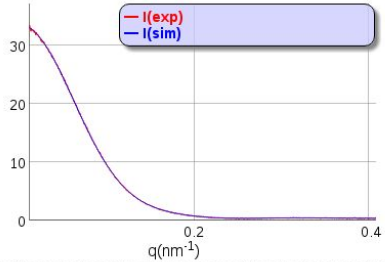
	Pipeline	SpaceGroup	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	Shell	Resolution (Å)	Multiplicity	Completeness %	<I/Sigma>	Rmeas	Rmerge	Rpim	cc(1/2)	ccAno	sigAno	ISA	Download	
BEST	XDSAPP	P 61	91.1	91.1	115.8	90.0	90.0	120.0	Overall	9.5-2.1	20.9	99.7	11.1		18.0			-5	0.713	9.41		
									Inner	100.0-9.5	20.2	99.5	39.1		8.8			-36	0.593			
									Outer	2.2-2.1	18.8	96.2	0.6		607.4			-2	0.614			
	XIA2_DIALS	P 1 21 1	90.1	114.6	90.3	90.0	119.8	90.0	Overall	64.6-2.1	7.1	98.9	6.6		16.0		100					
									Inner	64.6-5.8	7.2	100.0	16.7		6.2		100					
									Outer	2.2-2.1	7.3	94.6	1.1		180.8		50					
	grenades_parallelproc	P 1	89.9	90.1	114.4	90.0	90.1	120.0	Overall	100.0-2.4	3.8	91.9	8.5		10.4							
									Inner	100.0-10.7	3.4	96.1	23.7		5.0							
									Outer	2.5-2.4	3.3	88.7	1.1		116.8							
rMerge > 10	autoPROC_staraniso	P 61	90.9	90.9	115.5	90.0	90.0	120.0	Overall	65.0-2.3	20.8	92.9	12.5		18.7		100					
									Inner	65.0-6.6	21.6	100.0	34.7		10.6		100					
									Outer	2.4-2.3	22.9	49.8	1.4		273.9		50					
rMerge > 10	autoPROC	P 61	90.9	90.9	115.5	90.0	90.0	120.0	Overall	65.0-2.6	20.5	100.0	15.2		16.2		100					
									Inner	65.0-7.0	21.4	100.0	35.4		10.7		100					
									Outer	2.6-2.6	21.3	100.0	2.3		163.8		80					

BIOSAXS

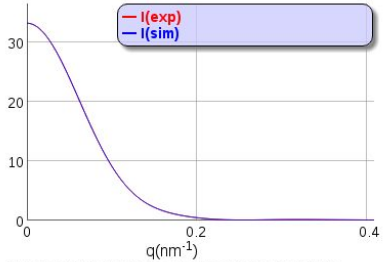
Ab Initio Modeling display



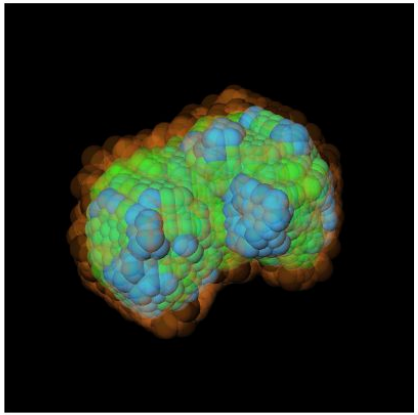




Fit of the simulated scattering curve versus a smoothed experimental data (spline interpolation)

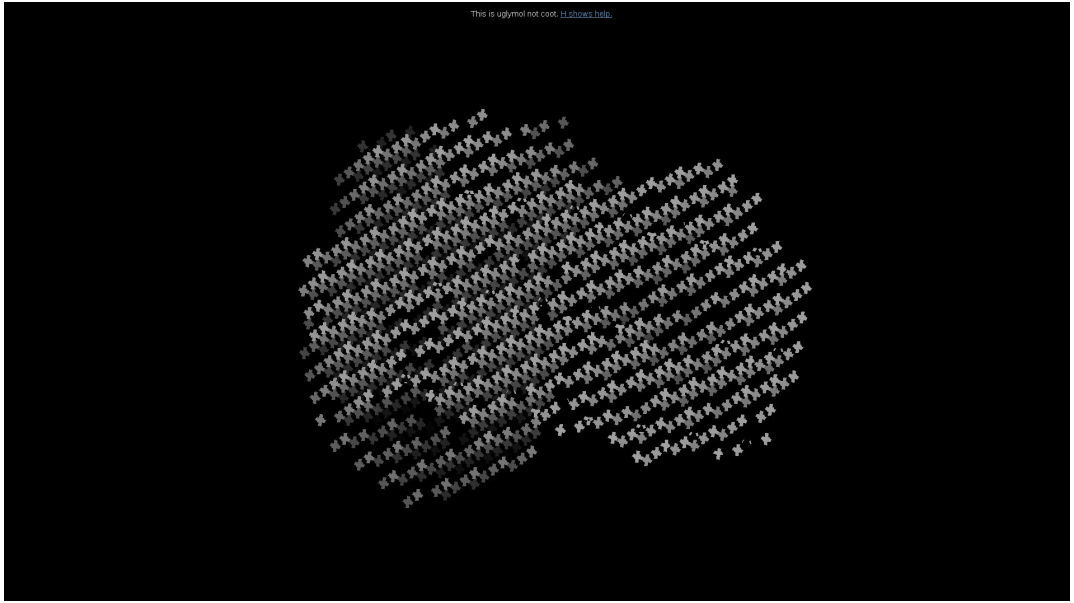


Fit of the simulated scattering curve versus the experimental data.



Type	chiSqrt	rFactor	Rg	PDB	Fir	Log
Reference				damaver		
Refined	0.827	0.001	19.700	dammin	dammin	dammin
Model	4.162	0.001	19.628	model_00	model_00	model_00
Model	3.924	0.001	19.632	model_06	model_06	model_06
Model	4.152	0.001	19.639	model_04	model_04	model_04
Model	4.241	0.002	19.631	model_01	model_01	model_01
Model	4.173	0.001	19.632	model_07	model_07	model_07
Model	3.979	0.001	19.632	model_05	model_05	model_05
Model	3.945	0.001	19.636	model_03	model_03	model_03
Model	3.860	0.001	19.636	model_02	model_02	model_02

Ab Initio Modeling display



Cryo-EM

Session stats

Thanks

- **Scientists**
  Stephanie Malbet-Monaco
  Martha Brennich
  EMBL, ESRF, ATF, scientists

- **Developers**
  Olof Svensson
  Solange Delageniere

- **Sys admin**
  Emmanuel Eyer
  Antoine Roux

- **ISPyB collaboration**