

Recent ISPyB Developments

@ESRF

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ESRF
Trieste 12/09/2018

MX

Shipments

[Information](#)[Transport history](#)

Name **mx2082**

Date **10-09-2018**

Beamline **ID30A-3**

Status **sent to User**



Send shipment to the facility

Comments:

Edit

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 **ESRF - France**

Courier company **colissimo**

Allowed Reimb. parcels

2

Return address **ESRF - France**

Billing Reference **colissimo**

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**



DLS-237



DSL-238



DLS-236



DLS-235



DLS-239

Add container

Edit

Reimburse

Print labels

Shipments

Content (1 Parcels (1 reimbursed selected out of 2 allowed.) - 96 Samples - 38 Measured)

+ Add Parcel

Import from CSV

Export PDF View

#1

Name: ESRF0316001 (R)

Status: sent to User

Location: ID30A-3



DLS-237



DSL-238



DLS-236



DLS-235



DLS-239

+ Add container

Edit

Reimburse

Print labels

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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+ Add Parcel

Import from CSV

Export PDF View

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Name: ESRF0316001 (R)
Status: sent to User
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DLS-237



DSL-238



DLS-236



DLS-235



DLS-239

+ Add container

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Print labels

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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

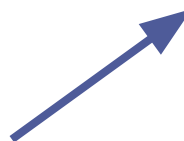
Collaborator

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	I
⊗		⊗ ⊗		⊗	⊗		▼							▼							▼	S

CSV Upload

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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-CS>

V

ispyb/ EXI

Unwatch 10Star 2Fork 10

CodeIssuesPull requestsProjectsWikiInsights

Fill shipment from CSV

StephMonaco edited this page on Mar 1, 22 revisions

Import shipment from CSV data file

Pages

EXI allows to fill in a shipment uploading a CSV file. Such file should contain information about the sample, container, parcel and diffraction plan. Some parameters are mandatory and others will be optional.

What is a CSV file?

A CSV file is a plain text format mainly used to store tabular data. CSV means Comma-Separated Values then each value is separated with a comma. Example:

Devar1,CA288,SPINepuck,1,ACR0,xta1101,HX56286A,P121,87,55,8,112,6,90,90,4,90,HXpressE,1

This line describes a sample located in a parcel called 'Devar1' that contains one container called 'CA288' which type is SPINepuck.

If a column has no value then it is left empty. Example:

Devar1,CA288,SPINepuck,1,ACR0,xta1101,.....

Why a CSV file and not a Excel file?

CSV is a standard format capable to be read for all different operating systems and it does not depend on any program.

Supported format

Value	Description	Example
parcel name	mandatory identifier of the parcel	Devar1

Session view and Protein and crystals view

The screenshot displays the 'Session view' of the ExiMX software. The interface includes a top navigation bar with 'Home', 'Shipment', 'Prepare Experiment', 'Data Explorer', 'Manager', and 'Help'. A search bar is present, and a 'Log out' button is visible. The main content area is divided into a left sidebar with a 'MODES' dropdown and a central panel. The central panel shows a summary of the experiment, including a table of parameters and three visualizations: a diffraction pattern, a fluorescence image, and a fluorescence spectrum. The table lists parameters such as Wavelength, Power, Sample, Path, Exposure Time, Fluorescence, and Fluorescence. The bottom section shows a list of experiments with columns for 'Wavelength', 'Power', 'Exposure Time', 'Fluorescence', and 'Intensity'.

Parameter	Value
Wavelength	1.58 Å (1.58 Å)
Power	12.812 keV (0.477 Å)
Sample	0.18"
Path	0.18"
Exposure Time	0.05 s
Fluorescence	2.55e-12 phos
Fluorescence	1.75e-12 phos

The screenshot displays the 'Protein and crystals view' of the ExiMX software. The interface includes a top navigation bar with 'Home', 'Shipment', 'Prepare Experiment', 'Data Explorer', 'Manager', and 'Help'. A search bar is present, and a 'Log out' button is visible. The main content area is divided into a left sidebar with a 'MODES' dropdown and a central panel. The central panel shows a summary of the experiment, including a table of parameters and three visualizations: a diffraction pattern, a fluorescence image, and a fluorescence spectrum. The table lists parameters such as Wavelength, Power, Sample, Path, Exposure Time, Fluorescence, and Fluorescence. The bottom section shows a list of experiments with columns for 'Wavelength', 'Power', 'Exposure Time', 'Fluorescence', and 'Intensity'.

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Exposure Time	0.05 s
Fluorescence	2.55e-12 phos
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The screenshot displays the 'Data Explorer' view of the ExiMX software. The interface includes a top navigation bar with 'Home', 'Shipment', 'Prepare Experiment', 'Data Explorer', 'Manager', and 'Help'. A search bar is present, and a 'Log out' button is visible. The main content area is divided into a left sidebar with a 'MODES' dropdown and a central panel. The central panel shows a list of experiments with columns for 'Wavelength', 'Power', 'Exposure Time', 'Fluorescence', and 'Intensity'. The bottom section shows a list of experiments with columns for 'Wavelength', 'Power', 'Exposure Time', 'Fluorescence', and 'Intensity'.

Wavelength	Power	Exposure Time	Fluorescence	Intensity
1.58 Å (1.58 Å)	12.812 keV (0.477 Å)	0.05 s	2.55e-12 phos	1.75e-12 phos

The screenshot displays the 'Fluorescence Spectra' view of the ExiMX software. The interface includes a top navigation bar with 'Home', 'Shipment', 'Prepare Experiment', 'Data Explorer', 'Manager', and 'Help'. A search bar is present, and a 'Log out' button is visible. The main content area is divided into a left sidebar with a 'MODES' dropdown and a central panel. The central panel shows a list of experiments with columns for 'Wavelength', 'Power', 'Exposure Time', 'Fluorescence', and 'Intensity'. The bottom section shows a list of experiments with columns for 'Wavelength', 'Power', 'Exposure Time', 'Fluorescence', and 'Intensity'.

Wavelength	Power	Exposure Time	Fluorescence	Intensity
1.58 Å (1.58 Å)	12.812 keV (0.477 Å)	0.05 s	2.55e-12 phos	1.75e-12 phos

Session vs Protein view

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

bsec_therm

Data Collections		Sessions (3)		Automatic SAD appears to have worked	
Energy Scans		ID30A-1	14-11-2014	Space Group	P212121
XRF	2	ID29	13-06-2016		
Samples	30	ID30B	20-07-2016		
Tests (< 4 images)	28				
Data Collections	160				

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

Triosephosphate isomerase

Data Collections		Sessions (2)	
Energy Scans		ID14-1	21-04-2008
XRF		ID14-1	19-05-2008
Samples	10		
Tests (< 4 images)	20		
Data Collections	1		

Ligands and PDBs

2dCD4 Collected last time on Oct 24, 2017 10:20:46 AM

Two-domain wild-type CD4 MX-1827 SANSAXS CHANNELL 09/06/16

[Summary](#)

Crystal Forms **6**

Space Group								Structures		
	a	b	c	α	β	γ		Group	Type	File
Edit	P21212	0	0	0	90	90	90	Add Structure		
								Trit-ase	PDB	model_01.pdb
								Trit-ase	PDB	model1.pdb
Edit	P6422	11	1	26	90	90	120	Add Structure	No structures defined yet	
Edit	I4132	100	120	130	90	90	90	Add Structure	No structures defined yet	
Edit	I4132	23	13	16	90	90	90	Add Structure	No structures defined yet	
Edit	Undefined							Add Structure	No structures defined yet	
Edit								Add Structure	No structures defined yet	

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

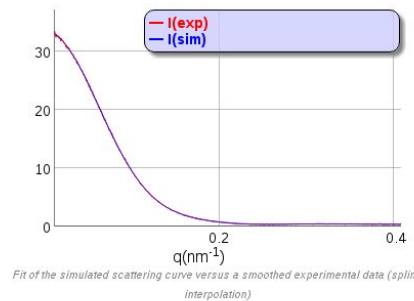
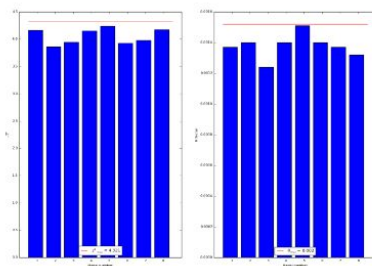
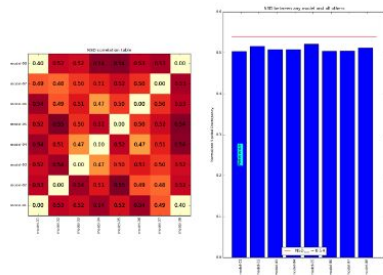
Field	Type	Null	Default
resolutionEllipsoidAxis11	float	YES	NULL
resolutionEllipsoidAxis12	float	YES	NULL
resolutionEllipsoidAxis13	float	YES	NULL
resolutionEllipsoidAxis21	float	YES	NULL
resolutionEllipsoidAxis22	float	YES	NULL
resolutionEllipsoidAxis23	float	YES	NULL
resolutionEllipsoidAxis31	float	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

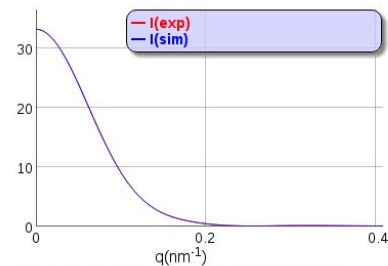
	Pipeline	SpaceGroup	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	Shell	Resolution (Å)	Multiplicity	Completeness %	<I/Sigma>	Rmeas	Rmerge	Rpim	cc(1/2)	ccAno	sigAno	ISA	Download	
BEST	XDSAPP	P 61	91.1	91.1	115.8	90.0	90.0	120.0	Overall	9.5-2.1	20.9	99.7	11.1		18.0			-5	0.713	9.41	⬇	📁
									Inner	100.0-9.5	20.2	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

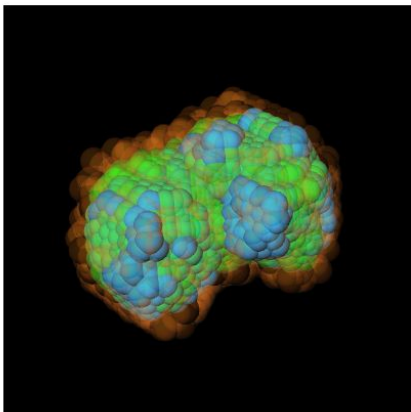
Ab Initio Modeling display



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

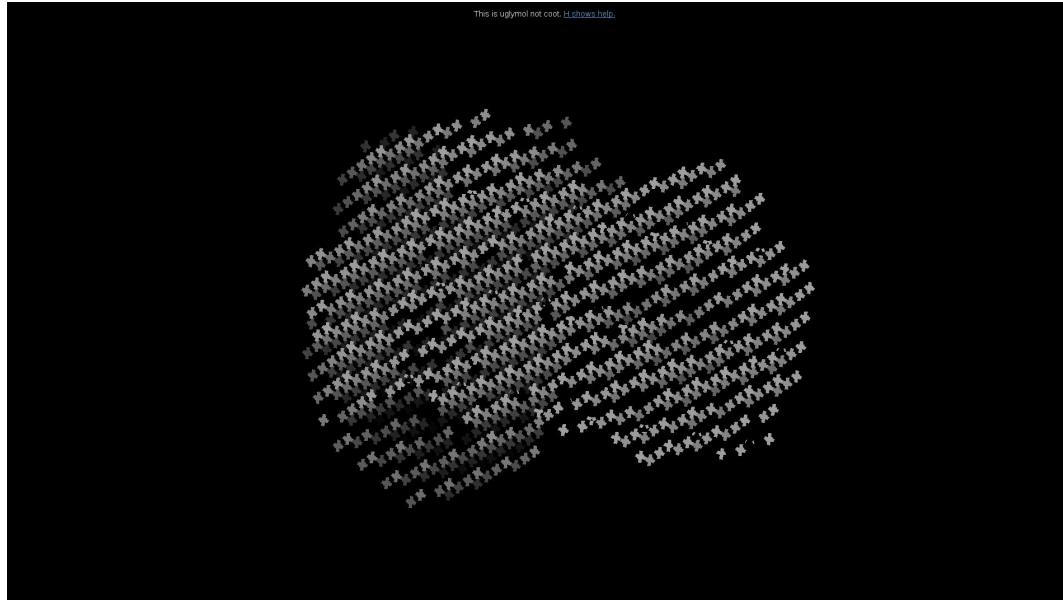


Fit of the simulated scattering curve versus the experimental data.



Type	chiSqr	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
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EMBL, ESRF, ATF, scientists
- **Developers**
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Solange Delageniere
- **Sys admin**
Emmanuel Eyer
Antoine Roux
- **ISPyB collaboration**