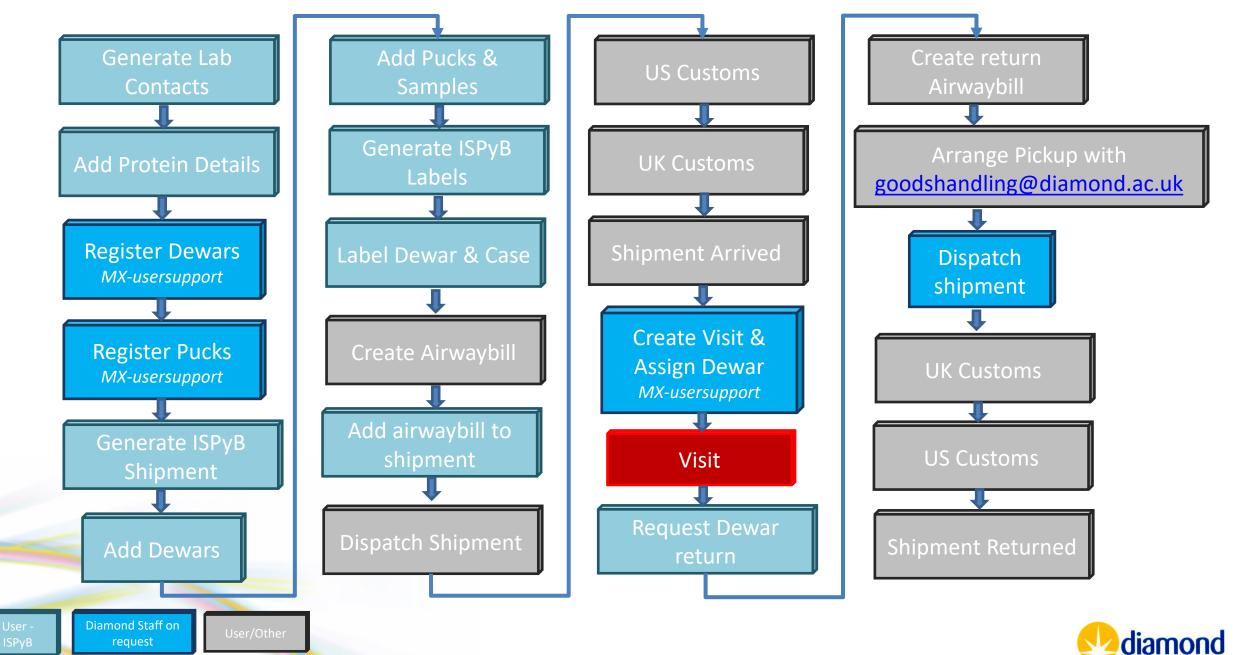
Shipping To / From Diamond





Shipments: Summary



- A lab contact is the address and details of the person that will ship a Dewar
- Select Lab contacts from the ISPyB Menu

Proposals	cm4950	Projects	Unit Cell Search		Feedback	Help
	View All Data					
Visits for cm49	Visits					
This page lists the visits ava	Calendar	proposal				
Show 10 + entries	Prepare Experiment					
Start Date	Shipments	\Rightarrow Number \Rightarrow	Beamline 🝦 Local (Contact 🔶 Comments	Data Collections	}
09:00 24-10-2014	Samples	↓ 5	i03	Click to edit	0	
09:00 15-08-2014	oumproo	1 4	i03	Click to edit	0	a b c ⁷
09:00 30-05-2014	Proteins	1 3	i03	Click to edit	0	
09:00 14-03-2014	Lab Contacts	1 2	i03	Click to edit	0	
		1 1	103	Click to edit	509	
09:00 01-01-2014	Statistics	•	100	Onok to cart	000	

https://www.diamond.ac.uk/Instruments/Mx/Common/Comm on-Manual/Using-ISPyB/Lab-contact.html



Generate Lab Contacts

• Select Add Home Lab contact

Home Lab Contacts

This page shows registered home laborate	ory contacts. This information	n is generally used to return shipme	ents back after an ex	periment		Create	a new contact
						+ Add Hor	me Lab Contact
Show 10 + entries							
Card Name	Person	Address	\$	Phone No.	•	Laboratory	♦ ♦
test	est t	lab address				labname	
Showing 1 to 1 of 1 entries						First Previous 1	Next Last

https://www.diamond.ac.uk/Instruments/Mx/Common/Comm on-Manual/Using-ISPyB/Lab-contact.html



Generate Lab Contacts

- Lab contact is a person that can be contacted regarding an associated shipment
 - Lab address used for pickup and collection
 - ZIP code or similar instead of post code
 - Include a country code in the phone number
 - Any issues contact <u>mx-</u> <u>usersupport@diamond.ac.uk</u>

Interpreter the Contact Card tact Details tity Name Threepu t Name Guybrus phone Number +442221 ail Address threepu versity / Institution / Company Details ne name of the university, institution or company et Address ireas for sourier luce post code and city Didcot	
Card Name Name for the Contact Card	Threepwood
Contact Details	
Family Name	Threepwood
First Name	Guybrush
Telephone Number	+442220911990 •••
Email Address	threepwoodG@example.co
lakansika (Institution (Company Dateile	
Jniversity / institution / Company Details	
Name The name of the university, institution or company	Diamond Light Source
Street Address Address for courier Exclude post code and city	Zone 8 stores Harwell Science Innovation Campus
Sity	Didcot
Postcode	OX11 ODE
Country	United Kingdom

https://www.diamond.ac.uk/Instruments/Mx/Comm on/Common-Manual/Using-ISPyB/Lab-contact.html



Generate Lab

Contacts

- As APS users will be arranging there own return shipments, these fields should be **left blank**
- For each shipment the courier company can be specified to help indicate to Goods Handling which company is due to pick up that shipment

Generate Lab Contacts

Dewar Return Details The following information is us	ed for each shipment associat
Courier Company Courier company to use to return dewars to home lab Courier Account No. Courier account number for returning dewars to home lab Billing Reference Billing reference to use when returning dewars to home lab Average customs value of dewar	
The average customs value of a dewar	
Average transport value of	

https://www.diamond.ac.uk/Instruments/Mx/Comm on/Common-Manual/Using-ISPyB/Lab-contact.html



Shipments: Protein Details

- For each protein defined in UAS, an equivalent record will be created in ISPyB
- In the proteins Interface, adding a sequence and PDB file will allow downstream processing such as MrBUMP and Dimple to run
- Alphafold structures will also be generated for provided sequences

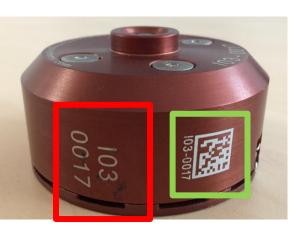
View Protein						
Clone Protein						
Name	TestLysozyme.1					
Acronym	TestLysozyme					
Molecular Mass	Click to edit					
Sequence A single protein sequence in single character format e.g. YPKN. No other characters or lines. Complexes are not supported at this time. This sequence is required for MrBUMP and will be used to generate an Alphafold model for future downstream processing tasks. This sequence will be used for the model building step of any Big EP phasing runs.	KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFES GCRL	SNFNTQ	ATNRNTDGSTDYGILQINSRWWCNDGRTPGSR/	NLCNIPC SAL	LSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGT	DVQAWIR
Component Type	Click to edit					
Concentration Unit	Click to edit					
Global	No					
Associated PDB Files A PDB format file of the protein, or subdomain. This is required to trigger the DIMPLE downsream processing task and is also used as an additional input to MrBUMP. Multiple PDB files can be provided and the best match will be used for the downsream task.	ranked_4.pdb [File]	×	ranked_3.pdb [File]	×	ranked_2.pdb [File]	×
+ Add PDB File	ranked_1.pdb [File]	×	ranked_0.pdb [File]	×	dls.lysozyme.pdb [File]	×



Add Protein Details

Shipments: Registering Dewar & Pucks

- Please provide <u>mx-usersupport@diamond.ac.uk</u> with your puck identifiers that you will use to send to diamond: IO3-0017
 - We will register these to your Proposal so they can be used in ISPyB
 - All pucks need to be registered, otherwise we cannot load and track the pucks on site
 - We will barcode pucks with 2D barcodes when on site
- Please ask <u>mx-usersupport@diamond.ac.uk</u> for Barcodes for each Dewar sent to Diamond
 - We will issue you a temporary paper barcode which we will replace with a 2D barcode on arrival





Register Dewars MX-usersupport

Register Pucks MX-usersupport



FOR USERS: this barcode needs to be attached to the dewar neck and its ID used for the shipment (in ISPyB/Synchweb)

FOR DLS-STAFF: This is a temporary barcode. Please replace it with a new sticker at the end of the visit (i.e. before returning to user). email mx-usersupport to notify this has happened or if you have any queries

For users -

print this page cut the square above and stick it to the dewar neck for shipment the dewar code will be associated with your proposal when the dewar arrives at Diamond we will substitute this temporary label with a permanent sticker

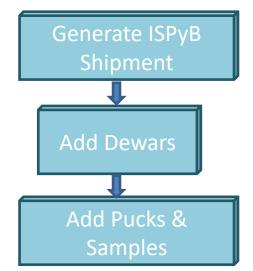


Shipments: Generating Shipment

- Select the "Shipment" page from the proposal menu
- This will take you to the shipments page, which lists all shipments for the currently selected proposal.
- Click the "Add Shipment" button on the top right hand side to register a new shipment

Shipments for cm4950

Proposals	cm4950	Pr
	View All Data	
Visits for cm49	Visits	
This page lists the visits avai	Calendar	proposal
Show 10	Prepare Experiment	_
Start Date	Shipments	\$
09:00 24-10-2014	Samples	÷
09:00 15-08-2014	oampies	1



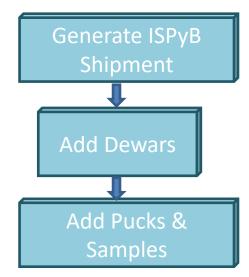
This page shows a lis	t of shipments associated with	the currently selected proposal					
In order to register yo shipment	ur samples you need to create a	shipment. Shipments contain dewa	ars, dewar contain containers, and d	containers individual s	samples. These can	be created sequentially by view	ing a particular
						Create a new shipment	+ Add Shipment
Show 10 + entrie	s					Search:	
Name 🔶	Creation Date	Outgoing Contact	Return Contact	Status 🍦	# Comp 🔶	Comment	
t2	13-02-2014	test	test	opened	1		
test	13-02-2014	test	test	opened	1	test please ignore	



- Once a shipment is created
- Click the + icon to add a container

Shipment Contents

Select a dewar by click	king on the row in the table below. D	ewar details are then she	own below. Click the + icc	n to add a container t	o the selected dewar				
									+ Add Dewar
Name	Barcode	Facility Code	First Experiment	Tracking # to	Tracking # from	Status	Location	Containers	
DLS-01-0001	cm4950-0003872	Click to edit	Click to edit	Click to edit	Click to edit	opened		0	₽ +
Dewar1	cm4950-1-i03-0003870	Click to edit	cm4950-1	Click to edit	Click to edit	opened		Click to add a co	ontainer +
rt	cm4950-0003871	Click to edit	Click to edit	Click to edit	Click to edit	opened		0	a +
DLS-01-0001	cm4950-0003873	Click to edit	Click to edit	Click to edit	Click to edit	opened		0	-
DLS-01-0001	cm4950-0003874	DLS-01-0001	Click to edit	Click to edit	Click to edit	opened		0	₽ +





- Select a Puck
- Registered container name
 - i.e. CPS-032
- Priority processing determines which pipeline will run first
 - xia2/DIALS
 - xia2/XDS
 - autoPROC.
 - autoPROC with <u>STARA</u> <u>NISO</u> is run as an additional task to running autoproc.

dd Container			Sinpine
hipment	test fixes	Container Sample Status	
ewar	Dewar1		Add Dewa
ontainer Type	Puck		Auu Dewa
ontainer Name			
egistered Container			Add Puck
iority Processing her data reduction pipelines will run on a wer priority queue	xia2/DIALS 🗸		Sample
how all spacegroups			
WNOF is user will be emailed with container dates. Check your email is up to date!	Elliot Nelson [You]		
omments omment for the container		$\bigcirc \bigcirc$	
ueue For UDC			
oc Protein Acronym	Name Sample Group Anomalous	Barcode Comment Status	
c Protein Acronym	Name Sample Group Anomalous	Barcode Comment Status	

https://www.diamond.ac.uk/Instruments/Mx/I04-1/I04-1-Manual/Using-ISPyB/Create-a-shipment.html



Generate ISPyB

Shinment

- The owner of each puck will be contacted for UDC collections
 - This can be changed here
- Pucks should be queued for UDC if relevant

hipment	test fixes	Container Sample Status	
ewar container Type	Dewar1		Add Dewars
container Name			
legistered Container	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~		Add Pucks
triority Processing ther data reduction pipelines will run on a wer priority queue	xia2/DIALS V		Samples
how all spacegroups			
WNEF his user will be emailed with container pdates. Check your email is up to date!	Elliot Nelson [You] View		
comments iomment for the container		\bigcirc \bigcirc	
Queue For UDC			

https://www.diamond.ac.uk/Instruments/Mx/I04-1/I04-1-Manual/Using-ISPyB/Create-a-shipment.html



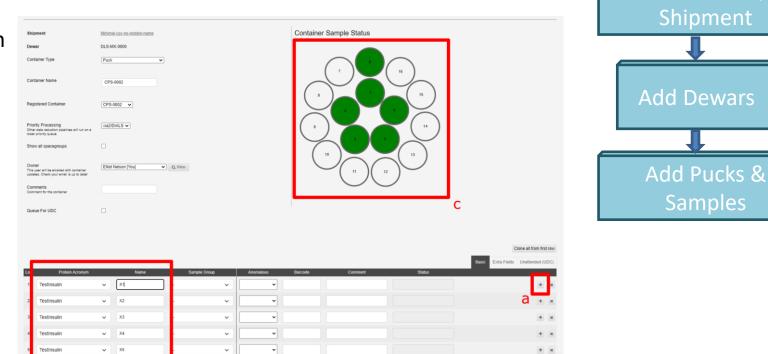
Generate ISPyB

- The sample table is split into three tabs:
 - Basic
 - Extra Fields
 - Unattended
- Every sample needs:
 - Unique name
 - Protein Acronym
- Anomalous scatter can be added to allow phasing pipelines to run

Loc Prote	ein Acronym	Name	Sample Group	Anomalous	Barcode	Comment	Status	Basic Extra Fields Unattended (UDC)	Shipment
1 TestLysozyme	e 🗸	X001	· v	· ·				+ x	
2	~		· v	~				+ x	
3	~		- v	·				+ x	Add Dewars
4	~		- v	·				+ x	Aud Dewars
5	~		- v	~				+ x	
6	~		· v	~				+ x	
7	~		· v	~				+ x	Add Pucks &
8	~		· v	`				+ x	
9	~		· v	`				+ x	Samples
10	~		· v	`				+ x	
11	~		· v	`				+ x	
12	~		· v	`				+ x	
13	~		· v	`				+ x	
14	~		· v	`				+ x	
15	~		· v	`				+ x	
16	~		- v	~				+ ×	



- The + button a allows you to duplicate the previous sample with a sequential name (i.e. X1 > X2).
- The x button d below, allows you to remove a sample
- Clone all from first row allows duplication of samples
- Anomalous scatter can be added to allow phasing pipelines to run
- The samples in b are shown in the puck view c above, green filled circles implies sufficient information has been provided.



https://www.diamond.ac.uk/Instruments/Mx/I04-1/I04-1-Manual/Using-ISPyB/Create-a-shipment.html

✓ X6



Generate ISPyB

 The add container button submits the table information into the shipment

	Generate IS Shipmer	Clone all from first row Basic Extra Fields Unattended (UDC)	Status	Comment	Barcode	Anomalous	Sample Group	Name	n	Protein Acronym	Loc
	1	+ x				~	- •	X1	~	TestInsulin	1
ī		+ x				~	- •	X2	~	TestInsulin	2
		+ x				~	- •	Х3	~	TestInsulin	3
ars 📗	Add Dewa	+ x				~	- •	X4	~	TestInsulin	4
		+ x				~	- •	X5	~	TestInsulin	5
		+ x				~	- •	X6	~	TestInsulin	6
0		+ x				~	- •		~		7
ks &	Add Pucks	+ x				~	- •		~		8
es	Sample	+ x				~	- •		~		9
		+ x				~	- •		~		10
		+ x				~	- •		~		11
		+ x				~	- •		~		2
		+ x				~	- •		~		13
		+ x				~	- •		~		14
		+ x				~	- •		~		15
		+ x				~	- •		~		16



Shipments: Generating Shipment

- The International shipment messages refers to booking airwaybills for EU users
 - As Diamond will not book APS shipments, this is not relevant
- Multiple Dewars can be added to a shipment
 - Dewars need all belong to the same proposal
 - Be the same collection method
 - Pre-assigned visit
 - UDC
 - (Responsive) Remote visit
 - If you want to ship Dewars with the same carrier under one airwaybill
 - Add same airwaybill details to multiple ISPyB Shipments

Add New Shipment		Generate ISPyB Shipment
Please note that international shipping is currently disabled from th	is application. Please see the link here	
Name Name for the shipment		Add Dewars
Number of Dewars Number of dewars to automatically create for this shipment	1	
Facility Dewar Codes Unique code for each dewar of the shipment. No facility codes listed? Make sure they are Registered to this proposal.	Please select one ~	Add Pucks &
Safety Level The safety level of the shipment	Green ~	Samples
First Experiment / Scheduling Select first experiment or if it's for an automated or responsive remote mail-in session	cm33904-1 (i04-1: 09:00 01-01-2023) ~ Aut	omated / Imager CResponsive Remote / Mail-in
Hard drive enclosed A hard drive is included with this shipment		
Tools enclosed Tools are included within this shipment		
Comments Comment for the shipment		

- Note that the carriage of Dewars is likely subject to dangerous good provisions. Typically, road and air transport require declarations, as below, please confirm these with your courier.
 - Not restricted as per <u>ADR A346</u> as per packing instruction 203.
 - Dry shipper not restricted as per IATA special provision A152.

stant dia 😓

Shipments: Generating Shipment

- Print shipment labels
- Add courier details to the shipment
- Arrange shipment with your courier
- Add a airwaybill tracking number to the ISPyB shipment
- Click sent to DLS once sent

Shipment: mx12345	-54 DDMMYY			
				Concrato ISDVP
This page shows details and contents of	the selected shipment. Most parameters	can be edited by simply clicking on them.		Generate ISPyB
Shipments need to have an outgoing and	return home lab contact before shipmen	t labels can be printed		Labels
You can print your Airway Bill by clicking	"Print Airway Bill" below			
		X Send to DLS	nent Contents 😝 Print Shipment Labels	
Created	03-07-2017	2.Click	1.Print	
Status	opened	send to	shipment	Label Dewar & Case
Outgoing Lab Contact	DemoUser	DLS once sent	labels	Laber Dewar & case
Return Lab Contact	DemoUser	DES ONCE SENT		
Safety Level	Green			
Courier	Click to edit			· · · · · · · · · · · · · · · · · · ·
Courier Account No.	Click to edit			
Shipping Date	05-07-2017			Create Airwaybill
Shipping Airway Bill	1173084614			
Shipping Pickup Location	Stores			
Shipping Ready By	09:00			1
Shipping Close Time	16:00			
Shipping Pickup Confirmed	Yes - Confirmation Number: 22			Add airwaybill to
Shipping Confirmed Ready By	18:00			
Shipping Confirmed Call In	18:00			shipment
Estimated Delivery Date	00-00-0000			
Comments	Click to edit			
oment Contents				

Shipment Contents											
										+ Add Dev	ewar
Name	Barcode	Facility Code	Weight (Kg)	First Experiment	Tracking # to	Tracking # from	Status	Location	Containers		
Dewar1	cm33904-0060701	Click to edit	18	Click to edit	Click to edit	Click to edit	opened		0	8+4+	⊷



Shipments: Labelling Shipment



Generate ISPyB Labels Label Dewar & Case

Dewar barcode

1. Dewar tracking label

Permanent

Per Shipment

Outbound address label
 Return Address label (behind)

Per Shipment



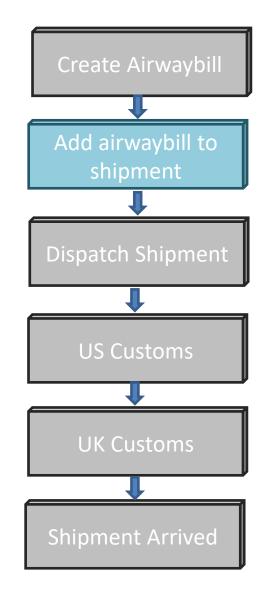
Shipments: Shipping

- Diamond does not cover shipping costs for users outside the EU
- User will need to arrange shipment and Airwaybill with their carrier of choice
- Dewars should be shipped to:

Goods Handling, Synchrotron Zone 8, Diamond Light Source Ltd, Harwell Science & Innovation Campus, Didcot UK OX11 0DE

- Diamond Goods Handling is only able to receive shipments between:
 - Monday Thursday 8.00am to 4.00pm.
 - Friday 8.00am to 3.00pm.

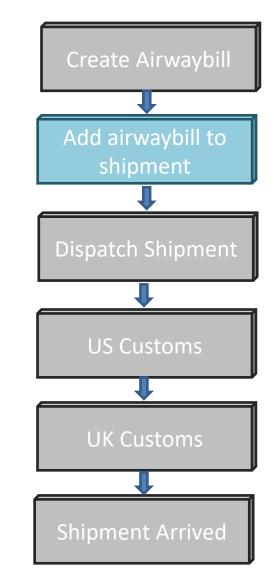
https://www.diamond.ac.uk/Instruments/Mx/Common/Common-Manual/Shipping-Samples/Academic_Shipping_to_Diamond/ROW-Other-Couriers.html





Shipments: Shipping

- Instructions to clear customs in your origin country should be discussed with the shipper
 - It may be beneficial to engage a customs broker
 - If you are required to undertake temporary import and export, or are declaring a high value permanent export
 - Instructions to clear at UK customs should be given under <u>CPC4000C13</u>. These instructions should be given to your courier with a request to contact <u>goodshandling@diamond.ac.uk</u> for a copy of the NIRU certificate and confirmed that such entry can be made.
- Shipment should be arranged under Delivered Duty Paid <u>Incoterms</u>, subject to duties/taxes



https://www.diamond.ac.uk/Instruments/Mx/Common/Common-Manual/Shipping-Samples/Academic_Shipping_to_Diamond/ROW-Other-Couriers.html

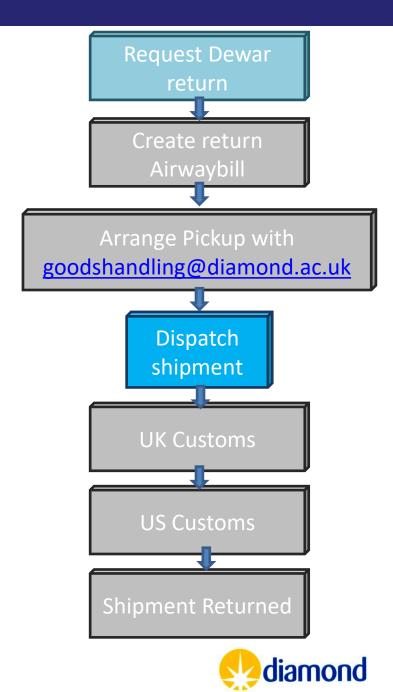


Shipments: Return Shipping

Shipment Contents										
Select a dewar by clicking on the row in the table below. Dewar details are then shown below. Click the + icon to add a container to the selected dewar										
										+Add Dewar
Name	Barcode	Facility Code	Weight (Kg)	First Experiment	Tracking # to	Tracking # from	Status	Location	Containers	
Dewar1	lb28214-3-i04-1-0046529	DLS-MX-1117	18	lb28214-3	Click to edit	Click to edit	at facility	tray-1d	2	⊖ + # ↔
							Only ship when dewar has left beamline		Ship dewar home	

- Select shipment that contains the Dewar you want dispatch back home.
- Click the small "house" symbol in the last column of the information for the Dewar that you want to dispatch.

https://www.diamond.ac.uk/Instruments/Mx/Common/Comm on-Manual/Shipping-Samples/Shipping_dewar_home.html



Shipments: Return Shipping

- Fill in the dewar dispatch form
- Email the airwaybill and collection details to

goodshandling@diamond.ac.uk

- We can arrange pickup with DHL, FedEx or UPS
- Collection should be at least one day from request of dispatch to allow time to prepare shipment

https://www.diamond.ac.uk/Instrumen ts/Mx/Common/Common-Manual/Shipping-Samples/Shipping_dewar_home.html

