

CryoFlow 1.28

User Guide

PN 1553194

Revision A • April 2025

Limited Rights

Copyright and Trademarks

Technical Publications

Technical Publications Team - Hillsboro

Copyright © 2024 by FEI company, a part of Thermo Fisher Scientific. The information and materials contained herein are proprietary to Thermo Fisher Scientific and are provided for your organization's internal use on a need-to-know basis. They cannot be duplicated, published or disseminated for any third party without the express written consent of Thermo Fisher Scientific.

Trademark Acknowledgments

All trademarks are the property of Thermo Fisher Scientific and its subsidiaries unless otherwise specified. FEI and the FEI logo are registered trademarks of FEI Company (part of Thermo Fisher Scientific and its affiliates). All other trademarks belong to their respective owners.

Excel and Microsoft are registered trademarks of Microsoft Corporation.

Limited Rights

The following notice applies to the U.S. Government and other purchases with federal funds:

Contractor Name: Thermo Fisher Scientific

Contractor Address: 5350 NE Dawson Creek Drive, Hillsboro OR 97124

The Government's rights to use, modify, reproduce, release, perform, display, or disclose these technical data are restricted to those rights specified in DFARS 252.227-7015(b)(2), FAR 52.227-14(g)(2)(Alternate II) and FAR 12.211. Any reproduction of technical data or portions thereof marked with this legend must also reproduce the markings. Any person, other than the Government, who has been provided access to such data, must promptly notify the above named Contractor.

Document History

Rev A, April 2025

Introduction

This product is a data management and workflow orchestration platform for all use cases using Thermo Scientific instruments. Intended for scientists who need to manage multiple projects, the platform facilitates collaboration between teams and data sharing between tools. Since projects and their data are centralized, securely sharing files, recipes, images and results is easily done between collaborators. The platform interfaces with other Thermo Scientific software for data acquisition to enable seamless integration into scientific workflows.

Users manage their projects and experiments with capabilities such as the following:

- Workflow customization
- Workflow status overviews
- Sample registration
- Visualization of acquired and processed data
- Data Referencing Functions: linking relevant samples, plus associating notes and external files.

Get Started

To access the platform portal, a web browser and access credentials are required. Supported web browsers are Edge™, Google Chrome™ and Safari™. For best results, it is recommended to update to the most recent version of the supported web browsers.

The installation of your software is configured according to customer-specific requirements, please see your administrator for access details and credentials.

Workspace Hierarchy

The workspace hierarchy helps keep folders well organized, especially when multiple people are working simultaneously. From general to specific, the hierarchy is the following:

1. Folder
2. Workflow
3. Step
4. Dataset
5. File

Folder

Each instance can contain one or more folders. A folder is simply a container for one or more folders or workflows. Only the user who created a folder can delete it.

Folder is the top-level in the workspace hierarchy. The platform allows folders to have a public or private mode:

- Public: visible and/or editable by everyone.
- Private: only visible or editable to selected users.

To modify privacy settings, see [Change the Privacy Setting of an Element](#) in the [Sharing](#) section.

Workflow

In the workspace hierarchy, *Workflow* follows *Folder*. At this point, the interface becomes specialized to address the business needs of different industrial and academic sectors. The platform provides users with several workflow template options. The appropriate workflow templates are distributed within the platform according to the business need. Therefore, depending upon the installed distribution, one of the following types of workflows are available:

- Free: an open, customizable workflow that contains user-defined steps
- Single particle analysis (SPA)
- Single particle analysis with Embedded CryoSPARC Live
- Single particle analysis with quality monitor
- Cryo-electron tomography with Tomo Live

The workflow is created with predetermined steps. Once created, you cannot change the workflow type.

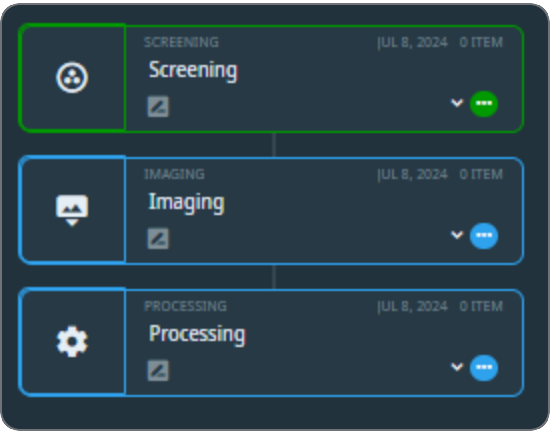
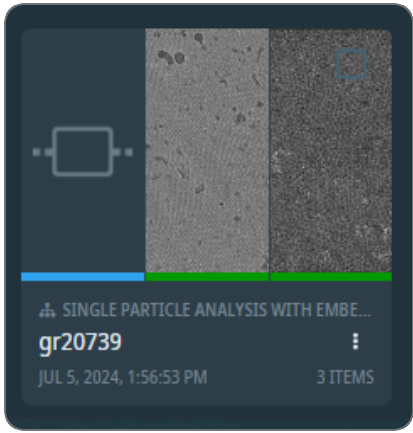
Step

Hierarchically, *Step* is an element of *Workflow*. The step defines a particular stage in a workflow. The logical decomposition of a step may be determined, for example, by moments where manual intervention or an instrument change is required.

Steps have status values, such as:

- Not started
- In Progress
- Completed
- Suspended
- Warning

The step's status is visible in the workflow and folder that contains it (for folders displayed as cards).

Workflow View	Folder View
	
<p>A workflow with completed steps, a running step and a step that has not started yet</p>	<p>The same workflow in the folder view</p>

Steps can contain custom data. See the [Upload](#) function.

Steps are sorted by their order in the workflow (from top to bottom).

Dataset


Depending on the workflow that has been instantiated, datasets can be different types such as free, EPU Run, Tomo Run. The type of datasets that can be used depends on the installed distribution.

- Free: the dataset can contain custom data. See the [Upload](#) function.
- EPU run: the dataset is filled automatically by EPU™. No custom data can be added.
 - See [Create EPU Run Dataset](#) for more information on EPU runs.
- Tomo run: the dataset is filled automatically by Tomography 5. No custom data can be added.
 - See [Create a Tomo Run Dataset](#) for more information on Tomo runs.

Datasets can have one of the status values:

- Not started
- In Progress
- Completed
- Suspended
- Warning

3D Dataset

After uploading 2D files that comprise a 3D stack, a Free dataset can be opened with the Volumetric Data Viewer. Switch to the 3D view at the top: . See [Volumetric Data Viewer](#) for more information about this viewer.

File

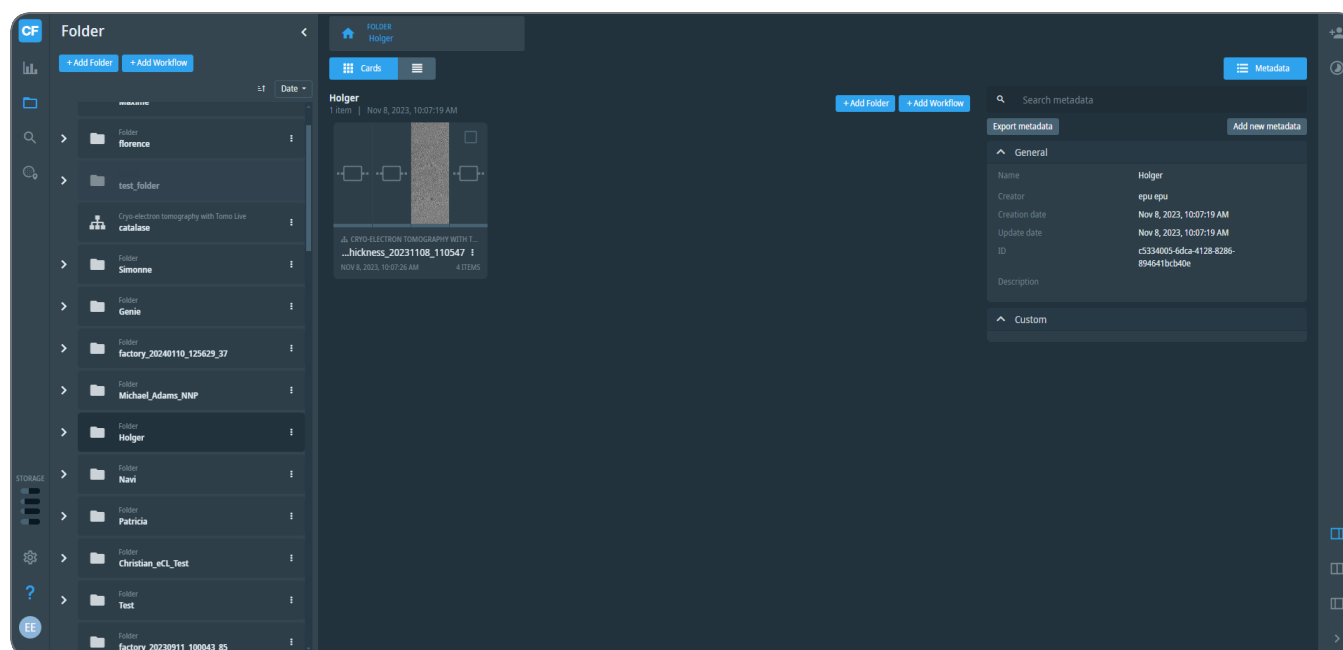
The file is the smallest element of the hierarchy. When clicking on a step or a dataset element, for example, a file uploaded to the platform or an EPU™ micrograph, the file is displayed in the appropriate viewer. See [Viewers](#) for more information.

User Interface

The main layout of the user interface is composed of the following:

- A left-side toolbar which propose a set of icons that point to core features (i.e., Dashboard, Workspace, Search, etc.).
- A central area where the current element is displayed with its children.

An extra left-side panel is also available to display other dedicated specific plugins like the Discovery-Viewer used in Single Particle Analysis workflows.



Main Tabs

The first four main tabs are at the top of the toolbar, while the last three are at the bottom.

Dashboard



The dashboard is composed of two parts. The first one gathers in the central panel:

- The most recently used Workflows
- The most recent used folders
- The storage usage by the different platform services
- The copyright information

The second one sums up in the right-panel the [Monitor Jobs](#) related information.

Workspace



The workspace tab displays the list of all existing elements (Folder, Workflow, Step, Dataset and File).

To create a new element:

- Click the **+Add *element*** button
- Enter the element's name
- Click **Create *element***

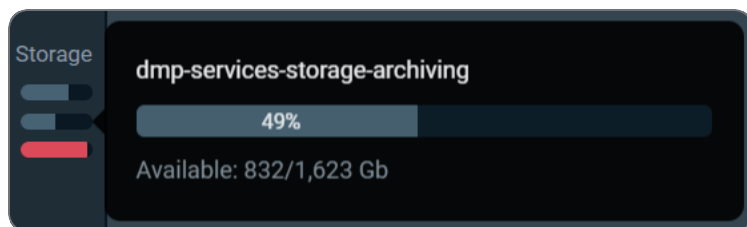
The workspace tab is detailed further in [Workspace](#).

Search



The search function works on all visible objects. By default, the search is done in the whole elements (name, metadata, notes) and returns all kinds of objects (workflows, folders, etc). Use the "Search in" and "Filter by" checkboxes to make the search more efficient.

Storage



Displays the storage currently connected to the platform, with the disk usage. Hovering a storage displays a tooltip with more details. There is an automatic refresh every 5 minutes.

User Guide



This page displays this current user guide.

User Icon

Clicking on the user icon opens a menu with an give access to the user name, the [Preferences](#) page, the user Profile, the Software License Agreement (SLA) and the Logout action.

Administrator Tabs

As an administrator, the user can access three extra features which allows them to manage high-level settings and users' rights:

- [Settings](#)
- [License](#)
- [User Administration](#)

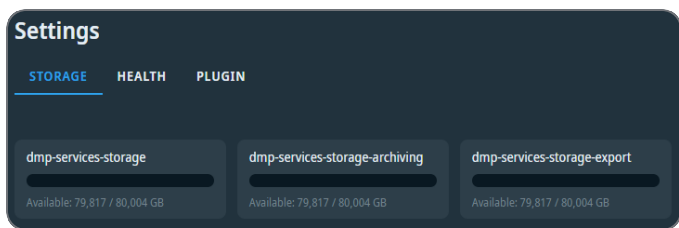
Settings



This page contains tabs available from the central area that allows the administrator to manage versioning and health check of his platform instance.

The Storage Tab

The *Storage* tab displays the storage components and their respective usage currently connected to the platform.



The Health Tab

The *Health* tab displays the *System status* sub panel that gathers the status and version of each service running in the platform.

- In the *Data engine* section, click **Reindex** to refresh the data engine service. Be aware that this operation may take many hours to complete and will impact the platform usability.
- For platform updating purposes, all live export jobs must be completed. To do so, it is possible to stop all the running or waiting to start jobs by clicking **Stop all live export jobs** in the live export section.

Settings

STORAGE **HEALTH** PLUGIN

System Status ● Stable ● Down ● Waiting

● ElasticSearch service (version 7.16.3)	● Entity service (version 123.0.0)
● Export service (version 123.0.0)	● Import service (version 123.0.0)
● License service (version 123.0.0)	● Lifecycle service (version 123.0.0)
● Registry service (version 123.0.0)	● Portal service (version 123.0.0)
● Storage service (version 123.0.0)	● Storage Monitoring service (version 123.0.0)

Data engine

If you feel data are inconsistent, you can force a reindex of the data engine service.
Watch out, it can take from a few minutes up to many hours depending on the amount of data stored in the platform! You won't be notified once the reindex is done.
During this process, the navigation in the workspace will be hazardous.

Reindex

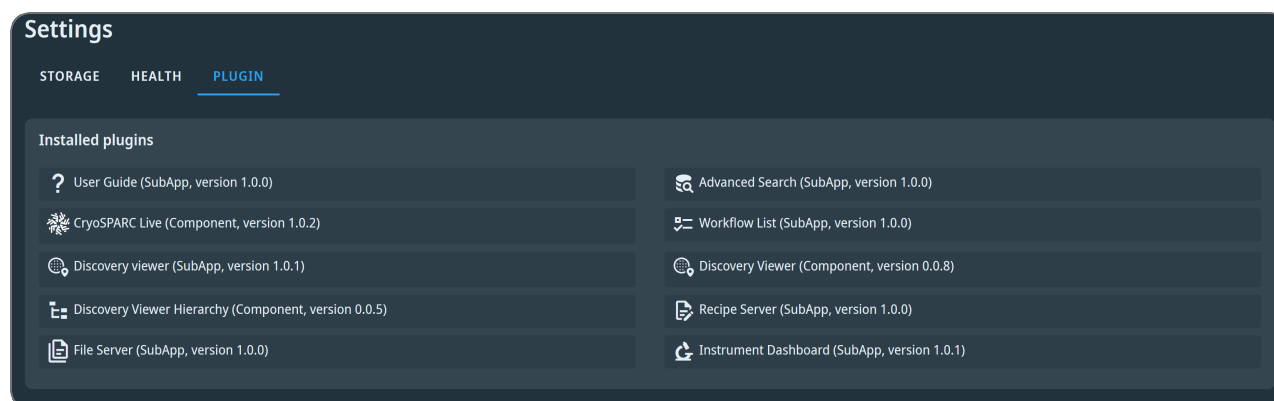
Live export

Upgrading the platform requires all live export jobs to be stopped.
You may stop all of them at once by clicking the following button.


Stop all Live Export jobs

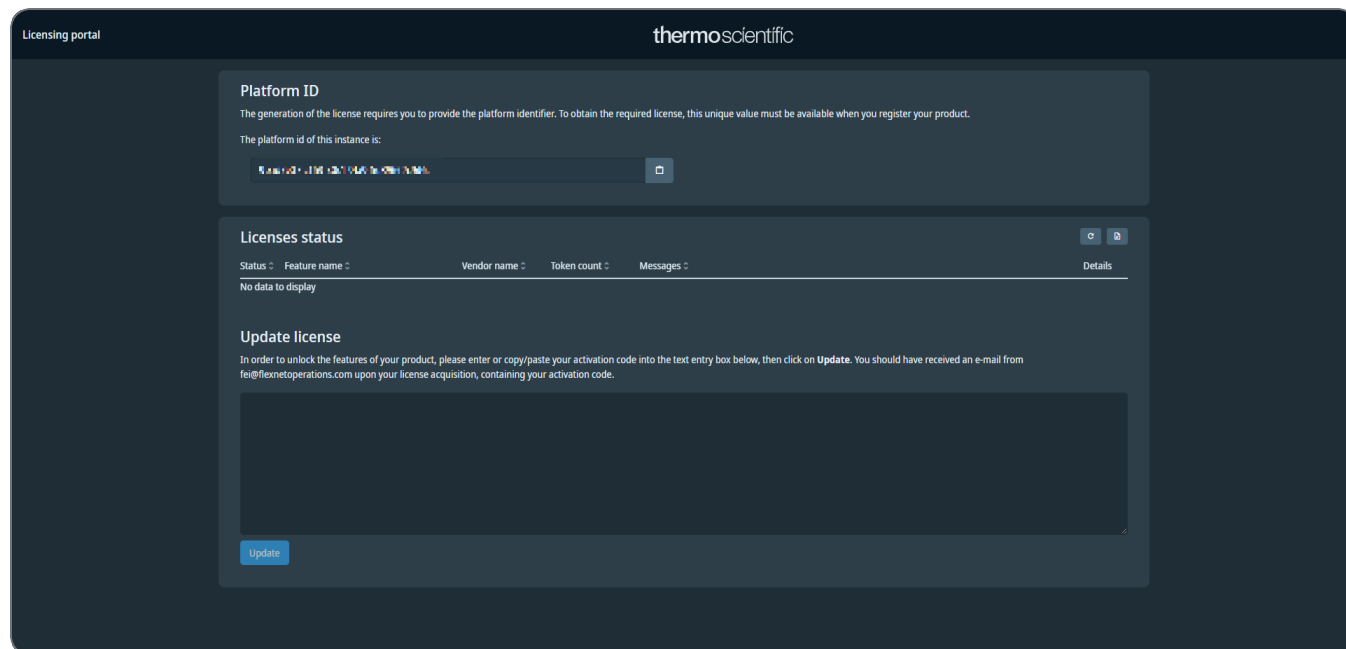
The Plugin Tab



The *Plugin* tab lists the installed plugins by displaying their names, types and versions.



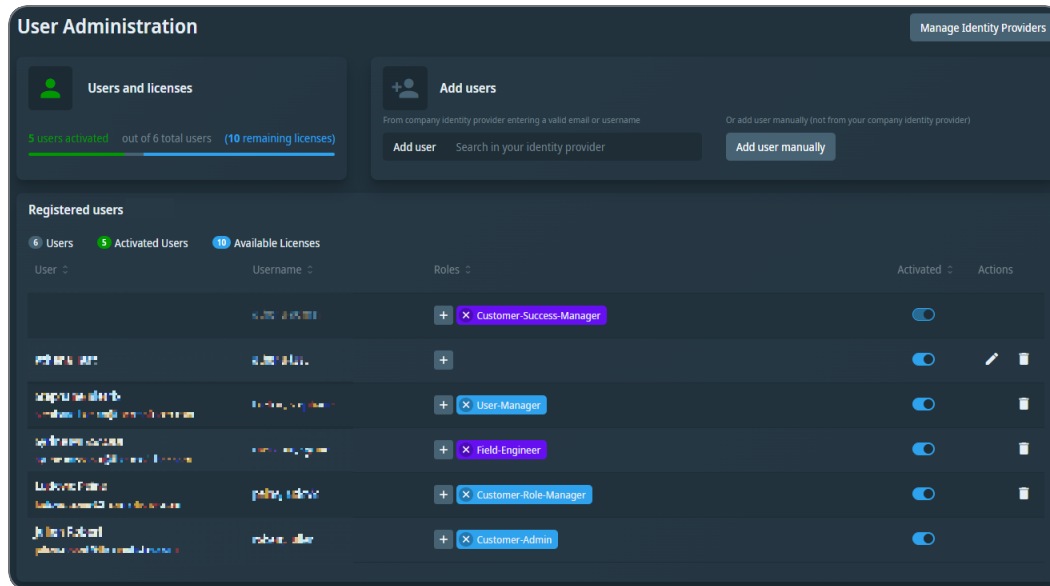
License

The icon  manages the licenses installed on the platform. An administrator user can reach the licensing portal that contains all information concerning his platform instance and licenses status.



- The top panel displays the platform id required to generate a license.
- The bottom section resumes the installed licenses details.
 - One can enter a new license key in the **Update license** form. If the license is valid, a message will confirm the license validity and the license information will be available in the **Licenses status** table. If the license is invalid, the reason will be displayed in the **Messages** column. After a new try, click the refresh license button  to update the license status.
 - The **Show license file**  button displays a dialog with the raw license file used by the license server.

User Administration



Roles

- Admin:
 - Can manage (create/update/delete) any Folder/Workflow/Step elements.
 - *Will be renamed in the coming releases as Workflow-admin.*
- License-manager:
 - Can visualize all registered users with their roles.
 - Can assign/unassign licenses.
- User-manager:
 - Can create/update users.
 - Can update users information.
- Customer-role-manager:
 - Can assign/unassign roles to users.
- Customer-admin: Mutualize the following scopes of action:
 - Admin (workflow-admin)
 - User-manager
 - Customer-role-manager
 - License-manager



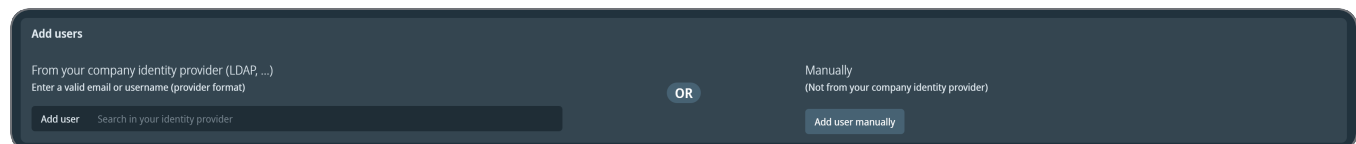
Note: The *customer-admin* role is protected, so that there is always a customer-admin user on the platform instance.

User Administration Panel

The User administration panel is accessible to the users with at least one of the following roles:

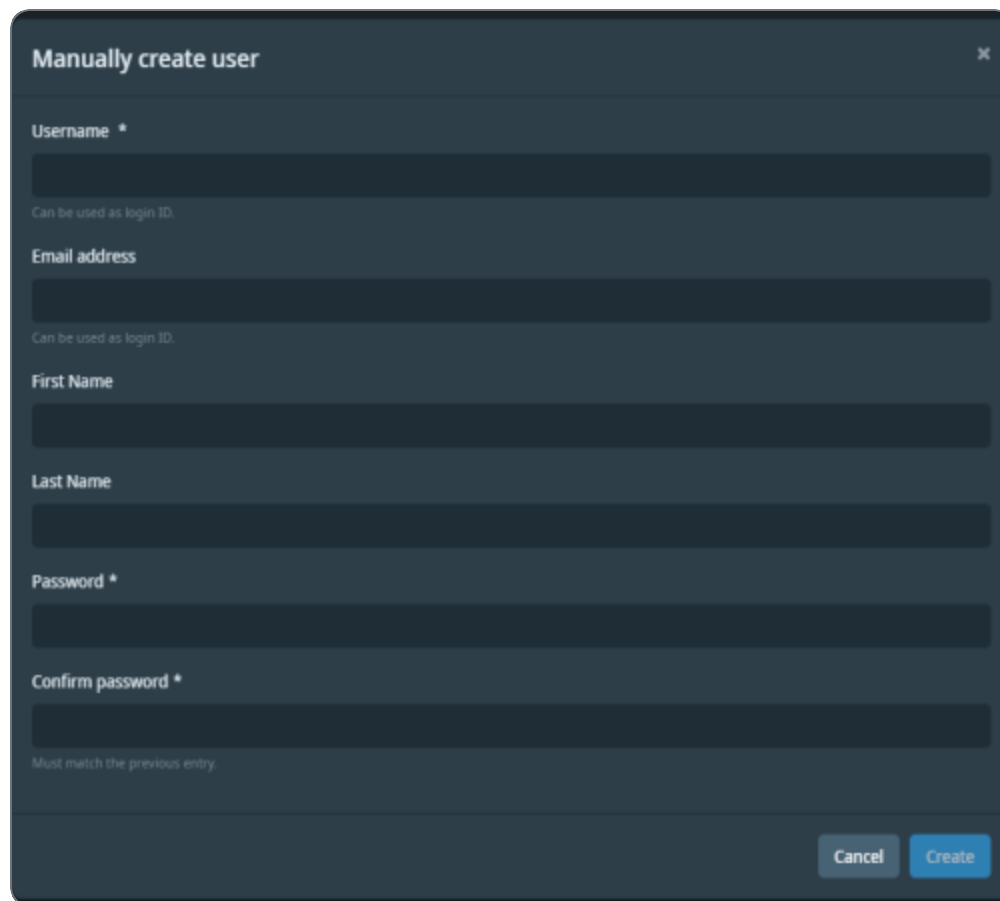
- User-manager
- License-manager
- Customer-role-manager
- Customer-admin

The **admin** role is not allowed to access User administration panel. This role is dedicated to enable full access to the workspace elements within the platform. See figure below to add a user.



The screenshot shows a dark-themed 'Add users' interface. It is divided into two main sections by an 'OR' separator. The left section, titled 'From your company identity provider (LDAP...)', instructs the user to 'Enter a valid email or username (provider format)' and features a search bar with the placeholder 'Search in your identity provider' and an 'Add user' button. The right section, titled 'Manually (Not from your company identity provider)', contains an 'Add user manually' button.

- If the user is part of the company, and that the company LDAP has been setup:
 - Start entering their work email address.
 - Select the relevant user from the auto-completion list.
 - If the auto-completion list does not appear, enter the user's full email address.
- If the user is not part of the company:
 - Click **Add user (Manual)**



The image shows a dark-themed modal window titled "Manually create user" with a close button (X) in the top right corner. The form contains the following fields and labels:

- Username ***: A text input field. Below it, a small grey note says "Can be used as login ID."
- Email address**: A text input field. Below it, a small grey note says "Can be used as login ID."
- First Name**: A text input field.
- Last Name**: A text input field.
- Password ***: A text input field.
- Confirm password ***: A text input field. Below it, a small grey note says "Must match the previous entry."

At the bottom right of the modal, there are two buttons: a grey "Cancel" button and a blue "Create" button.

Fill the following fields in the form:

- Username: can be used as Login **required**.
- Email: can be used as login.
- First Name, Last Name.
- Password **required**.
- Click **Create**.

Manage the Registered User List

The screenshot shows the 'User Administration' dashboard. At the top, there's a 'Users and licenses' section with a progress bar indicating '3 users activated' out of 6 total users, with '10 remaining licenses'. To the right is an 'Add users' section with options to add from a company identity provider or manually. Below this is the 'Registered users' section, which includes a summary of 6 Users, 5 Activated Users, and 10 Available Licenses. The main part of the dashboard is a table of registered users with columns for User, Username, Roles, Activated, and Actions.

User	Username	Roles	Activated	Actions
		+ X Customer-Success-Manager	<input checked="" type="checkbox"/>	
		+	<input checked="" type="checkbox"/>	
		+ X User-Manager	<input checked="" type="checkbox"/>	
		+ X Field-Engineer	<input checked="" type="checkbox"/>	
		+ X Customer-Role-Manager	<input checked="" type="checkbox"/>	
		+ X Customer-Admin	<input checked="" type="checkbox"/>	

The following information displays at the top of the registered users table:

- User Count:

6 Users

- Activated Users:

5 Activated Users

- Available License:


10 Available Licenses




Note: The *athena-admin* user is not counted as an activated user and cannot be deleted.

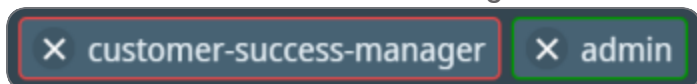
For each user, you can:


- Assign / Unassign roles to a user.
- Assign / Unassign licenses to a user.
- Edit the user.

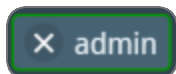
 **Note:** A user created from the company identity provider (for example, LDAP,...) cannot be edited.

Assign / Unassign User Roles

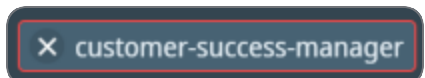
- The  icon accesses the list of available roles
- Visualize the list of available roles
 - Available roles, are all the authorized roles that are not assigned to the current user.
- Visualize roles that have been assigned to a user:



- Unassign a role from a user, by clicking  included into the **Role Tag**.
- Customer authorized roles are **framed** in green:



- ThermoFisher roles are **framed** in red:



- Available roles list:
 - Admin
 - License-manager
 - User-manager
 - Customer-role-manager
 - Customer-admin

Assign / Unassign User Licenses

When you create a new user, the system automatically assigns them a license if one is available. Otherwise, this error message displays:



At any time, you can disable a user's license or enable it again. Note that:

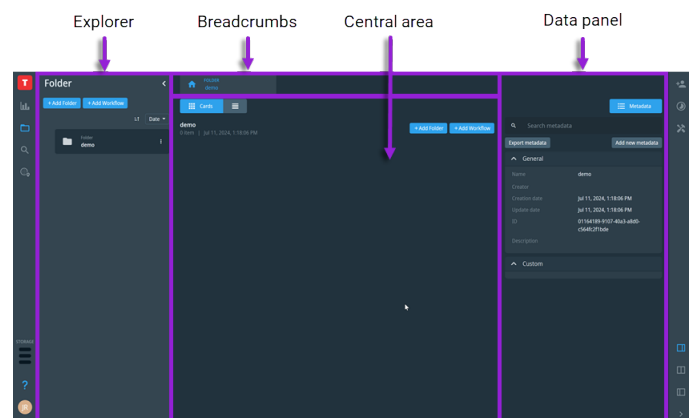
- Only a User with License-manager role can Assign/Unassign a License.
- A user without a license can not connect to the platform portal.

Edit the User's Details

-  Edit the user's details

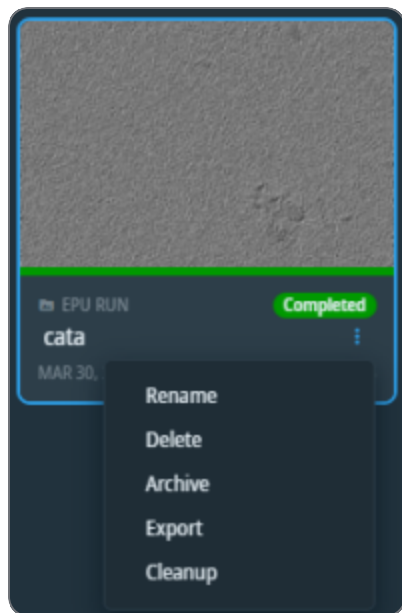
Workspace

The interface of the workspace tab is laid out as follows.



Action Menu

In the explorer and the central view, an icon with three dots is displayed on objects the user can act on. Depending on the element and the user's privileges, one can access different editing actions.



Actions available for Dataset 1. The user is the owner of the folder

Rename

Change the name of the element.

Delete

- Only available with **owner** privilege
- Deletes the current element, including all the element content, whether it is archived or not.
- A deletion job is registered in the platform orchestration, but does not necessarily start immediately, depending on the system load. Refer to the [Monitor Jobs](#) for more information.
- An element scheduled for deletion is grayed out and can no longer be opened.



Archive

Change the location of the entity's contents to the cold storage server defined in the [Settings](#).

Export

Only available with **collaborator** privilege and for datasets. Copy the dataset's content to an export storage. It is important to note that the export storage must be defined during the platform's installation phase. This storage can be a local drive within the customer's local infrastructure, which can be directly connected using the NFS protocol to the DMP server.

The next figure displays some examples of the export modal, which after choosing some options:

- Folder path:
 - Relative path where the dataset will be copied inside the export directory on the export storage. The folder name is always suffixed with the export launch timestamp.
- Data to export:
 - Define if the whole dataset content is exported or a subset of it. The subset can be defined using the Dataviz panel. See the specific description in each workflow section.
- Data type to export:
 - Define which data are exported. Different options are available depending on the workflow type. See the specific description in each workflow section.

Export

The following data from "EPU run QM" will be exported in a folder.

Folder path

Specify an optional path name for the export folder. The folder name will be suffixed with a timestamp.

Path/To/Folder

Path cannot contain invalid characters, like : * ? \ < > | .

The exported folder can be found at the path below:

//path/to/export/folder

Data to export

All Data

Filtered Data only

Data type to export

Files:

☒ Raw

☒ Processed

Metadata:

☒ Raw

☒ Processed

☐ Generate Relion file (.star) associated with Motion Correction and CTF information

Cancel

Export

Dialog for choosing the export options of an EPU run

Export

The following data from "Free" will be exported in a folder.

Folder path

Specify an optional path name for the export folder. The folder name will be suffixed with a timestamp.

Path/To/Folder

Path cannot contain invalid characters, like : * ? \ < > | .

The exported folder can be found at the path below:

//path/to/export/folder

Data type to export

Files: ☒

Metadata: ☒

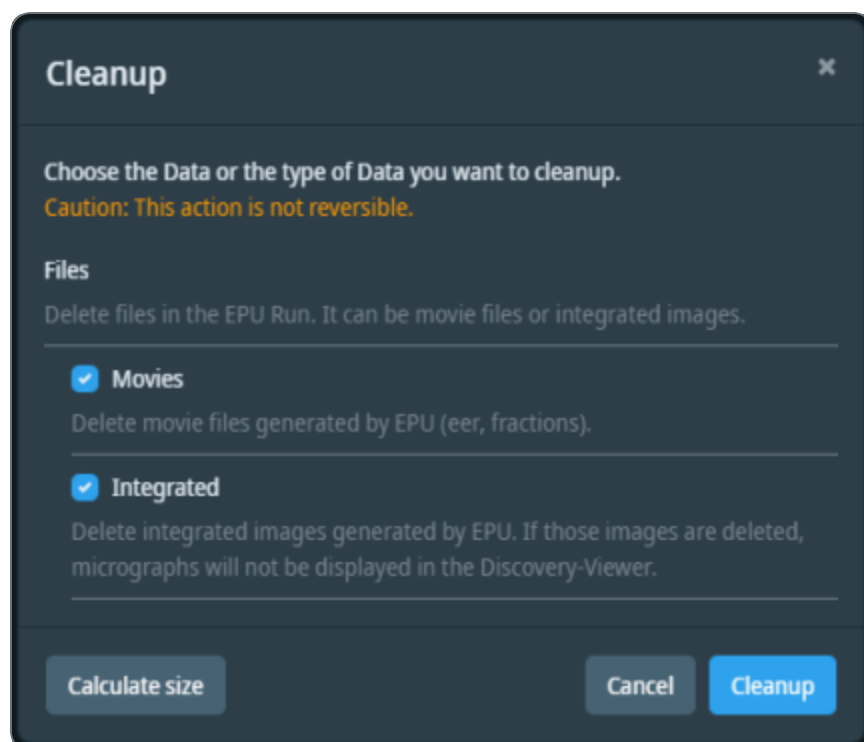
Cancel

Export

Dialog for choosing the export options of a free dataset

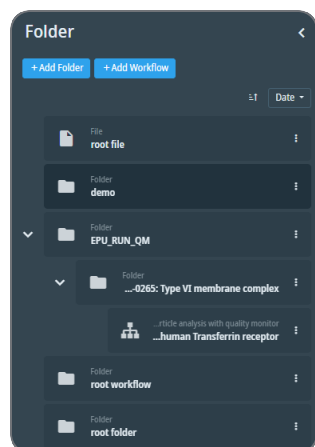
Cleanup

The cleanup functionality allows to clean a dataset in the platform according to specific rules. Those rules can be related to file type, properties or activities. Those rules depend on the type of dataset and the workflow used. When clicking on the cleanup action, a dialog is displayed. The rules that are applicable to this dataset are shown and can be selected or unselected using the checkboxes. It is possible to retrieve the amount of data present in this dataset by clicking the “Calculate size” button. Depending on the number of files present in this dataset, retrieve this piece of information can take some time. The figure below shows an example of cleanup dialog. The specific dialog for each workflow is explained on each dedicated workflow section.



Explorer Area

The left explorer panel displays elements structured as a tree that can be folded and unfolded (default state).



The explorer at the folder level. Root elements (folders, workflows, and files) are displayed.

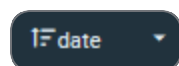
The explorer can be hidden by clicking the arrow on the left.

It is possible to create new objects from the Explorer by clicking **+Add element**. This is possible for:

- Folders: from root level
- Workflows: from root level
- Steps: from a Workflow
- Datasets: from a Step
- Files: from a Step or a Dataset (it is not possible to create a root file through the UI, you can only create them with the API)



For Folder creation, the hierarchy depth is managed by a platform preference (see [Preferences](#) for more information). By default, the depth is set to 2. This governance aims to guide the user in their work organization with optimized performances. If this value does not match your use case, an administrator can edit it (a user with the customer-admin role), see the [Role](#) section.

Objects can be sorted either by name or by date, descending or ascending.

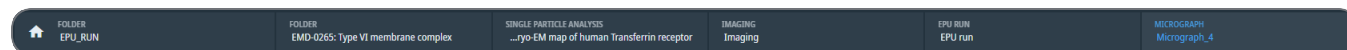


Sorting options in the explorer

- Click on name (or date) to switch between ascending and descending.
- Click on the arrow next to name (or date) to choose what to sort by.


Some objects can be displayed either as a simple list or as a list with thumbnails. Alternate between those options with the  **List** and  **List with thumbnails** icons. When you [Filter Micrographs](#), the explorer only displays filtered objects.

Breadcrumb Navigation



The breadcrumb navigation is visible in the workspace tab. It allows navigating up the hierarchy of elements.




For each level of the hierarchy, the type and the name of the element at that level are both visible.

Use the  **Home** button to go back to the root folder list.

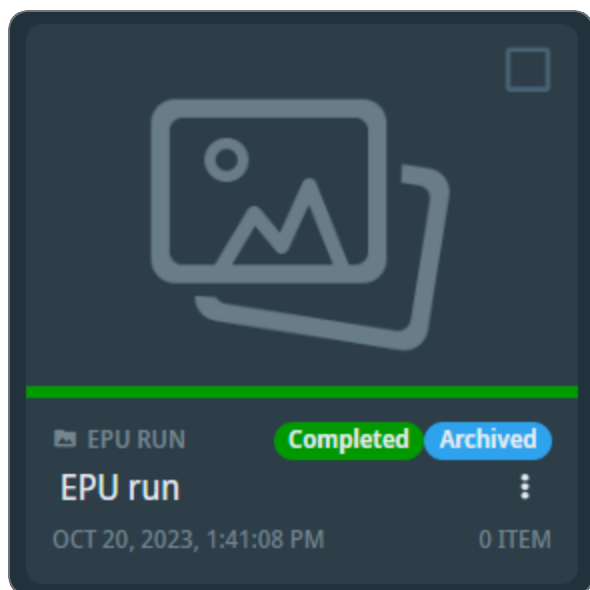
Central Area

The central area contains all children elements of the selected element, displayed as either a list or a collection of cards.

To switch between display modes, click on their icons at the top:

-  **List view** or  **Cards view** are always available.
- A display mode is available for EPU runs or Tomo runs; see [EPU Run Extended View](#) and [Tomo Run View](#).
- A display mode is available for Volumetric data in Free datasets ; see 3D View.

Cards can display a color-coded status for an element.



Card displaying a dataset that is both completed and archived

In **List view** and **Cards view**, multiple selection is available in order to apply an action to the selected elements.

Multiple selection is possible via a check box present on each displayed element.

Only simple actions common to the selected elements are supported such as: Delete, Download and Archive.





Data Panel

The data panel is located to the right of the Central panel. It always contains a [Metadata Panel](#). Depending on the context, it can also show:

- [Dataviz](#) panel
- Notes Viewer

Panel Resizing

Resizing option between the workspace and Data panel are located at the bottom right in a vertical toolbar.

-  the data panel fills two thirds of the space
-  the data panel fills half of the space
-  the data panel fills a third of the space
-  collapses or expands the data panel

Metadata Panel

The Metadata Panel displays two types of metadata:

- General metadata:
 - Name.
 - Creator.
 - Creation and last update dates, etc.
- Custom metadata/Group metadata:
 - Some custom metadata is added by previous steps, e.g. acquisition adds the type of microscope.
 - Custom metadata added manually.

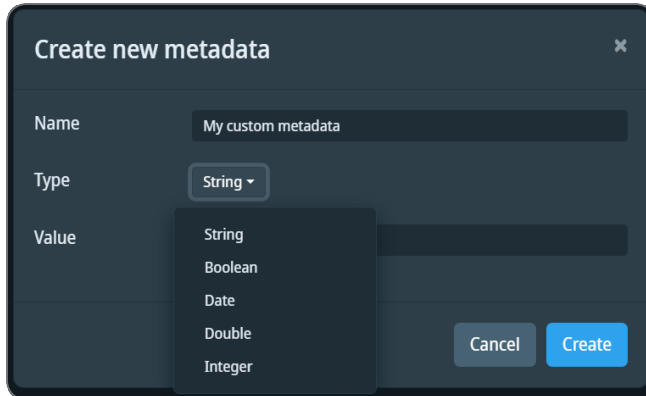
The screenshot shows the Metadata Panel interface. At the top right is a blue button labeled 'Metadata'. Below it is a search bar with the placeholder text 'Search metadata'. There are two buttons: 'Export metadata' on the left and 'Add new metadata' on the right. The panel is divided into four sections, each with a header and a list of metadata items:

- General**
 - Name: Recursive datasets
 - Creator: Athena Test
 - Creation date: Nov 20, 2023, 2:51:46 PM
 - Update date: Nov 20, 2023, 2:51:46 PM
 - ID: 9c295eb9-be74-4e5e-aa0c-feb288cb0444
 - Description:
- Core**
 - ApplicationSoftware: EPU
 - ApplicationSoftwareVersion: 2.4.0.3926
- Custom**
 - Image Type: Integrated
- Instrument**
 - InstrumentID: 123
 - InstrumentModel: TITANKRIOS2

Metadata Panel

To add custom metadata:

1. Click **Add new metadata** at the top right corner of the panel to open the creation dialog.
2. Enter the metadata name in the **Name** field. If the metadata already exists, select it from the list.
3. Choose the type to store the property.



Create new metadata [X]

Name: My custom metadata

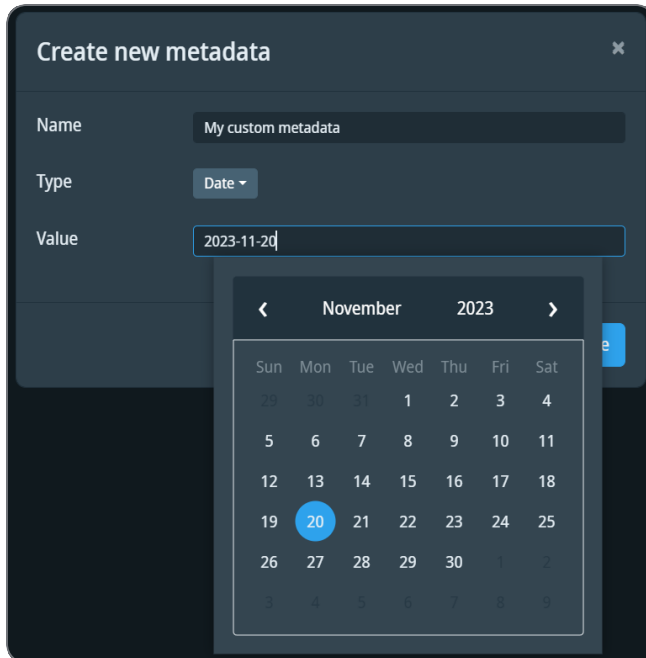
Type: String ▾

Value: [Empty]

String
Boolean
Date
Double
Integer

Cancel Create

4. Optional: Input the value you want to add at the same time.



Create new metadata [X]

Name: My custom metadata

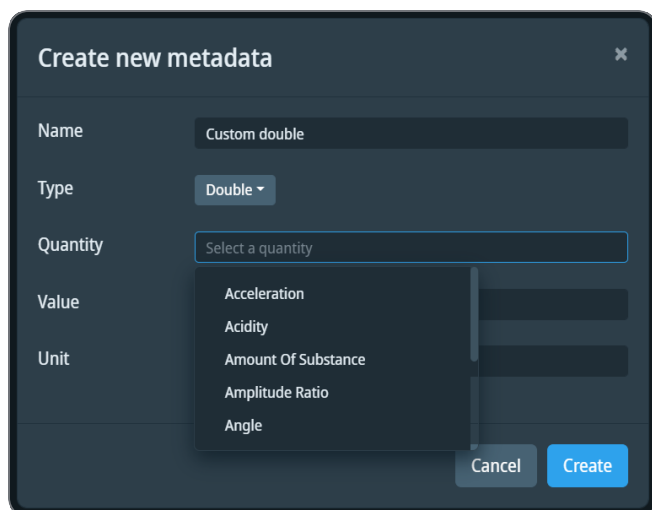
Type: Date ▾

Value: 2023-11-20

< November 2023 >

Sun	Mon	Tue	Wed	Thu	Fri	Sat
29	30	31	1	2	3	4
5	6	7	8	9	10	11
12	13	14	15	16	17	18
19	20	21	22	23	24	25
26	27	28	29	30	1	2
3	4	5	6	7	8	9

5. Optional: for "Double" and "Integer" types: Choose the physical quantity the property represents and unit of the physical quantity.



Create new metadata

Name: Custom double

Type: Double

Quantity: Select a quantity

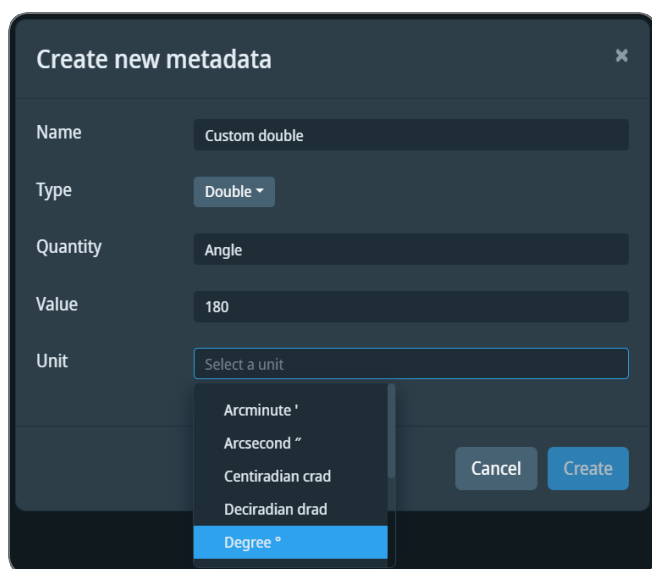
Value:

Unit:

Acceleration
Acidity
Amount Of Substance
Amplitude Ratio
Angle

Cancel Create

Type selection



Create new metadata

Name: Custom double

Type: Double

Quantity: Angle

Value: 180

Unit: Select a unit

Arcminute '
Arcsecond "
Centiradian crad
Deciradian drad
Degree °

Cancel Create

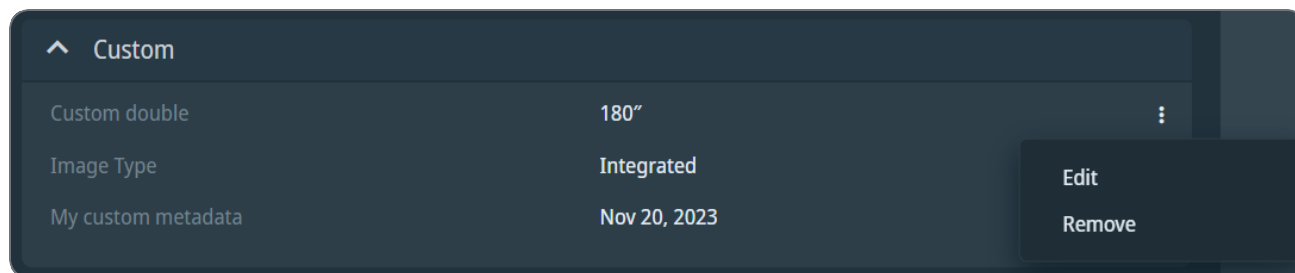
Unit selection

6. Click **Create**.

Metadata Panel

To remove a property:

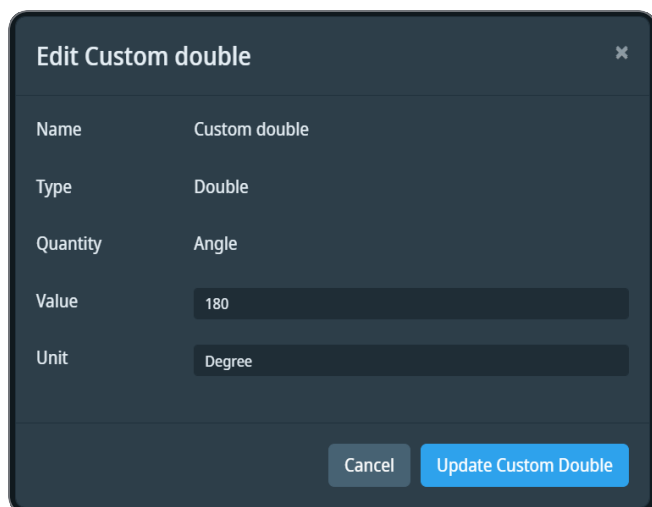
1. Hover over the property, click on the 3 dots icon, then click **Remove** in the menu that appears.



2. Click **Delete Metadata** in the message box.

To update a property's unit:

1. Focus on the property and click on the 3 dots icon to open the context menu, then click **Edit** to open the edit dialog.

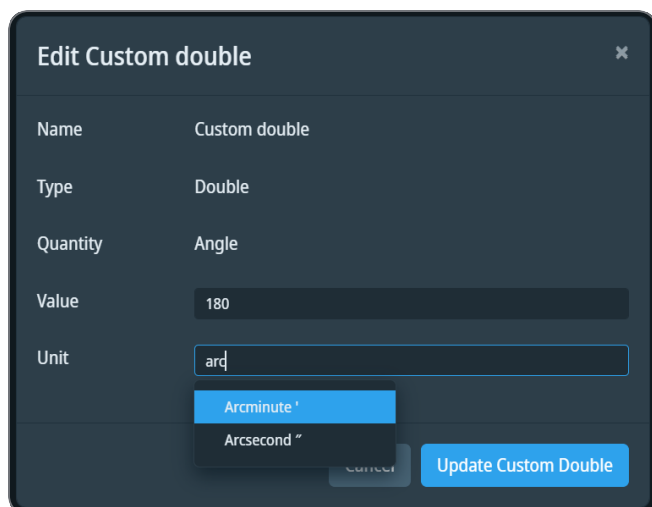


Edit Custom double [X]

Name	Custom double
Type	Double
Quantity	Angle
Value	180
Unit	Degree

[Cancel] [Update Custom Double]

2. Edit the previous value.
3. Search for a new unit and select it (tab, enter or click).



Edit Custom double [X]

Name	Custom double
Type	Double
Quantity	Angle
Value	180
Unit	arc

[Arcminute '']
[Arcsecond '']

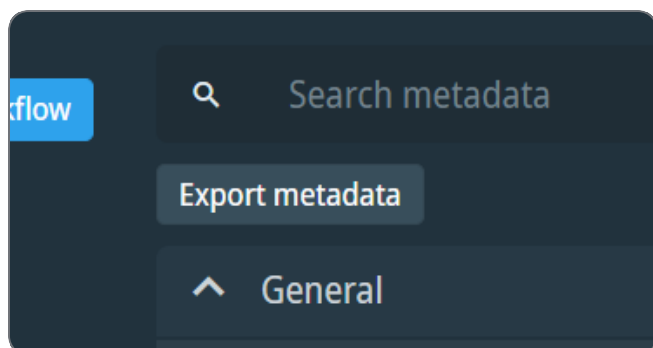
[Cancel] [Update Custom Double]

4. Click **Update [Metadata name]**

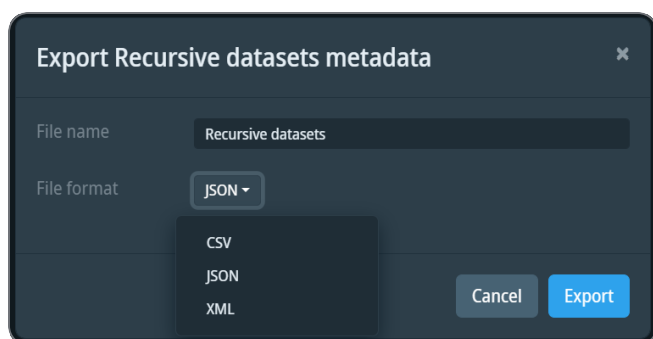
Metadata Panel

To export metadata:

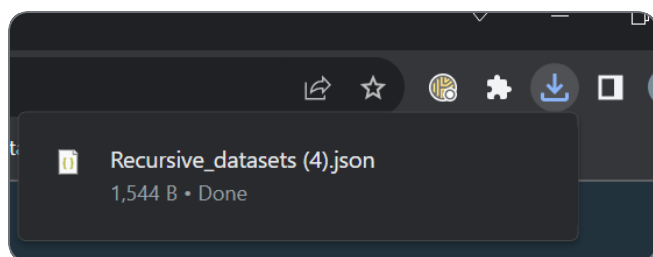
1. Click **Export metadata**, located on the top left corner of the panel.



2. Enter the desired file name or leave the default value (current element name).
3. Select the output format (CSV, JSON, XML).



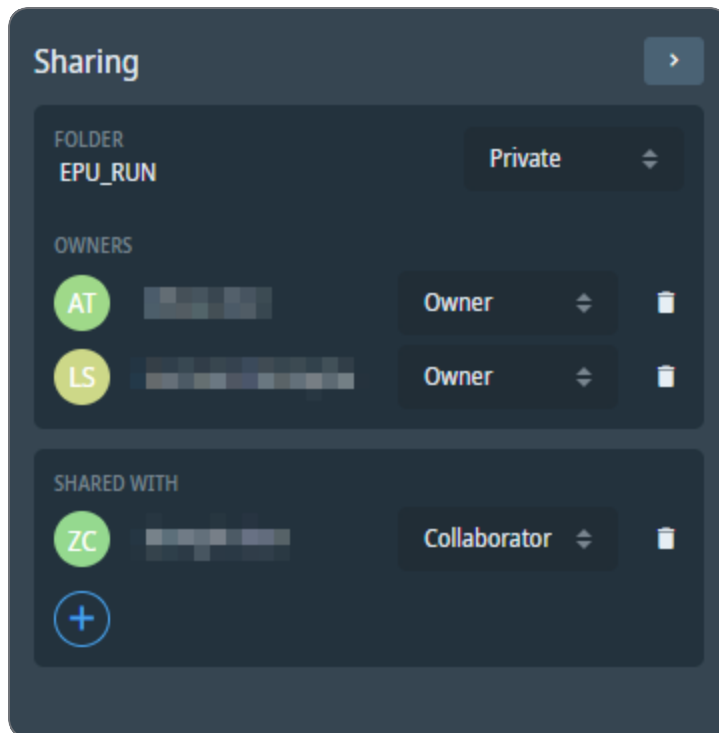
4. Click **Export**.
5. Your metadata file will be stored in the web browser download location.



Collaboration Tabs

The collaboration tabs are available from the toolbar on the right. They provide access to the Sharing settings.

Sharing



Only available for supported elements (Folder and Workflow).

By default, an element is private and only accessible by the owner (the creator). Only the owner or the Admin can edit the permissions of an element. An element must be owned by at least one person.

Permissions inheritance:

When a new element is created, inheritance is enabled by default, so that the new element inherits permissions from the element it is placed in. The reference of the permission set is stored on the element at creation time. It is also possible to break inheritance. When the permission levels for a child change, this breaks its inheritance. This means that it no longer inherits permissions from its parent.

For example, you might explicitly give permissions to a folder. All sub-folders created within this folder automatically inherit the permissions assigned to the parent folder.

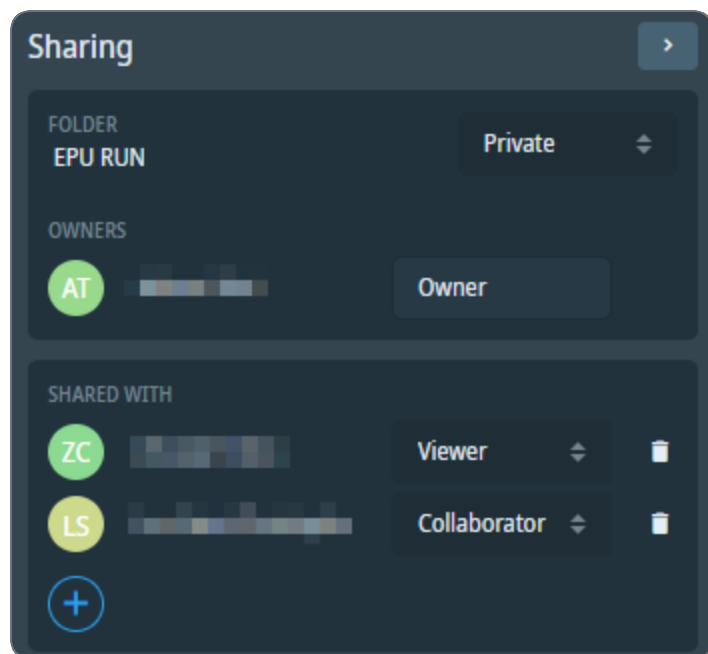
With the introduction of the tree explorer, you can now share elements in the middle of the hierarchy. For example, in a private root folder you can choose to share only one workflow (you give the right to see a small part of the entire project). The user with whom you share the workflow can then navigate it and all of its sub-hierarchy. They will be able to see it in the explorer from everywhere, even at the root level as the root folder card (title and sub-title only without navigation) is displayed to be able to unfold the private hierarchy to the shared one.

There are different permission roles:

- *Viewer*: reading rights for the element.
- *Collaborator*: reading and writing rights for the element.
- *Owner*: same as *Collaborator*, but can also delete the element, add and remove users, and modify their permissions.

The panel displays two lists of users:

- Owners.
- Viewers and collaborators.



The sharing panel, viewed by the owner. The owner can remove their own owner privilege if there was another owner.

The sharing panel is visible by anyone with access to the folder, but editable only by the owners.


Change the Privacy Setting of an Element

1. Open the Sharing tab.
2. Switch the privacy combobox to the right value.



When an element is set to Public, a special user called *Everybody* is added. *Everybody* may be either a viewer or a collaborator.

Add a New User to an Element

1. Open the Sharing tab.
2. Click  **Plus** in the "Shared with" section.
3. Select the user from the auto-completion list.
4. Set the chosen level of privilege for the user.

It is possible to change a user's privilege at any time after adding them to the element.

Remove a User from an Element

1. Open the Sharing tab.
2. Click the trash can in front of the user's name
3. Click **Delete Permission** in the confirmation message box.

Upload



Upload a file to an element. Only available for steps and free datasets.

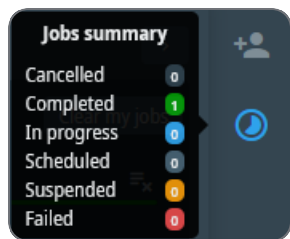
To upload a file:

1. Click the **Upload** button
2. Drag the files to the Upload area, or click the area to open a file explorer and select the files
3. The Upload area displays the upload progress for each file.

Uploading files is also possible by clicking **Upload File** at the top of the central area.

To cancel the upload, click the cross to the right of the progress bar.

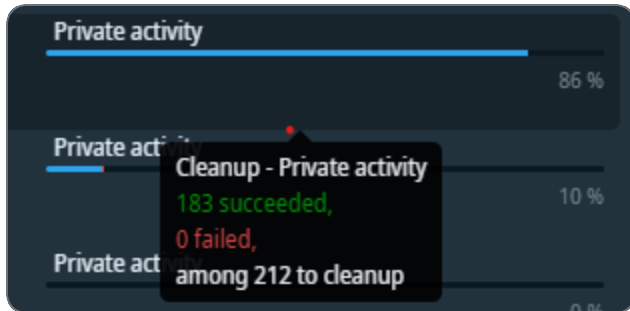
Monitor Jobs



Display information about the jobs in the platform, like dataset export tasks or deletion. The icon and its tooltip offer a summary. Click the icon to open the panel and view all the details.

The jobs are grouped by their status.

Job Details




Each line represents a job with its progress and the time it started.

Any user can see all the pending jobs. The element name related to the job is replaced by "Private entity" if the user has no viewer permission on the element.


The failed and completed jobs are only visible by the user who initiated the jobs.

Job Cancellation

Some jobs (like live export tasks) can be cancelled if they are not yet finished: . An administrator can cancel any of them. A regular user can only cancel the jobs he has launched.

Job Deletion

Once a job has completed (success or failure), the user can remove the job description from the view:

- Remove one job: 

An administrator can delete any job. A regular user can only delete the jobs he has launched.

- Remove multiple jobs: 

This button deletes all the jobs the current user has launched.

Preferences

The preferences page gives an access to some configurations, regrouped into two tabs:

- Platform
- User

Platform

The platform scope of a preference means the configuration will be global, for all users. This type of preference can be viewed by any user but is only editable by an administrator (a user with the customer-admin role; see [Roles](#)).

Specific constraints on preferences:

- Maximum folder depth: The value is an integer, with a range between 0 and 10 (any value less than 0 is set to 0 and more than 10 is forced to 10).
- Storage export folder path: The public path can be used from any computer connected to the network to retrieve the exported data.



Note: Do not use that preference to change the export configuration.

User

Preferences

PLATFORM **USER**

Please configure your own preferences

Main

Core

Language
Please choose your language

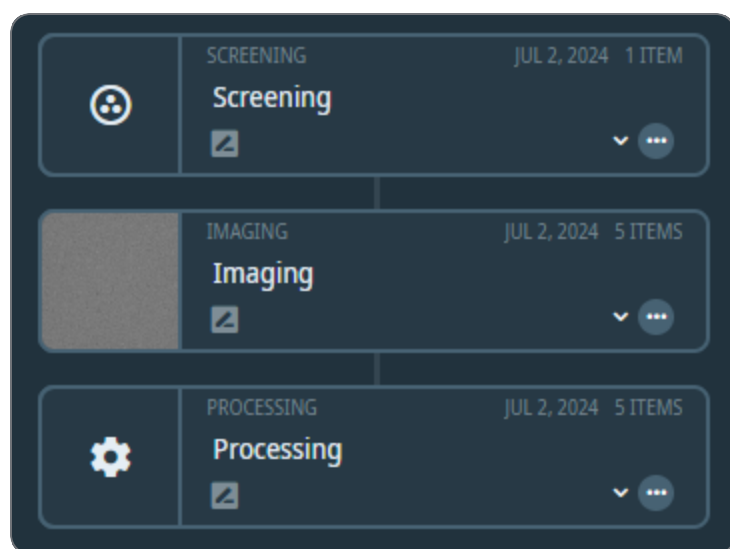
English (US English) ▾

The user scope of a preference means the configuration will be only for the current user. Changing a user configuration impacts only the current user (ex: changing the language for a user A do not impact the language for the user B).

Single Particle Analysis Workflow

This workflow is designed to manage data produced by instruments dedicated to a Single Particle Analysis workflow. At the moment only data coming from the transmission electron microscope can be pushed to CryoFlow. Three workflows are available, depending on processors licenses installed on the platform:

- **Single Particle Analysis:** generic workflow to manage data without any processing during TEM acquisitions with EPU.
- **Single Particle Analysis with quality monitor:** generic workflow management and EQM processing during EPU acquisition. See [Single Particle Analysis with Quality Monitor](#).
- **Single Particle Analysis with Embedded CryoSPARC Live:** generic workflow management and Embedded CryoSPARC Live processing during EPU acquisition. See [Single Particle Analysis with Embedded CryoSPARC Live](#).



Steps of the Single Particle Analysis workflow

The Screening and Imaging steps are dedicated to the cryo-EM acquisition using EPU. The Processing step allows to access the CryoSPARC Live session for the **Single Particle Analysis with Embedded CryoSPARC Live** workflow.

EPU Acquisition Workflow Setup

Create SPA Workflow

1. Go to the folder in which you want to create the workflow.
2. Click **Add Workflow** at the top of the central area.
3. In the creation dialog, choose a name for the workflow.
4. Choose "Single Particle Analysis" in the Type combo box.
5. Click **Create Workflow**.

Create EPU Run Dataset

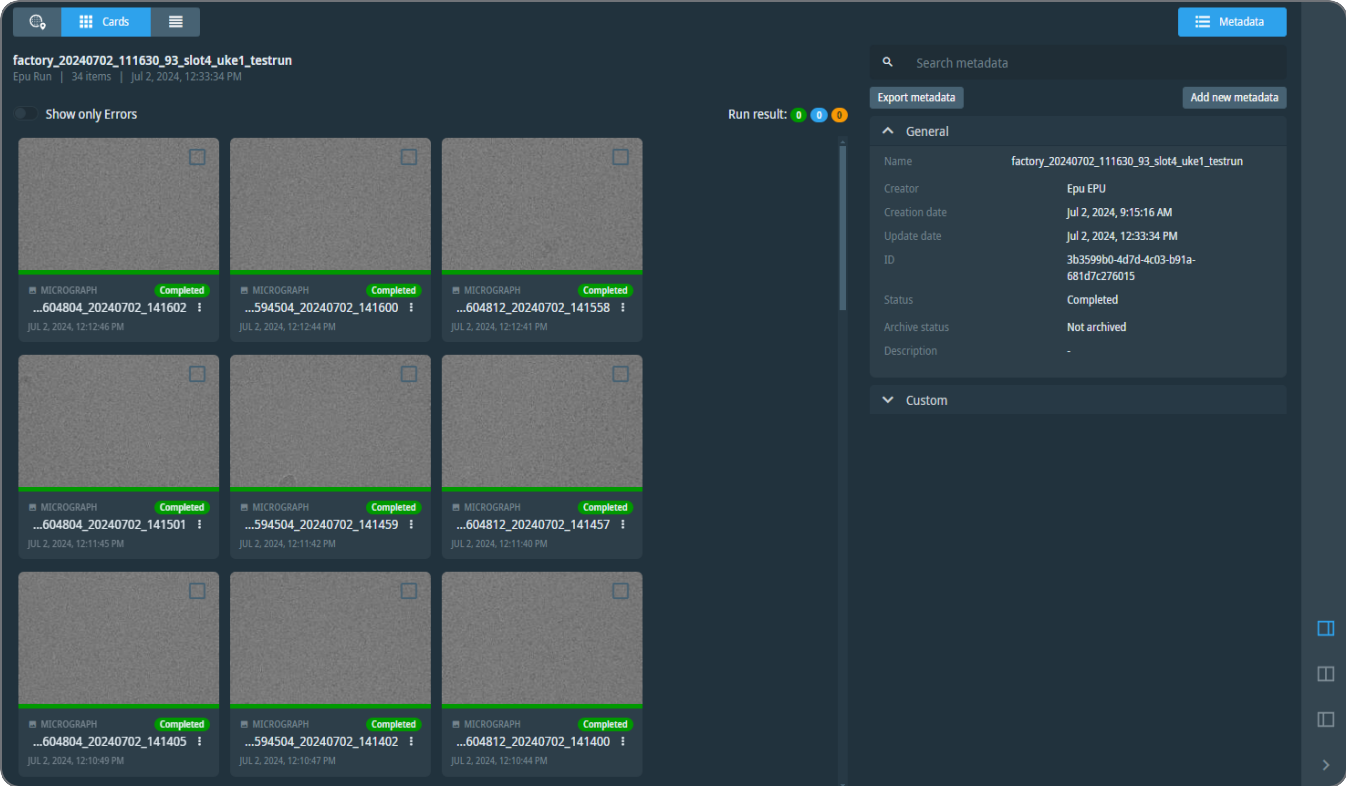
1. Go into the Screening or Imaging step to add the dataset.
2. Click **Add Dataset** at the top of the central area.
3. In the creation dialog, click **EPU run**.
4. Choose a name for the dataset.
5. Click **Create Dataset**.

EPU Acquisition

Refer to the EPU™ user guide manual for more information on EPU acquisitions.

EPU Run View

Micrographs acquired by EPU are visible in the EPU Run dataset. They can be displayed using the list or card display modes. Micrograph can be visualized by clicking on the image.



Normal EPU Run view with the card mode.

Acquisition Status

During the run or once the acquisitions are done, the workspace can be filtered by selecting only error micrograph where it displays acquisitions which encountered an error and did not finished successfully.



The top right of the workspace displays the number of acquisitions currently filtered (if toggled), and the number of acquisitions finished, in progress, and in error (at the current state of the run). Moreover, the dot beside the micrograph name indicates the status of the acquisition:

- Green for a completed pipeline.
- Blue for an in progress pipeline.
- Orange for a pipeline in error.

EPU Run Export

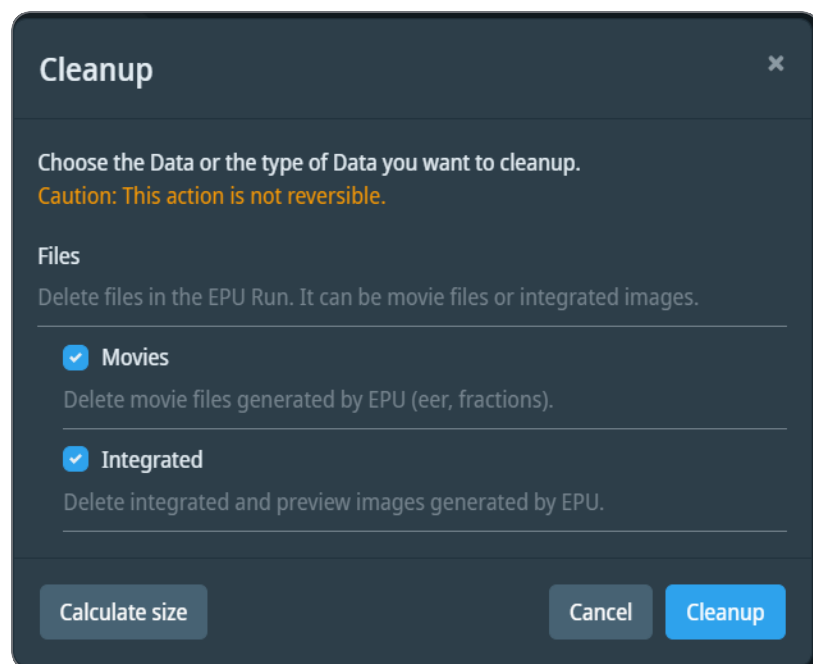
An EPU Run can be exported to the export storage by choosing the Export action. In that case the user can:

- Export all the files of the dataset, the raw files only.
- Export all metadata from the dataset and its content, just metadata related to the raw files. Metadata are written using a json format.

If the EPU Run is *In Progress* status, the user can, instead, start a live export. Data is exported when it arrives and until the run completes. Only one live export job at a time can run for a specific EPU Run. An export job is registered in the platform orchestration system, but does not necessarily start immediately, depending on the system load. Refer to the Job Monitoring for more information.

EPU Run Cleanup

For a normal EPU Run dataset, the cleanup functionality allows to specify which raw data you want to delete (see figure below). It is possible to choose to delete Movie (Fractions or EER files) or Integrated files that have been registered by EPU™ application.




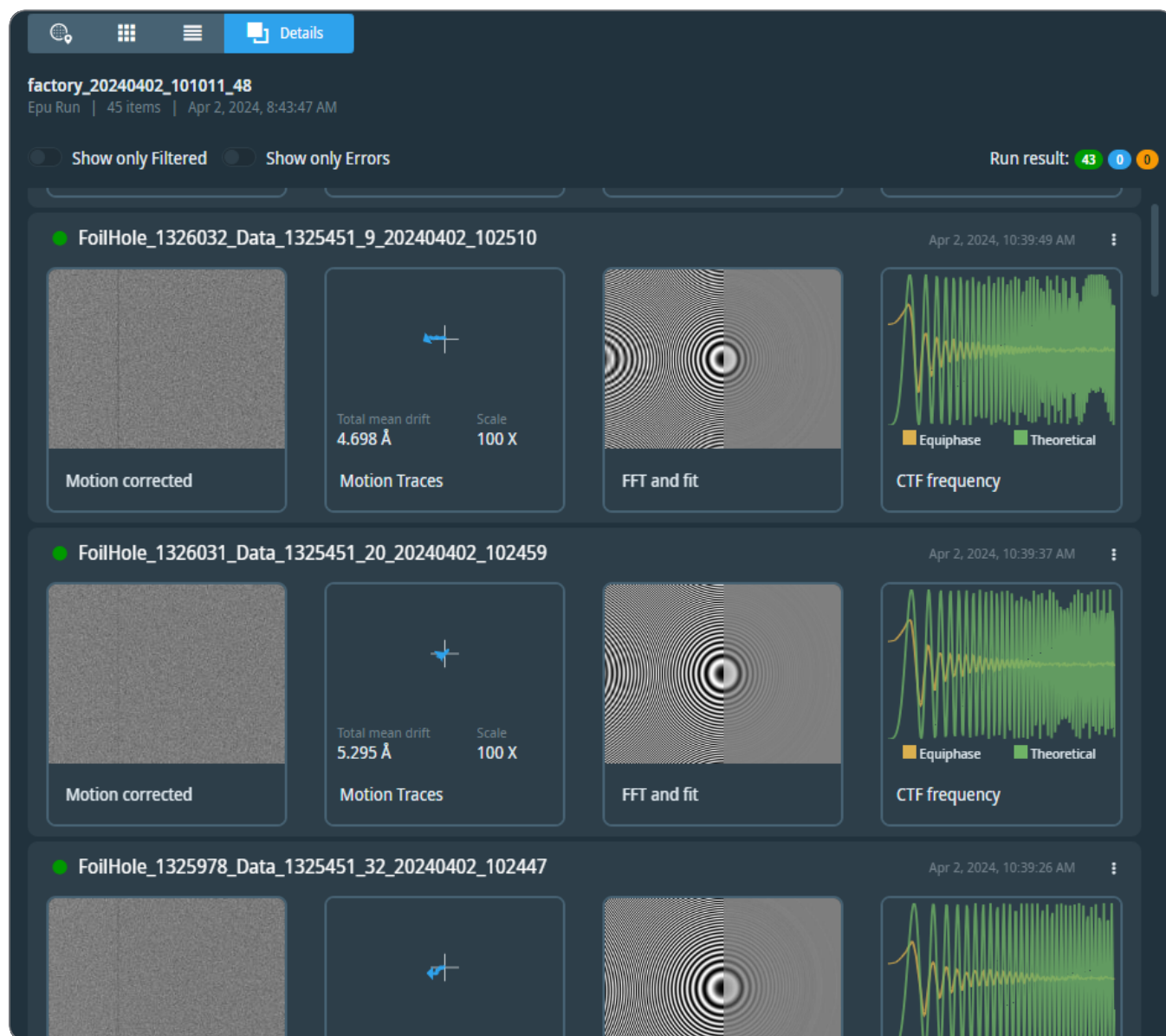
The cleanup dialog for a Single Particle Analysis workflow

Single Particle Analysis with Quality Monitor

EPU Quality Monitor (EQM) processing consists of a motion correction and CTF determination algorithm that provide quality metrics to help users to assess the quality of their acquisition. The processing is started automatically when images are acquired by EPU™ in a "Single Particle Analysis with quality monitor workflow". For the nominal workflow usage, see the normal [Single Particle Analysis Workflow](#) guide.

EPU Run Extended View

In addition to the list and card display modes, EPU runs can be displayed in a "Extended view mode" only if a "Single Particle Analysis workflow with quality monitor" has been created. This view allows visualizing a summary of the EQM processing results. To activate it, click on the icon  to enable it.



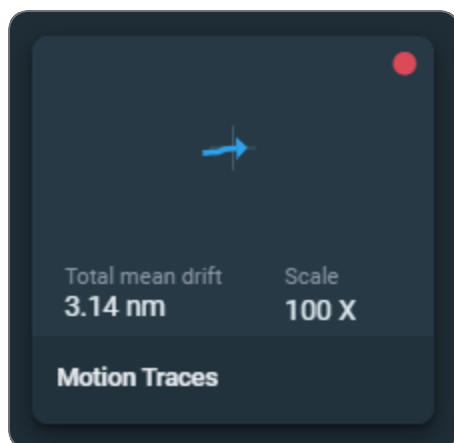
Extended view of an EPU run

In this mode, each micrograph displays:

- The thumbnail of the motion corrected micrograph.
- The motion traces card which displays the mean drift value and direction.
- The 2D CTF fit.
- The 1D CTF fit.

See the section [EPU Quality Monitor](#) for supplementary explanations about the EQM processing results available by clicking on the cards.

If the mean drift value is higher than expected then a red colored indicator is displayed on the top right of the motion traces card.



Mean drift out of range

Extended Acquisition Status

Either during the run or once all acquisitions have finished, the workspace can be filtered with the two following options:

- **Show only Filtered:** displays only the acquisitions matching the filter defined in the [Dataviz](#) panel.
- **Show only Errors:** displays acquisitions which encountered an error and did not finished successfully.



The top right of the workspace displays the number of acquisitions currently filtered (if toggled), and the number of acquisitions finished, in progress, and in error (at the current state of the run).

With the [EPU Run Extended View](#) or the cards view, the dot beside the micrograph name indicates the status of the EQM processing pipeline for each micrograph: completed, in-progress and in-error with color-coded in green, blue and orange, respectively.

EPU Run Export with Quality Monitor Data

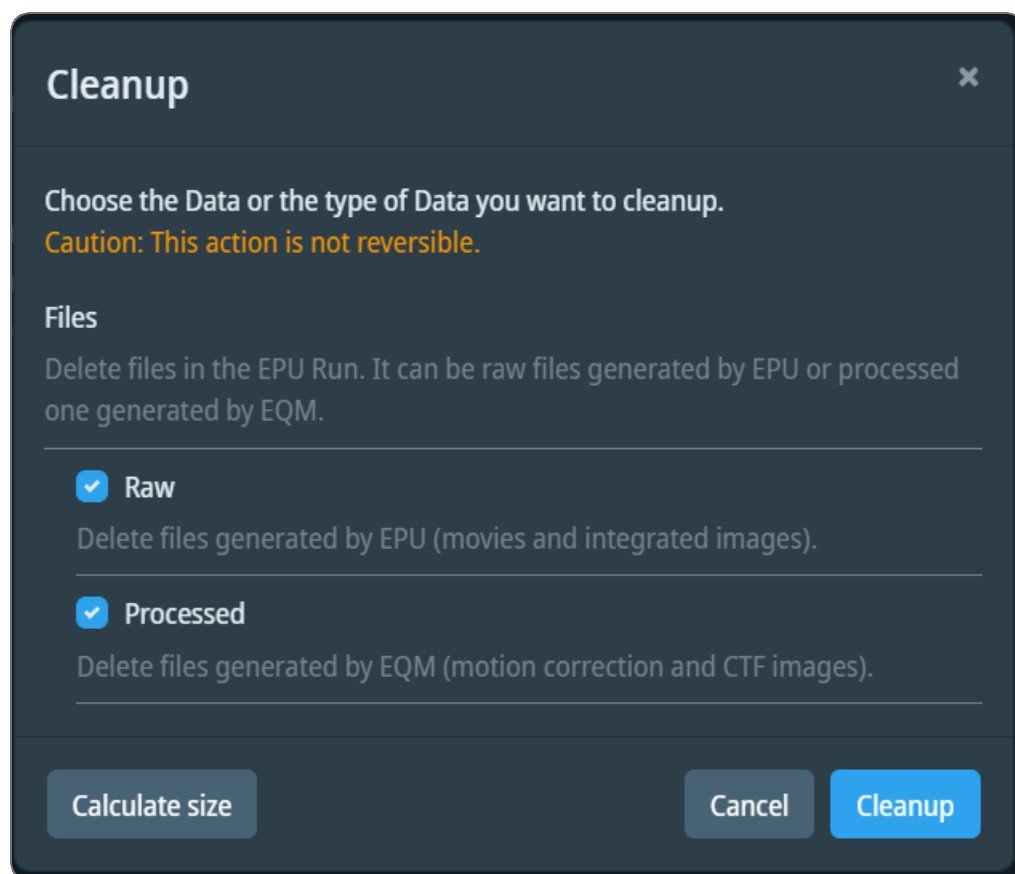
An EPU Run for which quality monitor has been enabled can be exported to the export storage by choosing the Export action. In this case you can:

- Export all the files of the dataset, the raw files and/or the processed one generated by EQM.
- Export all metadata from the dataset and its content, just metadata related to the raw files. Metadata are written using a json format.

If the EPU run is in the In progress status, the user can, instead, start a live export. Data is exported when it arrives and until the run completes. Only one live export at a time can run for a specific EPU run. An export job is registered in the platform orchestration, but does not necessarily start immediately, depending on the system load. Refer to the Job Monitoring for more information.

EPU Run Cleanup with Quality Monitor Data

For an EPU Run dataset with quality monitor data, the cleanup functionality allows to choose if you want to delete raw data (Movies and Integrated) and/or Processed one generated by EQM (Motion Corrected and CTF images). In this workflow, the Discovery-Viewer displays by default the motion corrected images.



Cleanup dialog for an EPU Run in a Single Particle Analysis with quality monitor workflow

EPU Quality Monitor

Motion Correction

The motion correction panel shows the parameters of the motion correction and the motion traces for each patch.



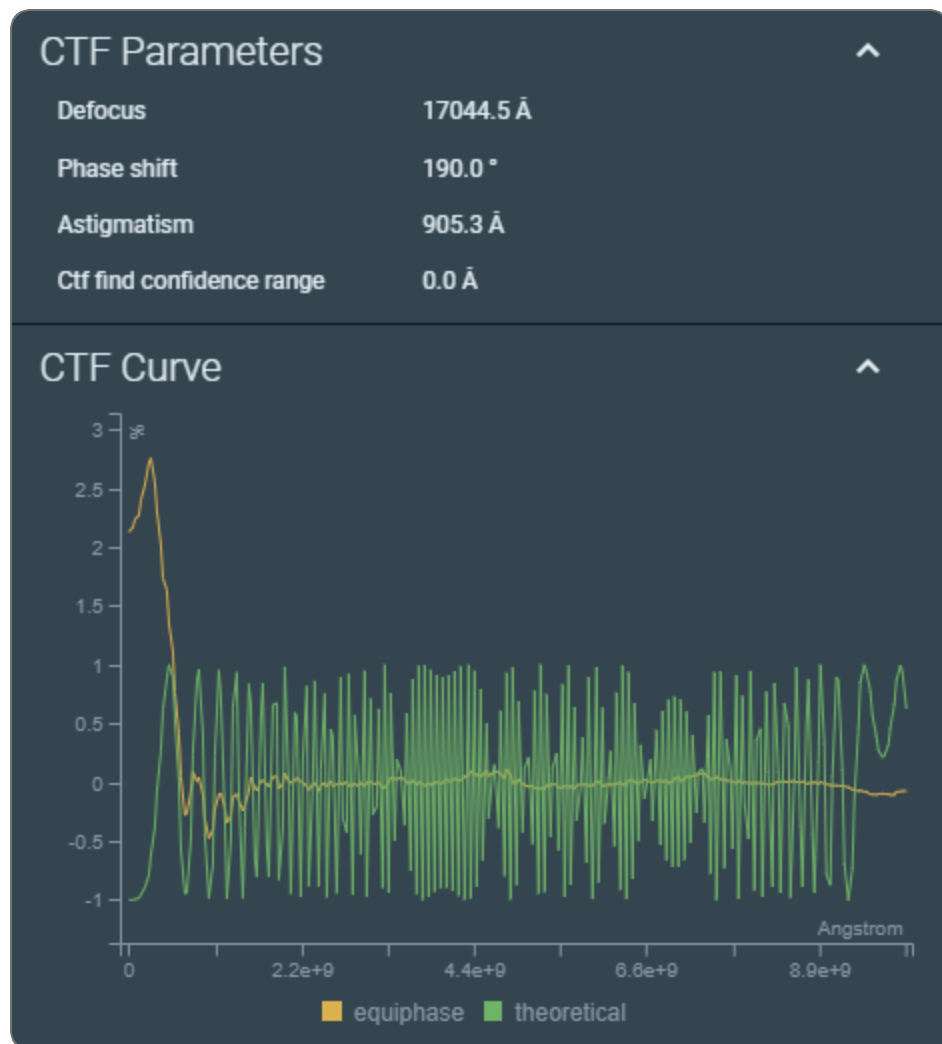
The motion correction panel

It is possible to change the scale factor of the displayed traces by using the control below the motion correction display.

CTF

The CTF panel shows the CTF parameters, the CTF curve with both experimental and theoretical results, and the FFT and fit.

CTF curve



The CTF parameters and curves

It is possible to toggle the visibility of both curves by clicking their label in the legend. The graph will automatically adapt its scale.

FFT Fit

The FFT fit is displayed in a basic image viewer with the following functionalities:

- An extraction of the 2D CTF fit to ease the analysis of the FFT fit, with a scale bar displaying the resolution in Ångström-1.



- The full image can be displayed with those functionalities:
 - ╕ Zoom in
 - ╔ Zoom out
 - 🔄 Reset the zoom
 - 🖥️ Toggle fullscreen viewing
 - It is also possible to exit the fullscreen mode by pressing the ESC key.

The following mouse and keyboard actions are available in the FFT viewer:

- Pan the image
 - Drag the image
 - Shortcuts: WASD keys, arrow keys
- Zoom in and out
 - Use the mouse wheel
 - Shortcuts: + and - keys
- Flip the image horizontally
 - Shortcut: F
- Rotate the image by 90°
 - Shortcuts: R (clockwise), Shift+R (counterclockwise)

A scale in Ångström-1 is also displayed to help the interpretation.

EPU Run Dataset Panels

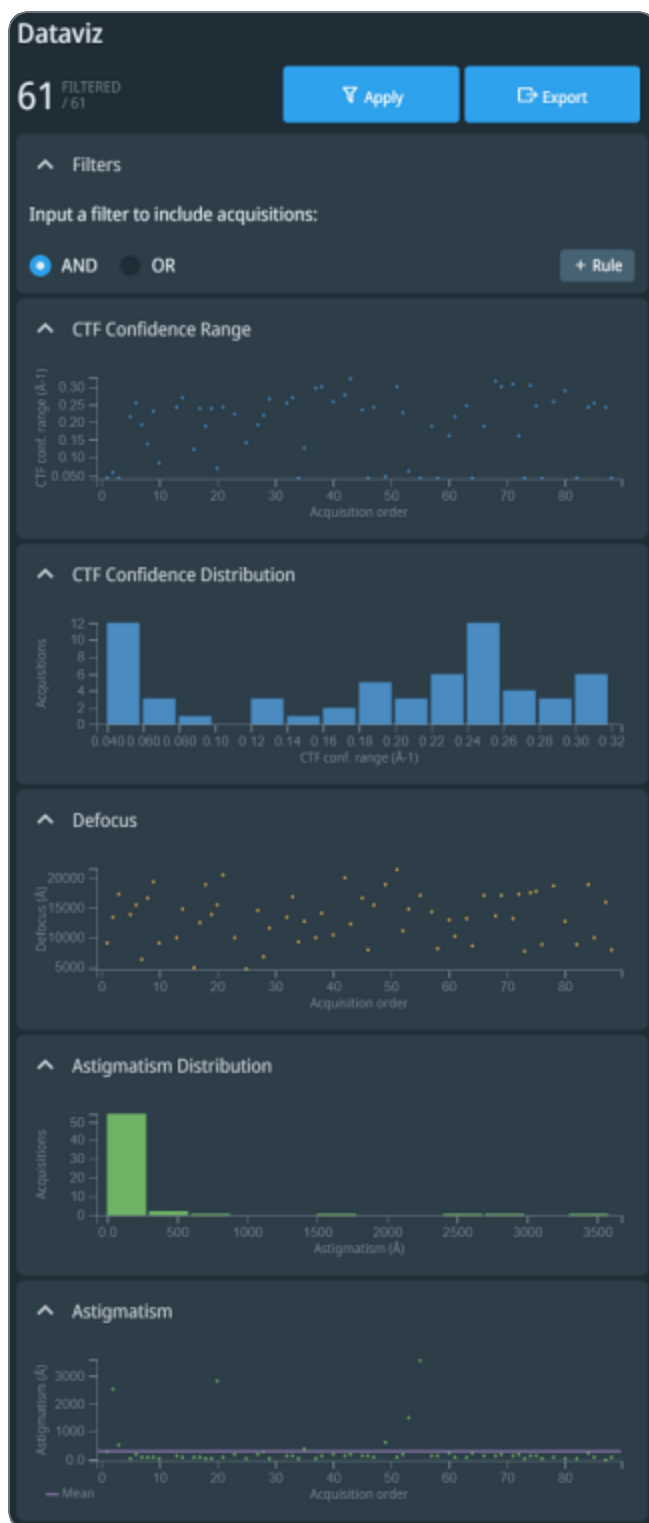
The **Dataviz** and **Quality report** panels are available on the EPU run dataset when using an SPA workflow with quality monitor

Dataviz

The Dataviz panel displays the following statistics on the whole EPU run:

- CTF confidence range
- CTF confidence distribution
- Defocus
- Astigmatism distribution
- Astigmatism
- Phase shift distribution*
- Phase shift*

** only if the phase plate detector is enabled*



The Dataviz panel for a completed run

Click **Export** (if the run is completed) or **Start Live Export** (when the run is in progress) to open the [Export](#) dialog.



When the run is in progress, click **Refresh** to update the information with newly-acquired micrographs.

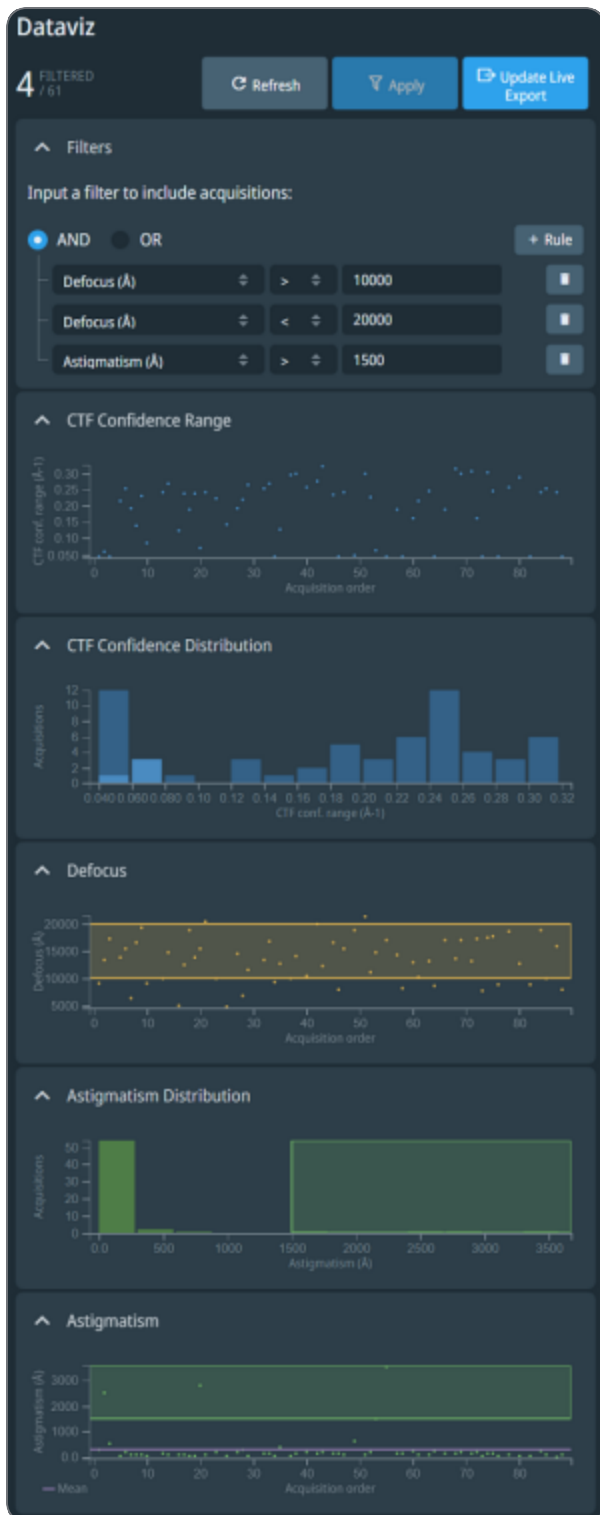


The Dataviz buttons for an in progress run

Filter Micrographs

To filter the micrographs to include in the view or in the export, specify values in the **Filters** sub-panel.

- Click the button to add a new rule  .
 - Choose a dimension to filter on (first input).
 - Choose an operator (second input).
 - Define the numerical value to filter on (third input).
- Delete a filter rule using the button .
- The charts reflect the filtered zones with boxes. For histograms, data corresponding to filtered-out plots change to a darker color.
- The number of matching micrographs appear in the bar at the bottom of the panel.
- Click **Apply** to save the filter.



Graphs with filters on

When a **live export** is running, after creating or modifying a filter, clicking on the **Update live export** button instructs the current live export to apply that new filter to upcoming data.


By default, the central area only shows filtered results. Even if no filters are on, micrographs that are being acquired, or whose motion correction/CTF are being computed, are incomplete and not show up in filtered results. Uncheck the **Show all results** checkbox in the top left of the central area to display all results, including incomplete ones. This also makes the **Show only errors** checkbox appear at the top-left of the central area.

Single Particle Analysis with Embedded CryoSPARC Live

Embedded CryoSPARC live (eCL) is a collaboration with Structura Biotechnology Inc. to develop an integrated version of CryoSPARC Live to enhance the efficiency of Thermo Scientific cryo-transmission electron microscopes significantly. Using the platform, the connection of eCL to EPU™ is automatic, no manual interactions are required. Only the picking parameters need to be provided by the user. Once the acquisition is started, Embedded CryoSPARC Live starts automatically to process the images. eCL is available using the workflow “Single Particle Analysis with Embedded CryoSPARC Live” in the platform.

Start CryoSPARC Live Processing

To start Embedded CryoSPARC Live, three parameters need to be provided. Refer to the EPU documentation to see how to start an EPU™ acquisition with Embedded CryoSPARC Live. Access to the Embedded CryoSPARC Live session page is made through the Embedded CryoSPARC Live Run in the Processing step which is created automatically when an EPU Run is created in a Screening or Imaging step using the dataset selection UI in the EPU™ application. Clicking on the Embedded CryoSPARC Live run opens a dedicated view that is shown below:

 Embedded Cr...

Embedded cryoSPARC Live (eCL) Settings

Fill the parameters in the “Input at EPU Run startup” column and press the Apply button to provide the data to eCL. When the EPU Run starts, eCL will automatically process the data, starting eCL Session manually is not needed.

To change the parameters while the acquisition is in progress or to stop the eCL Session, it is required to open eCL.

	Input at EPU Run startup		Currently used by eCL	
Minimum Particle Diameter*	100	Å	100	Å
Maximum Particle Diameter*	120	Å	120	Å
Extraction Box Size*	256	px	256	px

OPEN CRYOSPARC LIVE
 APPLY

The Embedded CryoSPARC Live view in CryoFlow.

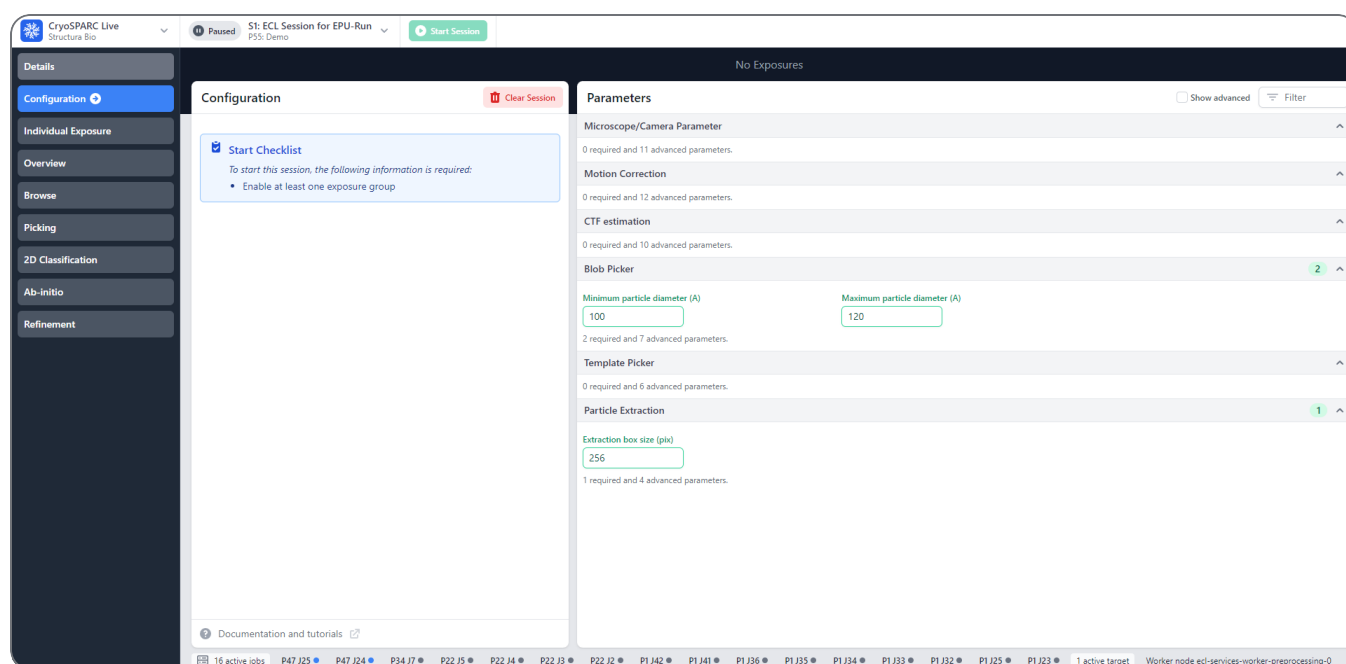
Single Particle Analysis with Embedded CryoSPARC Live

This view displays the three mandatory parameters that are required to start a CryoSPARC Live session:

- Minimum particle diameter (in angstrom)
- Maximum particle diameter (in angstrom)
- Extraction box size (in pixels)


If those parameters have been filled from the EPU application, the column "Input at EPU run startup" is filled. If the EPU Run has not started, you can still modify the input parameters and click the **Apply** button to send the values to the corresponding CryoSPARC Live session.

Clicking on the "Open CryoSPARC Live" button opens the CryoSPARC Live web page. For more information on CryoSPARC Live UI, refer to the online documentation available at this link: <https://guide.cryosparc.com/live/about-cryosparc-live>.



The CryoSPARC Live UI

As soon as the EPU Run starts, Embedded CryoSPARC Live will start processing automatically

as soon as the first micrograph has been acquired. Pressing the  button on the top of the page is not required anymore. If you need to change the picking parameters while the acquisition is in progress, these parameters can be directly modified in the CryoSPARC Live UI.

EPU Multigrid with Embedded CryoSPARC Live

Embedded CryoSPARC Live supports EPU Multigrid acquisition. Please read the EPU documentation to see on how to start an EPU™ Multigrid acquisition with Embedded CryoSPARC Live. During a multigrid acquisition, CryoSPARC Live will start and stop automatically on each grid without any manual intervention. Moreover, 2D Classification is launched automatically with a default of 50 classes when at least 5000 particles are picked.

Deletion Synchronization Between CryoFlow and Embedded CryoSPARC Live

Deletion action between CryoFlow and Embedded CryoSPARC Live are synchronized. The different behaviors are:

- From the CryoSPARC Live UI:
 - When a CryoSPARC Live Session is deleted from CryoSPARC Live UI then the corresponding eCL Run in the platform workflow is deleted.
 - When a CryoSPARC Live Project is deleted from CryoSPARC Live UI then all the eCL Run in the related platform workflow will be deleted. A new CryoSPARC Live project will be created if a new EPU Run is created in the platform workflow.
 - When the eCL Session is cleared then the corresponding eCL Run is cleaned. See [Cleanup](#).
- From CryoFlow portal:
 - When the workflow “Single Particle Analysis with Embedded CryoSPARC Live” is deleted then the corresponding CryoSPARC Live Project is deleted.
 - When an eCL Run is deleted then the corresponding eCL Session is deleted.
 - When a cleanup is performed on the eCL Run in the platform then the corresponding eCL Session is cleared.

Discovery Viewer


In the Single Particle Analysis and Tomography workflows, an initial assessment step is intended to investigate ice and particle quality on the grid in order to make decisions for the biochemistry and vitrification process, grid selection, and definition of the EPU or Tomography 5 setup. Performing data acquisition from various locations on the grid helps to determine which areas are suitable for further high-resolution imaging or increase data diversity. To simplify this time-consuming process, the Discovery-Viewer helps identify the imaged positions on the grid.

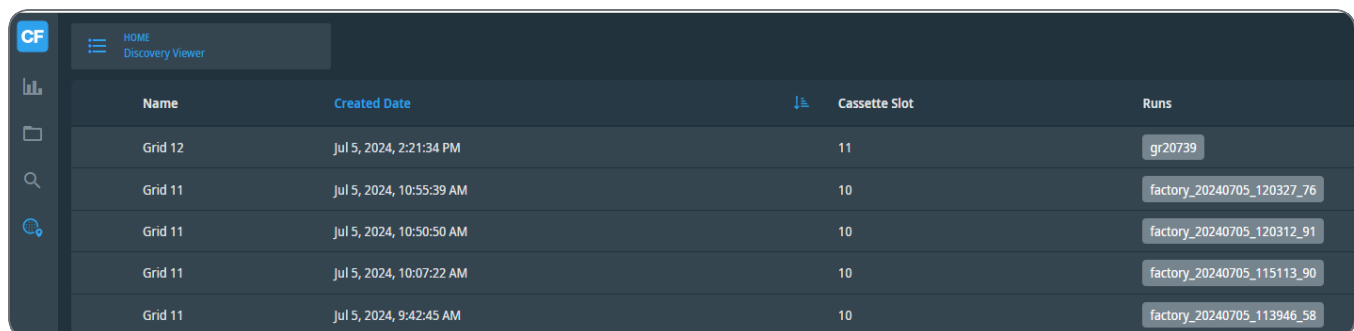
Access Discovery Viewer

The Discovery Viewer can be accessed in three different ways:

- From the sub-application icon
- From the EPU or Tomography 5 Run dataset view
- From each acquisition (micrograph or tilt series) view.

From the Sub-application Icon

To access the Discovery-Viewer using the sub-application icon, click on the icon  available on the left panel in the platform portal. The Atlas table displayed in the central view shows all the Atlas images that have been registered in the platform by the EPU™ or Tomography 5 application. See figure below for an example of Atlas table.




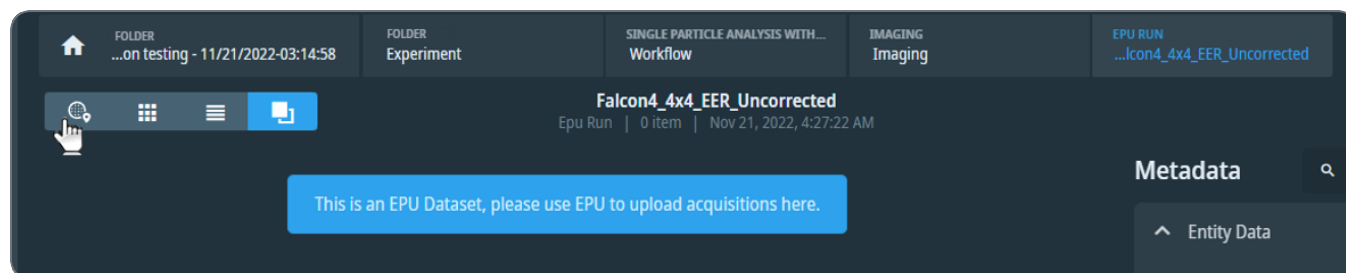
Name	Created Date	Cassette Slot	Runs
Grid 12	Jul 5, 2024, 2:21:34 PM	11	gr20739
Grid 11	Jul 5, 2024, 10:55:39 AM	10	factory_20240705_120327_76
Grid 11	Jul 5, 2024, 10:50:50 AM	10	factory_20240705_120312_91
Grid 11	Jul 5, 2024, 10:07:22 AM	10	factory_20240705_115113_90
Grid 11	Jul 5, 2024, 9:42:45 AM	10	factory_20240705_113946_58

You can sort them by Creation Date by clicking on the column header. Click on any row to display the related Atlas image in the Discovery-Viewer. For each Atlas image, the EPU or Tomography 5 Run that has been used for the data collection is shown in the "Runs" column. Clicking on the button navigates to the EPU or Tomography 5 Run view. To delete discovery-viewer data that are not useful, clicking on the trash can button will delete the atlas and Grid Square or Search Map images. The acquisitions are not deleted. To delete them the EPU or Tomography 5 Run needs to be deleted. When Atlas images have been deleted, it is shown clearly in the Atlas table. The line can be deleted from the table by clicking on the trash can

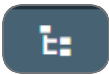
button .

From the EPU or Tomography 5 Run Dataset View

From an EPU or Tomography 5 Run dataset, when clicking on the icon  available on the top left of the central view (see figure below) displays the Atlas image where the acquisition has been performed. Clicking on the Grid Square or Search Map marker on the Atlas image opens the discovery-view sub-application.



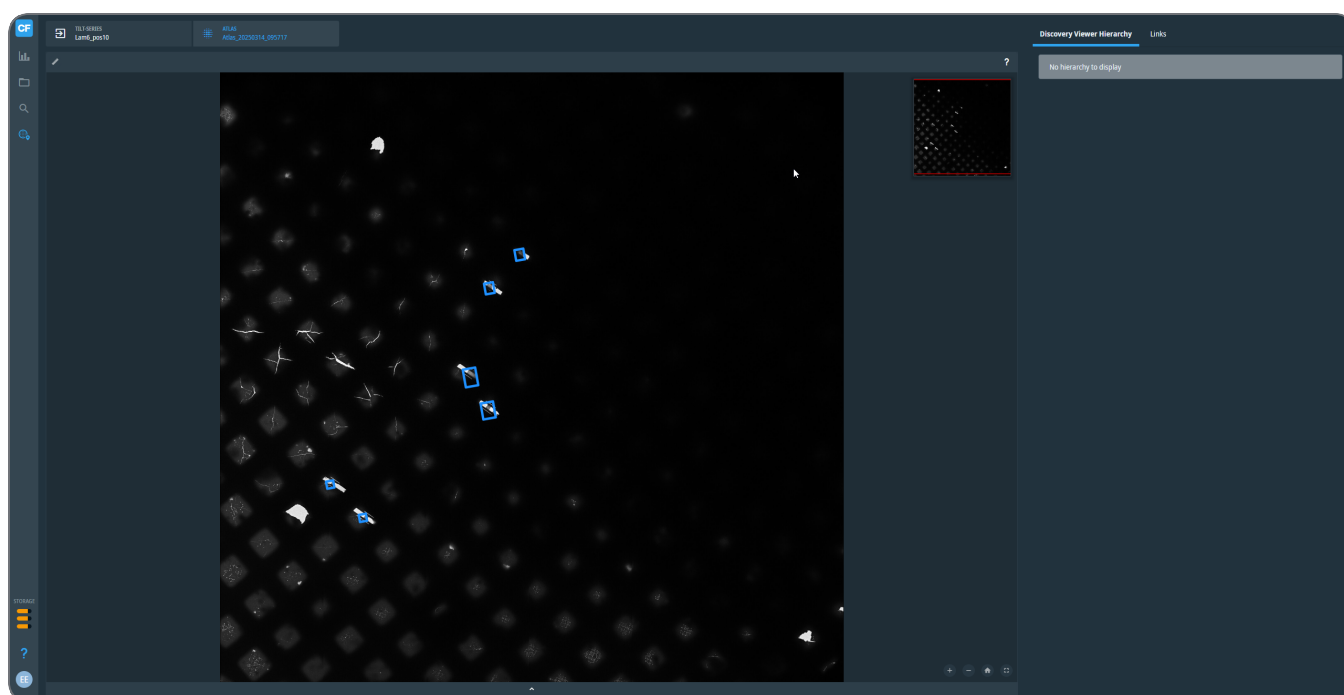
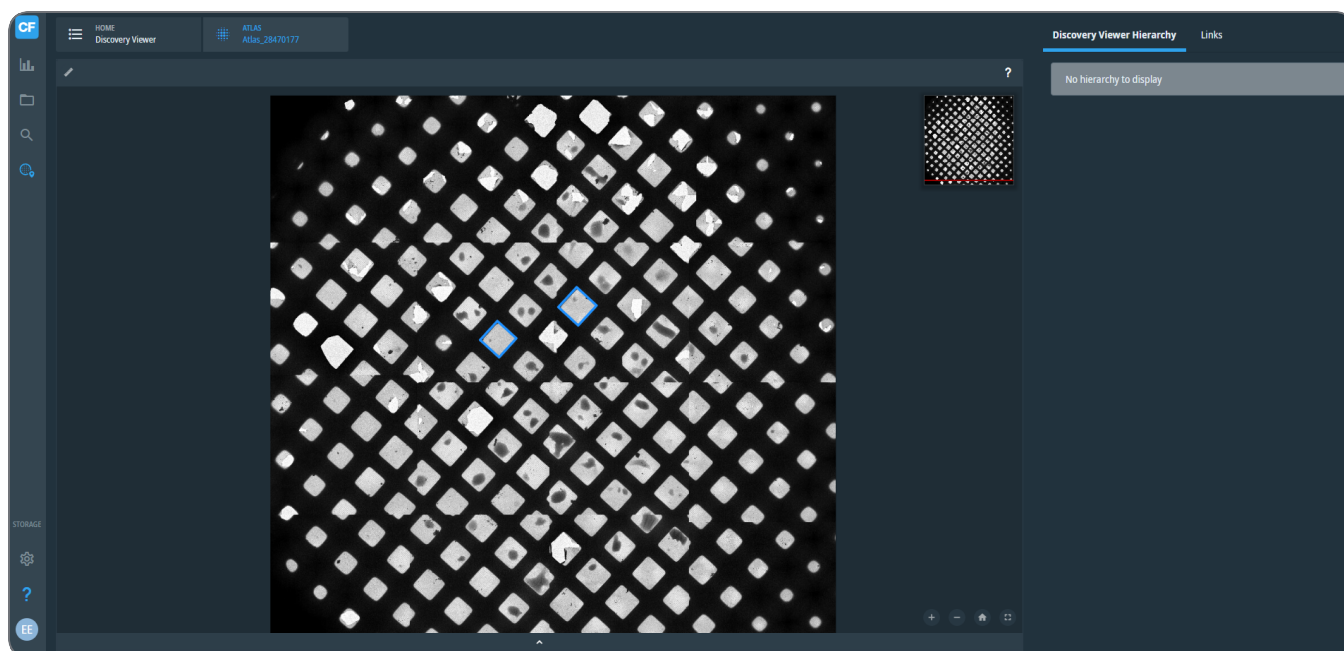
From the Acquisition View

To access the Discovery-Viewer from one of the acquisitions in an EPU or Tomography 5 dataset, open the right panel and select the hierarchy tab by clicking on the icon .

Navigation

Basic Navigation

In the Discovery-Viewer, you can navigate easily from Atlas images to acquisitions that have been acquired by EPU™ or Tomography 5 application. The figures below display an Atlas image displayed in the Discovery-Viewer.



Atlas Image from a Tomography Run Displayed in Discovery-Viewer

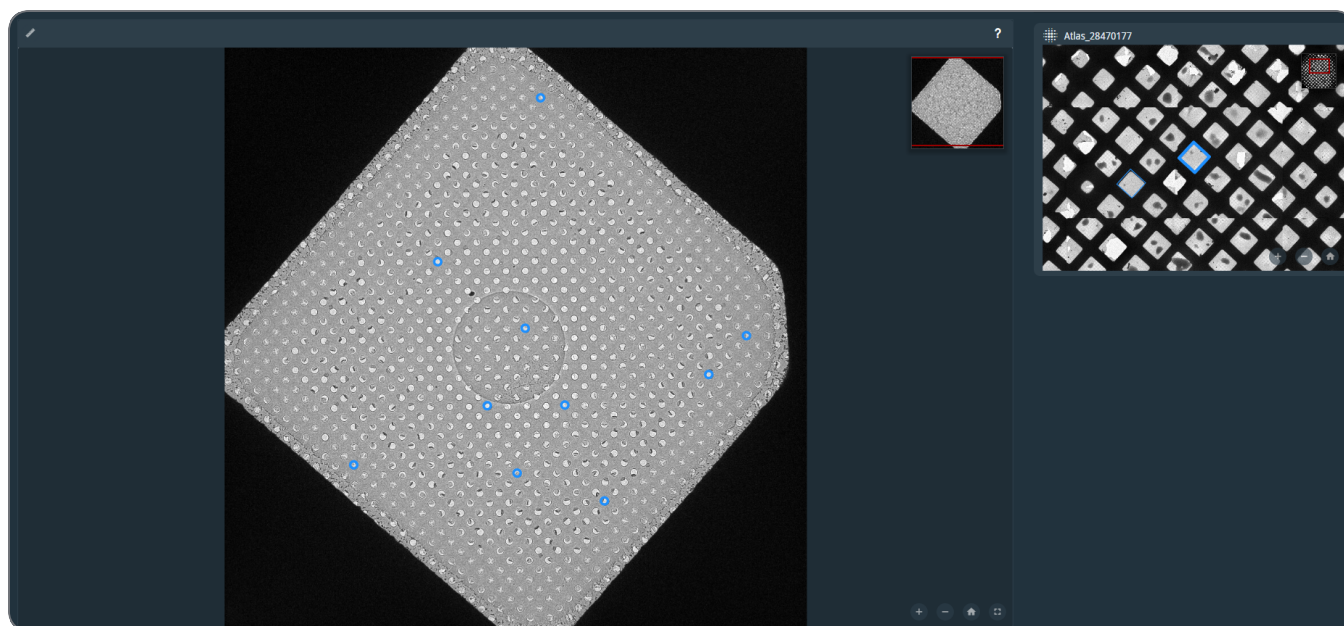
The displayed markers correspond to Grid Squares or Search Maps that have been acquired by EPU™ or Tomography 5. The colors are the same as EPU™ or Tomography 5 application and correspond to the status of each acquisition areas:

- Blue: Terminated
- Green: In Progress

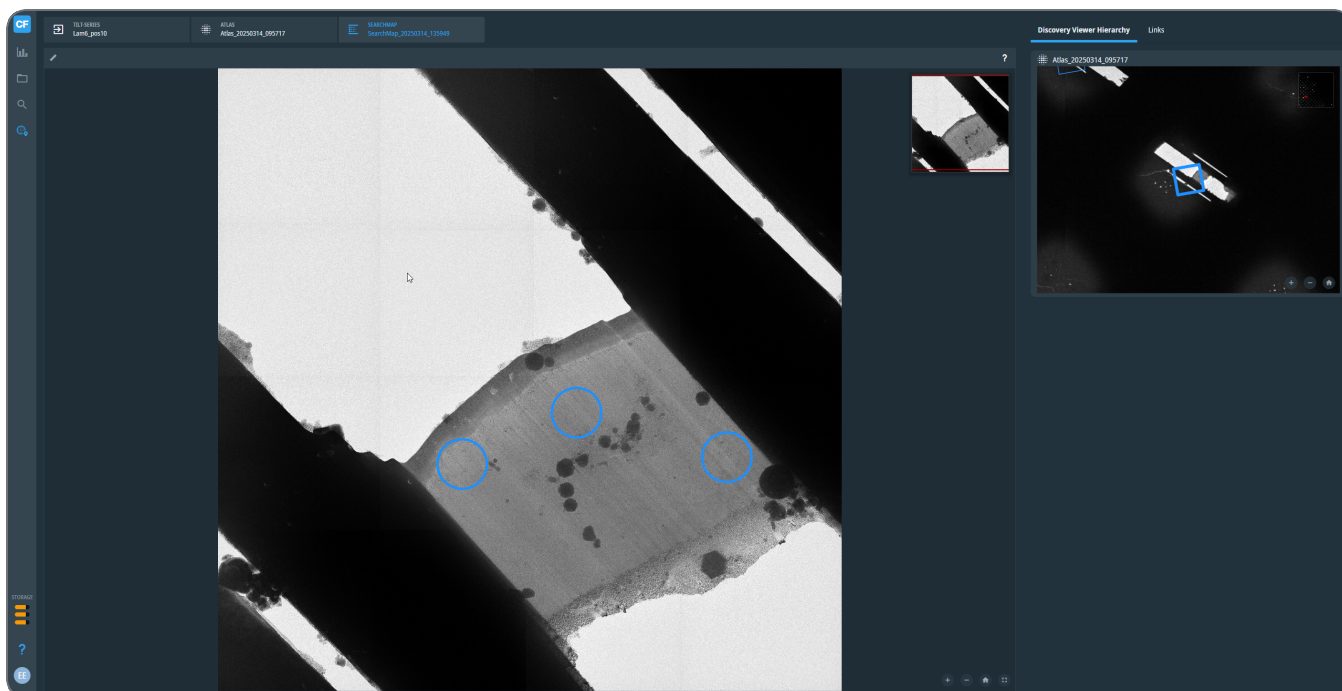


Note: The color scheme is reversed compared to the platform front-end application.

Clicking on a marker opens the Grid Square or Search Map image in the central view and displays the Atlas on the right. The location on the Atlas is highlighted and centered. The same viewer functionalities are available on the hierarchy panel on the right. The figures below display the corresponding view:

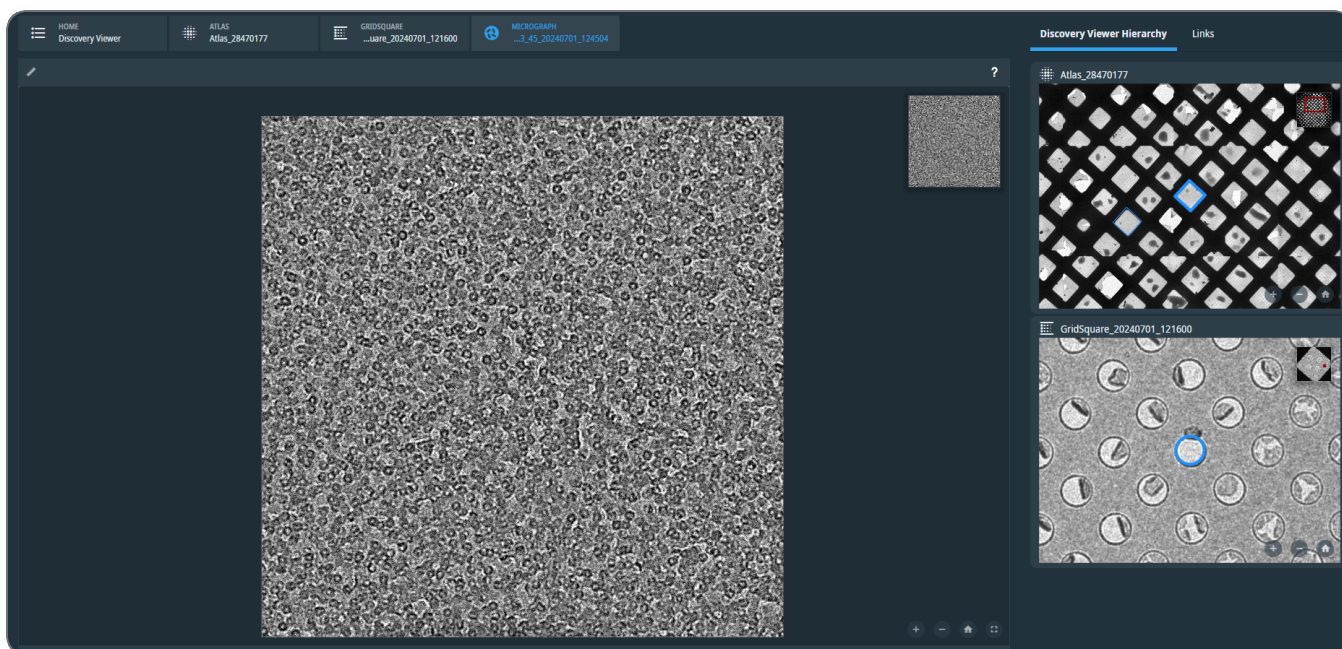


Grid Square image from an EPU run Displayed in Discovery-Viewer

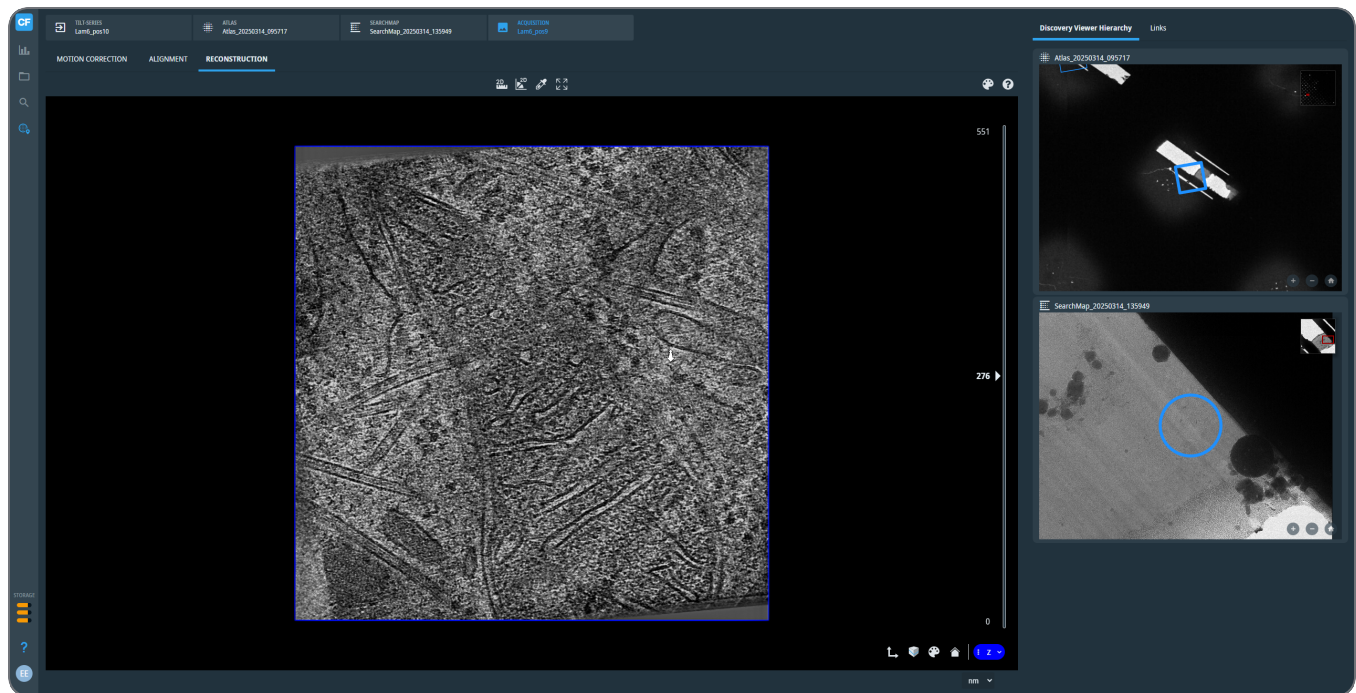


Search Map Image from a Tomography 5 run Displayed in Discovery-Viewer

Clicking on a marker on the Grid Square or Search Map image displays the acquisition in the central view and updates the navigation hierarchy on the right panel to display the Grid Square or Search Map. The figures below display an example of an acquisition view:



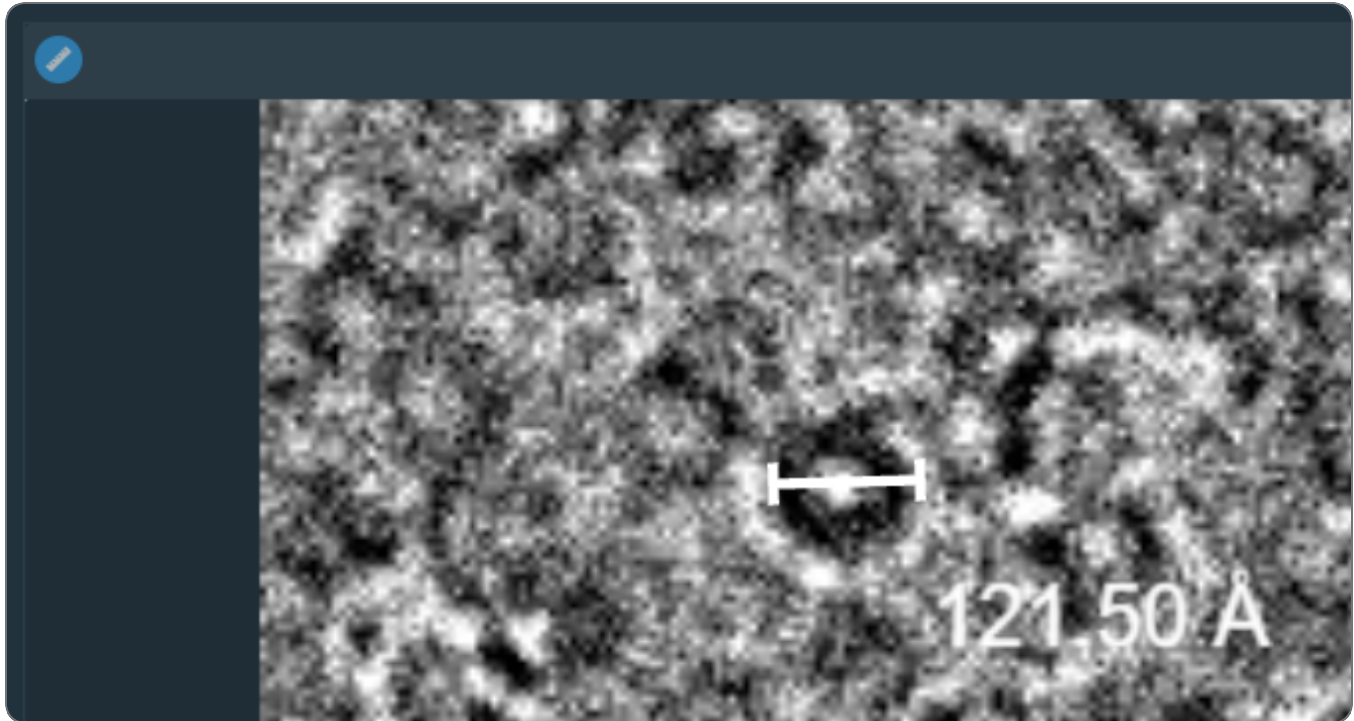
Micrograph Image from an EPU run Displayed in Discovery-Viewer



Tilt-series from a Tomography 5 run Displayed in Discovery-Viewer

Ruler

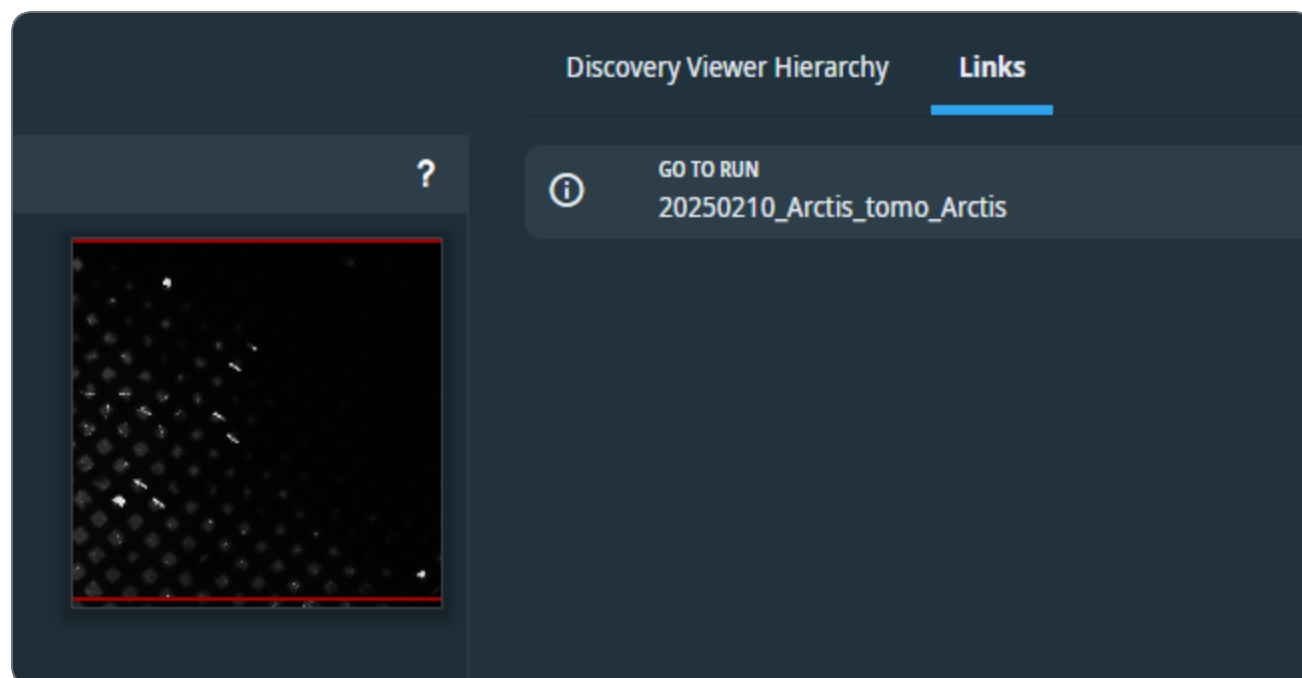
A ruler has been added to the top left of each image, allowing users to measure distances accurately. The pixel size of the image is retrieved to ensure reliable measurements.



Link Panel

Atlas Level

On the right panel in the Discovery Viewer, a link panel is available to navigate easily between the EPU or Tomography 5 Run dataset view and the Discovery Viewer. On the Atlas image, clicking on the link panel displays all EPU Run or Tomography 5 dataset that have been created on that Atlas:

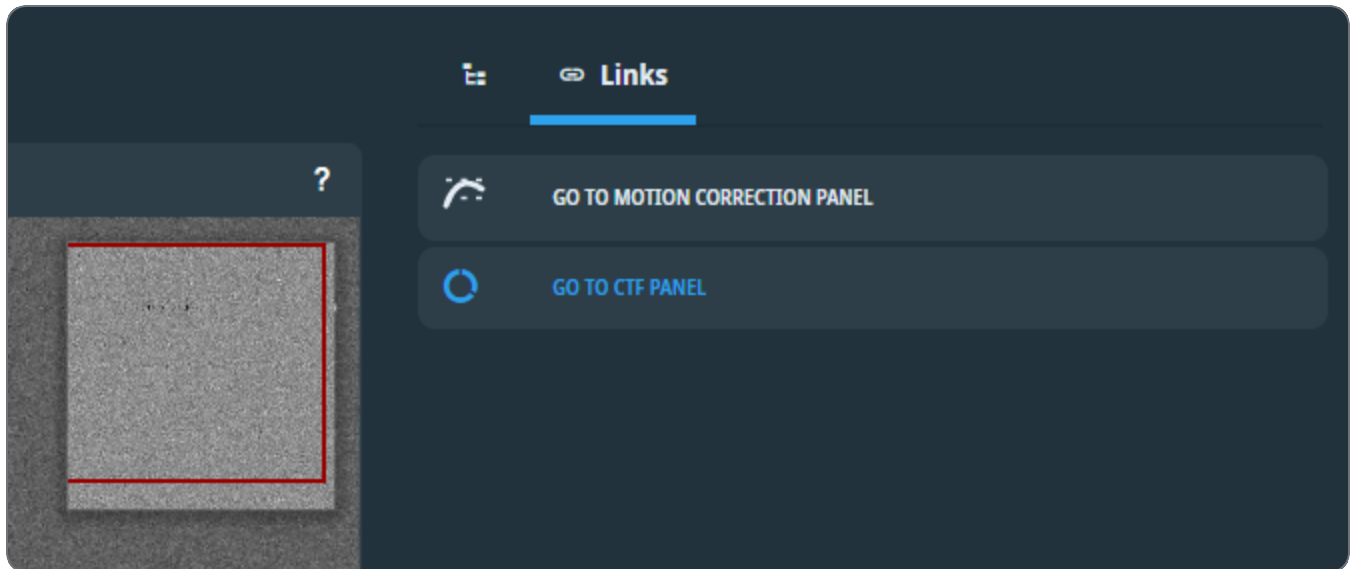


Acquisition Level

The same functionality is available at the acquisition level. It depends on the workflow type selected for the acquisition. If it's Single Particle Analysis workflow with a quality monitor (see [Single Particle Analysis with Quality Monitor](#)), the link panel redirects to the micrograph view in the EPU Run dataset:

- Clicking on "Go to Motion Correction panel" displays the micrograph view with the Motion Correction right panel.
- Clicking on "Go to CTF panel" displays the micrograph view with the CTF right panel.





See the figure below of the link panel at the acquisition level for the Single Particle Analysis workflow with quality monitor.





For other workflows, clicking on "Go to micrograph" or "Go to acquisition" displays the acquisition view with the metadata right panel.

Toolbar

On every image (except the acquisition view in Tomography workflow) displayed by the Discovery-Viewer a toolbar is available:

-  Zoom in
-  Zoom out
-  Recenter the image
-  Display the image in full screen

For the acquisition view in Tomography workflow:

- The view can be zoomed in or out by scrolling the mouse wheel.
- The view can be re-centered with the tool on the right bottom of the view 
- The acquisition can be displayed in full screen with the tool on top of view 

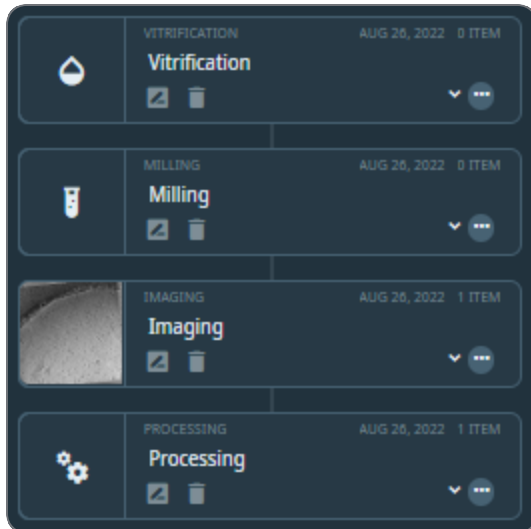
Data Availability

To ensure that the images are always available in the Discovery Viewer, even if the EPU or Tomography 5 Session folder is removed from the offload storage, the Discovery Viewer generates a downscale version of each image on-the-fly using "Fourier cropping" with a binning value that depends on the file type:

- **Atlas**: no binning is applied
- **Grid Square** or Search Map: binning 2
- **Micrograph** or Tilt-Series: binning 4

Cryo Electron Tomography Workflow with Tomo Live

This workflow is designed to manage data produced by instruments used in the Cryo-Electron Tomography workflow from sample preparation to processing. The image below shows the four steps of the workflow:



The four steps of the Cryo-Electron Tomography workflow

The Vitrification, Milling and Processing steps are not currently used. Only the Imaging step which is dedicated to cryo-EM data collection with Tomography 5. During the acquisition, the live reconstruction pipeline Tomo Live processing is automatically triggered. See the [Tomo Live](#) section for more details.

Tomography 5 Acquisition Workflow Setup

Create the Workflow

1. Go to the folder in which you want to create the workflow.
2. Click **Add Workflow** at the top of the central area.
3. In the creation dialog, choose a name for the workflow.
4. Choose "Cryo-Electron Tomography with Tomo Live" in the Type combo box.
5. Click **Create Workflow**.

Create a Tomo Run Dataset

1. Go to the Imaging step to add the dataset.
2. Click **Add Dataset** at the top of the central area.
3. In the creation dialog, click **Tomo Run**.
4. Choose a name for the dataset.
5. Click **Create Dataset**.

Tomography 5 Acquisition

For information about setting up an acquisition, refer to the Tomography 5 User Guide.

Tomo Live

Tomo Live is a live reconstruction pipeline, triggered during a tomography acquisition made by Tomography 5. The pipeline is divided into two steps.

Motion Correction

For each *fractions* or *eer* file that is registered in the platform by Tomography 5, the motion correction algorithm is triggered. It applies global drift correction on the input image. Depending on the electron dose, fractions or eer frames are averaged.

Processing Workflow

After generation of the motion corrected tilt series, the alignment and reconstruction algorithms are divided into several steps:

1. **Clean Stack**: clean obvious bad slices.
2. **Pair-Alignment**: align the raw stack using cross-correlation between pairs of slices. The 0° tilt angle is taken as a reference.
3. **Tomogram Positioning**: determine the X and Y tilt correction of the tomogram. Tilt angles take the Y tilt correction into account for next steps.
4. **Marker-less tracking**: use patch-tracking based on cross-correlation to track patches on the tilt series. Trajectories of patches are then used to determine rotation, magnification, and residual shifts to align the tilt series.
5. **CTF determination**: perform strip based CTF determination on the raw stack. Slices considered bad by the previous steps are removed.

6. **Reconstruction:** perform SIRT reconstruction with bin 4. Thickness of the tomogram is automatically determined based on contrast.
7. **Sample thickness determination:** the sample thickness is automatically determined from the 3D reconstruction.

Output Alignment Parameters

Tomo Live generates some parameters to assess the quality of the alignment.

Bad Slice Detection

Tomo Live can detect if the tilt series contains some bad slices and discards them automatically.

Tracking Correction

Value of the shifts applied between slices to correct for mis-tracking in Tomo 5.

Alignment Accuracy

The alignment accuracy value is the residual value between the fiducial positions used for tracking and theoretical positions. The theoretical positions are determined from the 3D object reconstructed using the projection of the feature positions of each tilted view and back-projected in 2D with corrections of displacements, rotations, and magnification. The process is iterated until convergence.

Rotation Correction

At the end of the alignment, rotation correction is applied on each slice. The value of the rotation considers the tilt axis value and correction around its value (called tilt axis correction).

Output CTF Parameters

Handedness Check

During CTF determination, the handedness of the tilt-series is checked by ensuring that variation of the defocus is coherent with the tilt angle value. The output can be:

- **Correct:** defocus is coherent with tilt angle values.
- **Uncorrect:** the defocus is not coherent with the tilt angle values. It can be due to reversed tilt-angles, tilt axis off by 180° or flipped projections.
- **Undetermined:** the handedness check algorithm has failed (too noisy, ...) to check the handedness.

Defocus Values

For each slice of the tilt-series, the algorithm determines the defocus value taken at the tilt-axis. The algorithm assumes that there is no variation of the z-height for each slice.

Astigmatism Values

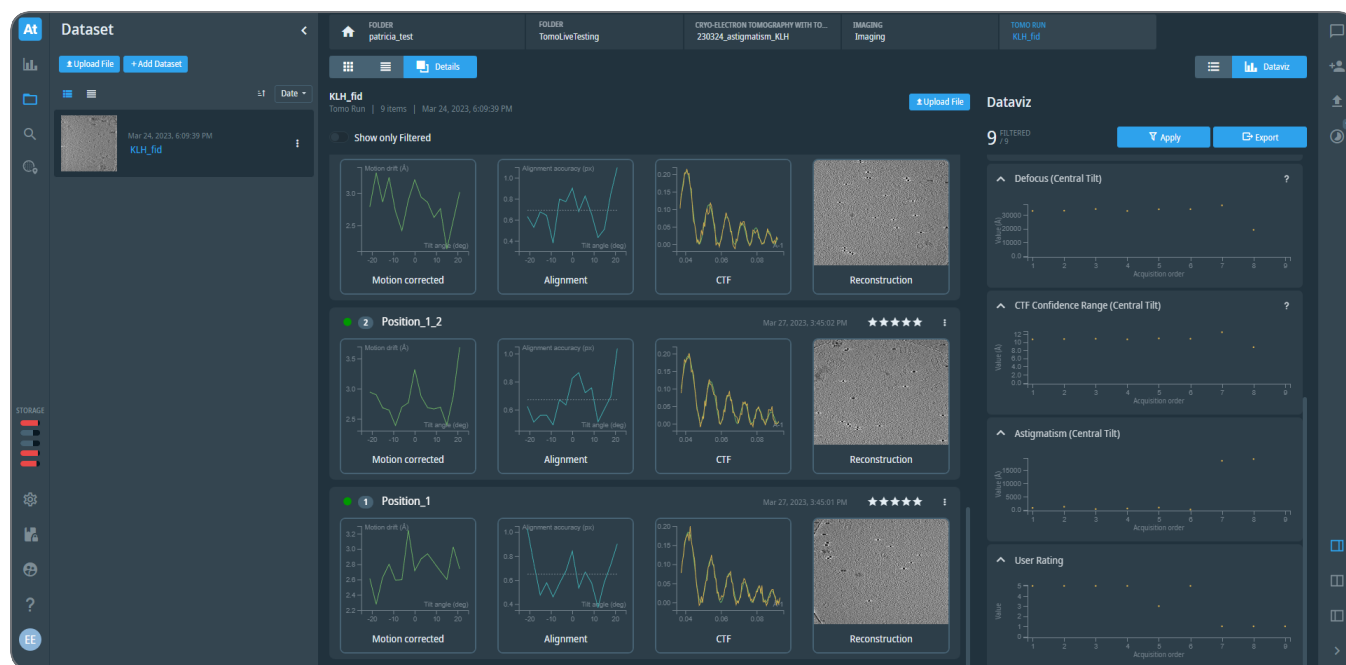
Tomo Live determines the astigmatism of the central slice only. This astigmatism value is then propagated to each image of the tilt-series to calculate the equiphase average power spectrum.

CTF confidence Range Values

For each slice of the tilt-series, the algorithm estimates a resolution in (1/Angstrom) based on the last point of the frequency used for the curve fitting. This last point is determined automatically based on the number of ctf zero that have been found by the algorithm.

Tomo Run View

When clicking on a Tomo run dataset, a dedicated front-end for cryo-electron tomography acquisition is displayed. The image below displays the front-end with the overview of the Tomo Live results in the central part and the Dataviz panel on the right (see [Dataviz for Cryo-Electron Tomography](#)).



Overview of Tomo Live Results

This view presents a quick overview about the alignment quality for each tilt-series. For each tilt-series, three cards are displayed:

- **The motion correction card:** the motion drift (in angstroms) as a function of the tilt angle (in degrees) is displayed.
- **The alignment card:** the alignment accuracy (in pixels) as a function of the tilt angle (in degrees) is displayed. The alignment accuracy is the residual value in pixels of feature positions and theoretical ones. Values close to zero increase confidence on the alignment success.
- **The CTF card:** the ctf fitting curve between experimental and theoretical is displayed for the central slice of the tilt-series.
- **The reconstruction card:** a preview of the central slice of the reconstruction is shown. An averaging of ten slices around the central slice is performed.

Dataviz for Cryo-Electron Tomography

A summary of some alignment parameters is shown in the Dataviz panel for each tilt-series in the Tomo run. Each tilt series has a corresponding acquisition order number. Three quantities are displayed as a function of the acquisition order. For filtering on those quantities, see [Filter Micrographs](#).

Alignment Accuracy

This is the average value (in pixels) of the alignment accuracy chart shown on the alignment card. Values close to zero increase confidence of the alignment success. A threshold at 4 pixels is displayed. Acquisition with values higher than the threshold have an exclamation point indicating that a manual check of the alignment quality needs to be performed. For more details, see [Alignment Accuracy](#).

Number of Deleted Slices

Number of slices of the raw tilt-series that are considered bad by Tomo Live and deleted during alignment. For more details, see [Bad Slice Detection](#).

Tilt Axis Correction

The tilt axis correction value (in degrees) determined by Tomo Live during alignment. If almost all tilt-series have the same average value, it may indicate a problem with tilt axis calibration. For more details, see [Rotation Correction](#).

Defocus (Central Tilt)

Defocus of the central (in Angstrom) determined during the CTF determination step. For more details, see [Defocus Values](#).

Ctf Confidence Range (Central Tilt)

CTF Confidence Range(in 1/Angstrom) determined during the CTF determination step. For more details, see [CTF confidence Range Values](#).

Astigmatism (Central Tilt)

Astigmatism of the central slice (in Angstrom) determined during the CTF determination step. For more details, see [Astigmatism Values](#).

User Rating

Rating values provided by the user for each tilt-series. To update the value in the Dataviz panel, the page needs to be reloaded.

Sample Thickness

Tomo Live automatically computes the thickness of the sample from the 3D reconstruction. The user can overwrite this value from the reconstruction panel in the platform portal when clicking on the reconstruction card.

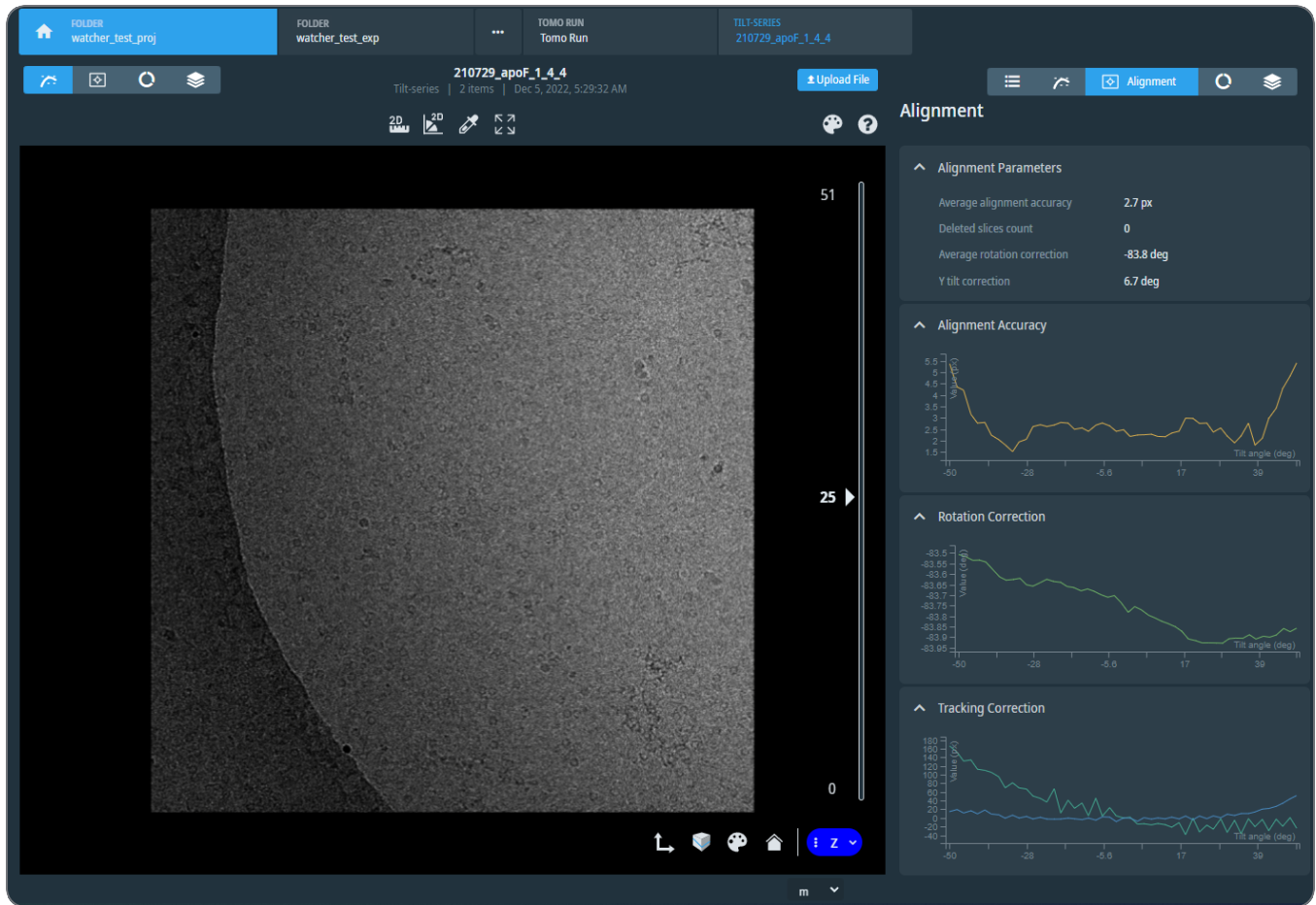
Inspect Reconstruction and Image Stack

To inspect the tilt-series generated at each step of the processing, you can:

- Click on the motion correction card to visualize the motion corrected tilt-series.
- Click on the alignment card to visualize the aligned tilt-series.
- Click on the CTF card to analyze CTF determination results.
- Click on the reconstruction card to visualize the 3D reconstruction.

On the right panel, dedicated information for each step is displayed.

An example of the alignment view is shown below.



Motion Correction Panel

The motion correction panel displays the motion drift (in angstroms) as a function of the tilt angle (in degrees).

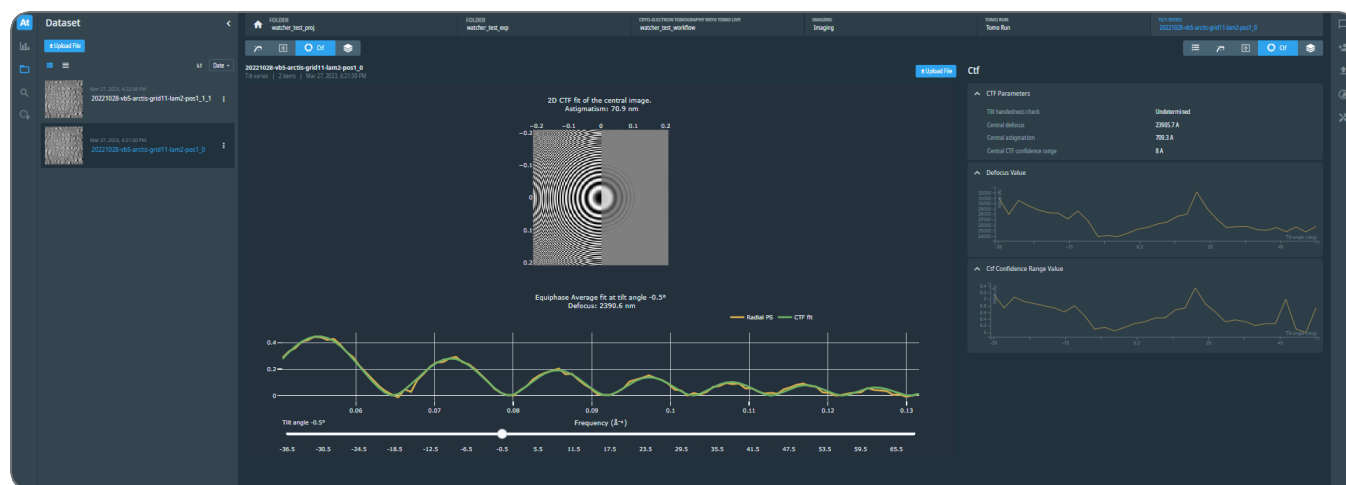
Alignment Panel

The alignment panel shows:

- Alignment parameters:
 - Average alignment accuracy: the average value of the alignment accuracy chart.
 - Deleted slices count: number of deleted slices.
 - Average rotation correction: the average rotation value.
 - Y tilt correction: the Y tilt correction applied to the tilt angle values.
- Alignment charts:
 - Alignment accuracy: for more details see [Alignment Accuracy](#).
 - Rotation correction: for more details see [Rotation Correction](#).
 - Tracking correction: for more details see [Tracking Correction](#).

CTF View

When clicking on the CTF card, the CTF fitting curves are displayed in the central view. See the image below for an example.



This view displays:

- The 2D CTF fit of the central slice.
- The equiphase average for each tilt angles that can be changed using the slider.

Drag and pan to zoom in on a chart or double click to zoom out. A toolbar is available for basic chart manipulation (screenshot, zoom, pan, auto-rescale, reset). On the right of the platform portal, the CTF panel displays some quality metrics regarding the CTF determination step:

- CTF Parameters:
 - Tilt handedness check: result of the handedness check algorithm. Values can be Correct, Uncorrect, Undetermined. See [Handedness Check](#) for more information.
 - Central defocus: defocus value of the central slice of the tilt-series.
 - Central astigmatism: astigmatism value of the central slice of the tilt-series.
 - Central CTF confidence range: resolution estimation of the central slice. It is based on the last frequency point used for the ctf fitting.
- CTF Charts:
 - Defocus value: defocus variation as a function of the tilt angle, for more details see [Defocus Values](#).
 - Ctf confidence range value: estimated resolution values as a function of the tilt angle, for more details see [CTF confidence Range Values](#).

Reconstruction Panel

The reconstruction panel contains two expandable panels:

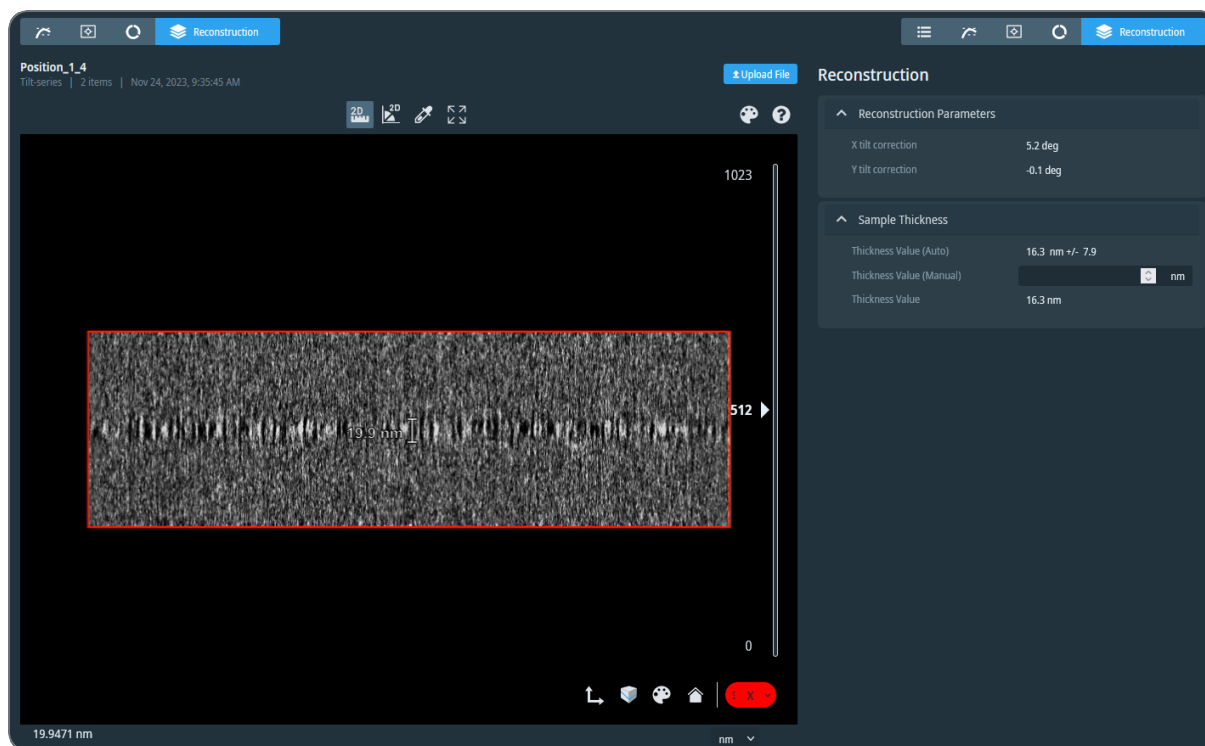
The **Reconstruction Parameters** expandable panel that displays the rotation applied to the tomogram to set the sample horizontal in the XZ and YZ plane.

- **Y tilt correction:** the Y tilt correction applied to the tilt angles to obtain a horizontal reconstruction in the XZ plane.
- **X tilt correction:** the X tilt correction applied to the reconstruction to obtain a horizontal reconstruction in the YZ plane.

The **Sample Thickness** expandable panel displays:

- The sample thickness determined automatically by the algorithm. The uncertainty of the measurement is also displayed.
- The sample thickness provided by the user. If the value provided by the algorithm is not accurate enough, the value can be overwritten manually. This updates the corresponding value in the Dataviz panel.
- The sample thickness value used by the Dataviz panel.

The figure below displays the reconstruction view with the different parameters. In this example with an Apoferritin reconstruction we can see that the value provided for the sample thickness by the algorithm is really close to the manual measurement.



Export Tomo Run with Tomo Live Data

To export a Tomo Run, select the **Export** action. If some filters have been defined with the Dataviz panel, the export only contains positions that fulfill the filtering.

There are two different export options: standard export and IMOD/Relion export.

Export

The following data from "Tomo Run for Export" will be exported in a folder.

Folder path
Specify an optional path name for the export folder. The folder name will be suffixed with a timestamp.
Path/To/Folder
Path cannot contain invalid characters, like : * ? \ < > | .

Data to export
☒ All Data ☐ Filtered Data only

Data type to export
Files: ☐ Raw ☒ Processed
Metadata: ☐ Raw ☐ Processed
☒ Additional Tomo Live metadata to import in IMOD and Relion ?

Cancel Export

Standard export

The standard export has two functions:

- Export all the files of the dataset. This includes the raw files and/or the processed file generated by Tomo Live.
- Export all metadata from the dataset as a .json file.

Relion export

Export Tomo Live data with additional files to allow Tomo Live results to be used in IMOD 4 or Relion 4. The additional files generated are:

- IMOD files: *.rawtilt, *.tilt, *.xf, *.defocus.
- Relion files: the order list per position (*.csv) and the *.star file.

If Tomo Live has removed some bad slices, then the export generates a *clean.mrc stack in which the bad slices have been removed.

Tomo Live data in IMOD or Relion

When the Relion export is selected, Tomo Live motion corrected stack and tilt-series alignment can be used directly in IMOD (see [Tomo Live in IMOD](#)) or Relion (see [Tomo Live in Relion](#)).

If Tomo Live has detected some bad slices during the export, it creates a new stack (*clean.mrc). When used in IMOD or Relion, this new stack must be used along with the other generated files.

Tomo Live in IMOD

When the IMOD/Relion export is selected, these IMOD files are generated:

- *.rawtilt*: raw tilt angles for the position without Y tilt correction.
- *.tilt*: tilt angles corrected with the Y tilt correction (see [Processing Workflow](#)).
- *.xf*: transformation matrix for each tilt-angle determined by Tomo Live to align the tilt-series.
- *.defocus*: defocus file in the Ctfplotter format.

Without performing any prior alignment steps in IMOD, Tomo Live stacks can be used directly in IMOD to:

- Generate new aligned stacks with a different binning.
- Use *Ctfplotter* to determine new defocus files.
- Perform new 3D reconstructions.

To obtain more information on IMOD, please visit <https://bio3d.colorado.edu/imod/doc/guide.html>.

Tomo Live in Relion

Relion 4 can perform a sub-tomogram averaging pipeline. For each position, the IMOD format alignment files (see [Tomo Live in IMOD](#)) are needed.

The Relion export generates two Relion specific files:

- The order list (*.csv) that stores the chronological order in which the images of the tilt-series have been acquired.
- The star file (*.star) that describes the location of the different tomograms needed to import data in Relion.

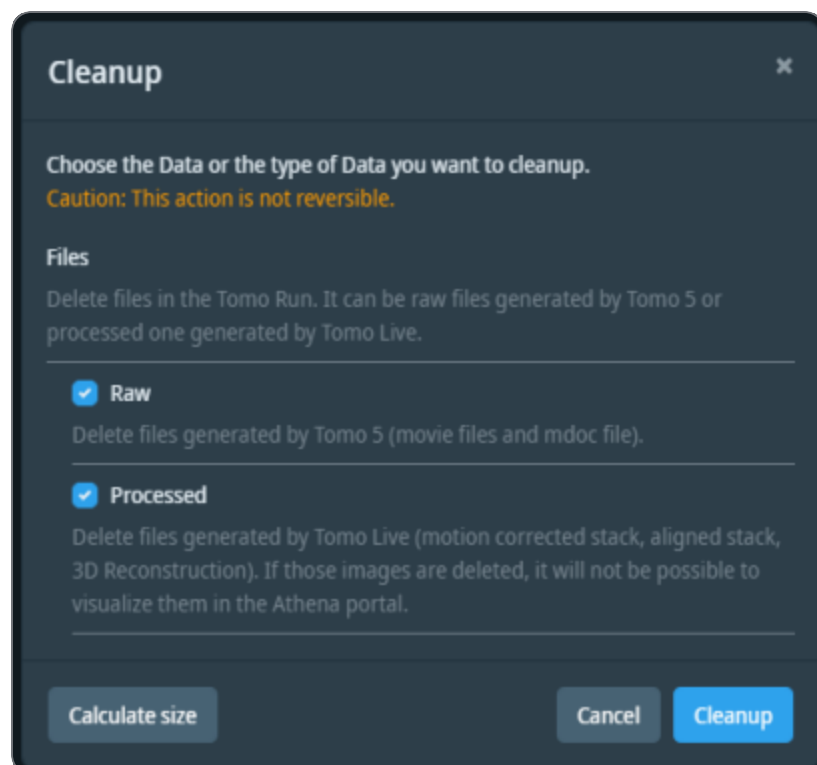
For more information please visit <https://relion.readthedocs.io/en/release-4.0/>.

To pick particles using Tomo Live data, first reconstruct a new tomogram with IMOD.

The reconstruction provided by Tomo Live corrects the object orientation in the tomogram around the axis perpendicular to the tilt-axis (x-tilt, also called "elevation"). Most subtomogram averaging pipelines do not support this.

Clean up a Tomo Run Dataset

On a Tomo Run dataset, the cleanup functionality allows you to choose if you want to delete raw data (Movies and mdoc files) registered in the platform by Tomography 5 and/or the processed one generated by Tomo Live (Motion Corrected stack, aligned stack and reconstructed stack).



Cleanup modal available on a Tomo Run in a cryo-electron tomography workflow.