



EOSC-Life

Science Demonstrator: CryoEM

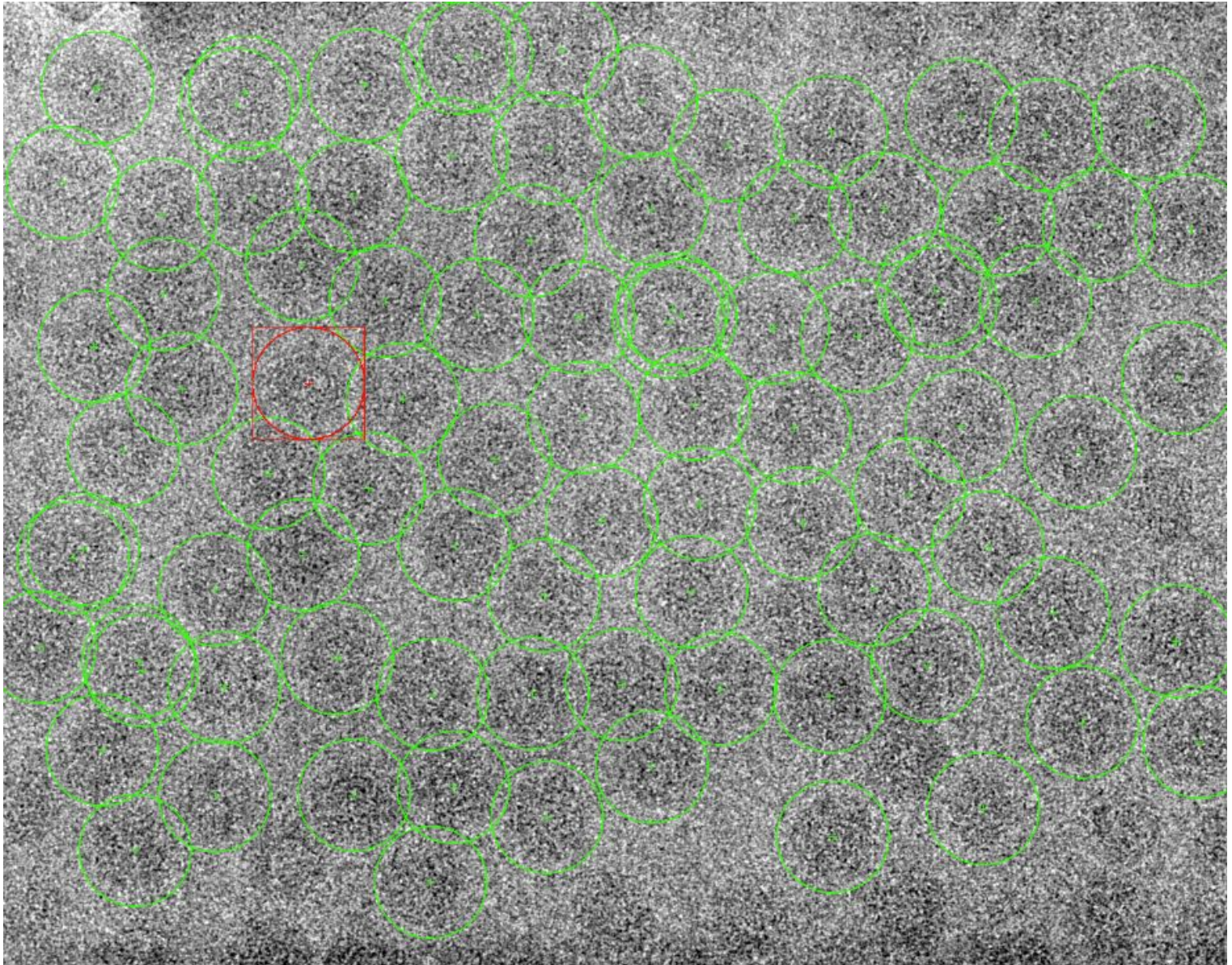
C.O.S. Sorzano

Biocomputing Unit, CNB-CSIC

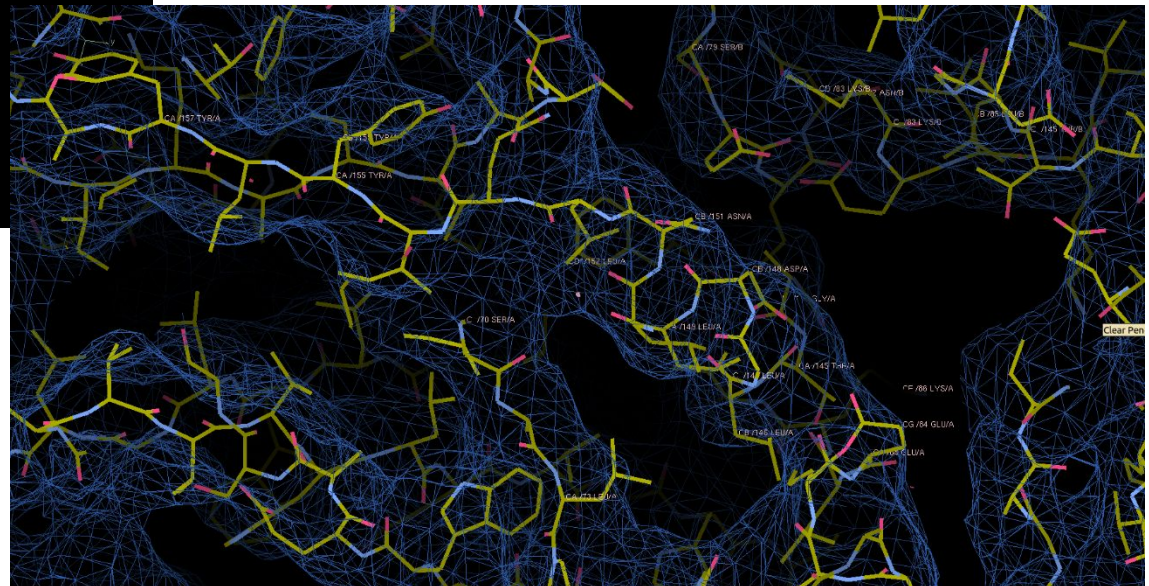
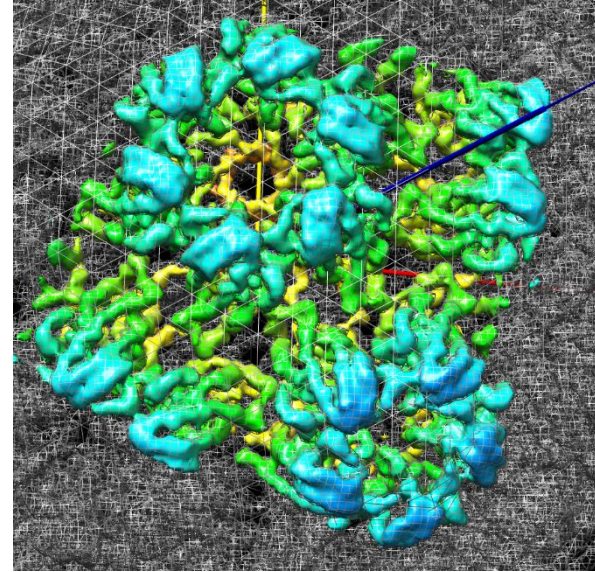
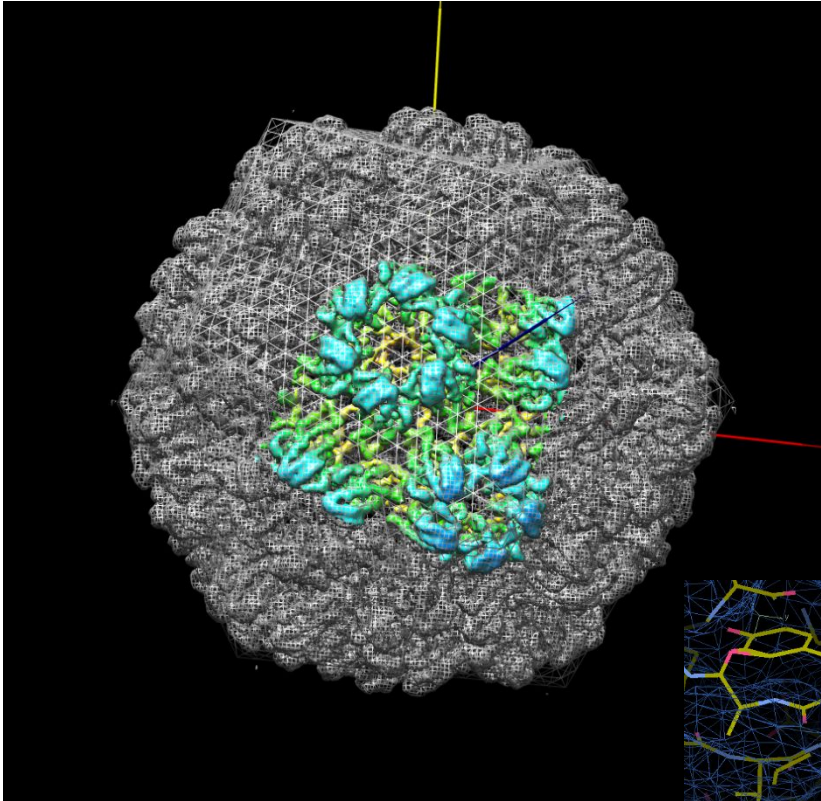
Instruct Image Processing Center

CryoEM

1 TB/day

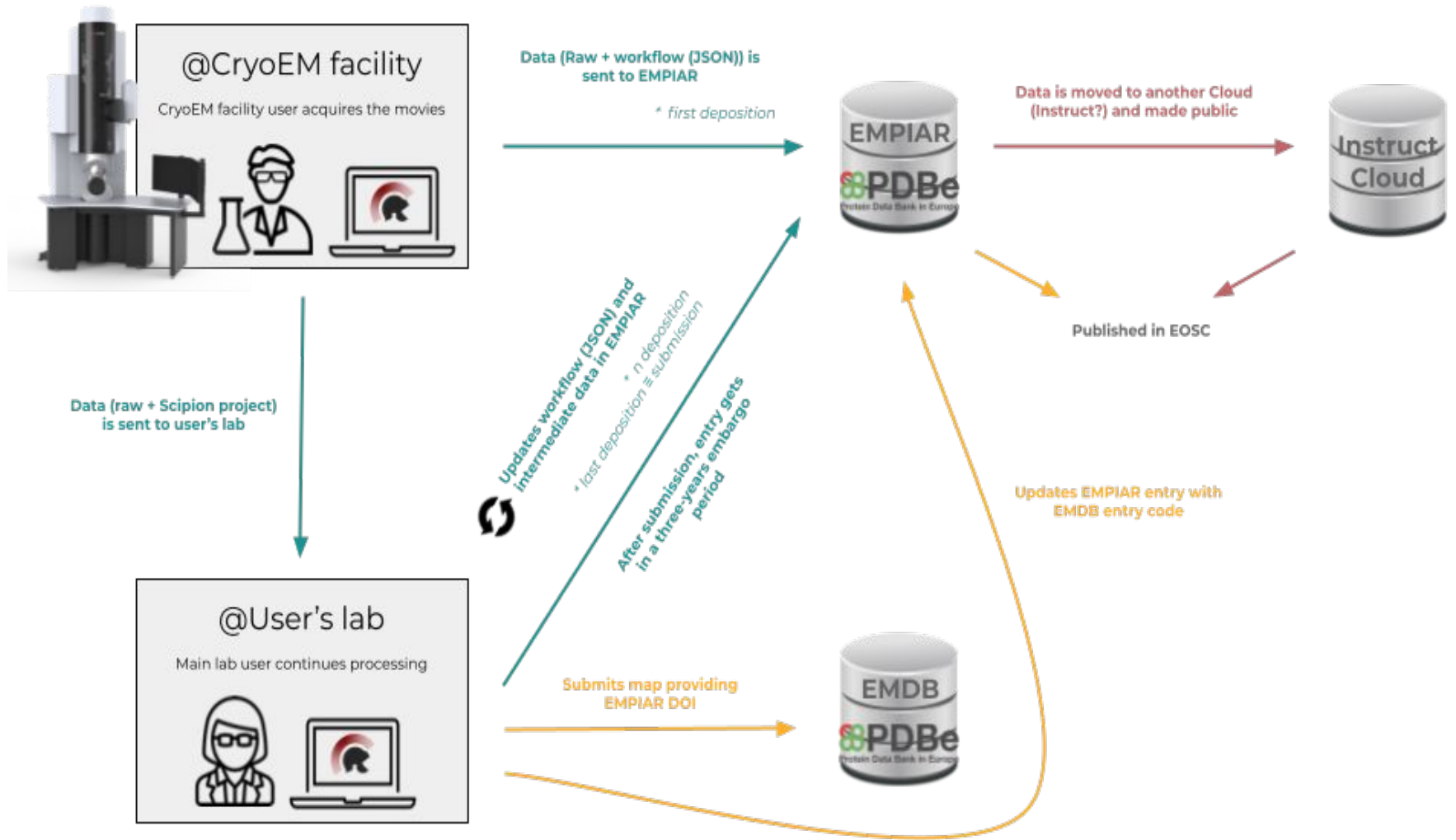


CryoEM



- The aim of the project was to increase the data **FAIR principles in CryoEM** from the moment of its acquisition.
- For doing so, the data is transferred from the CryoEM facility to a **centralized repository** (EMPIAR).
- During the image analysis the **data/workflow** can be **updated**.

CryoEM Science Demonstrator



When main lab user finishes:

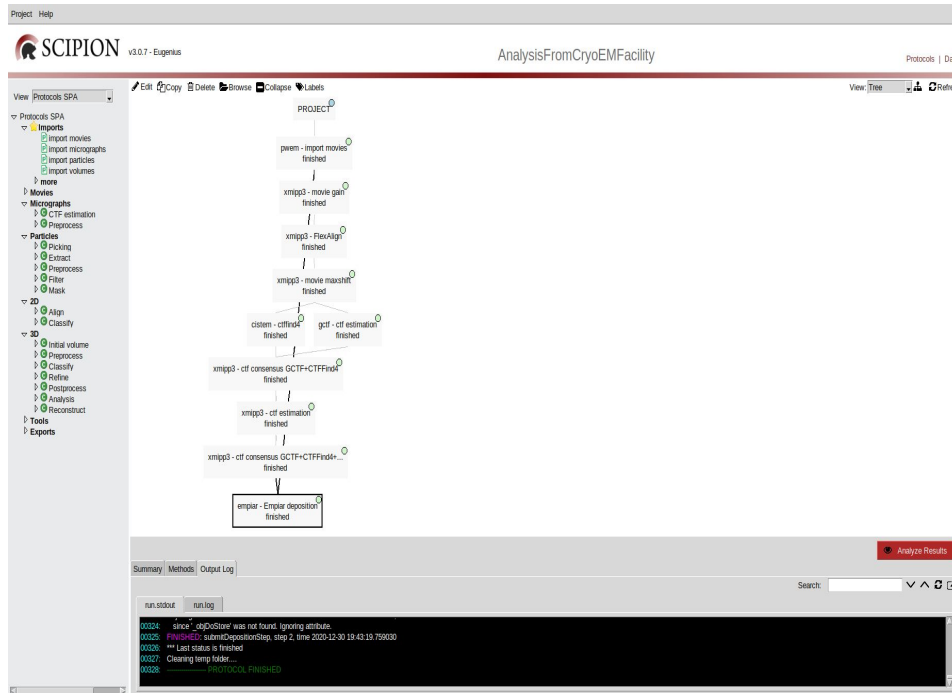
- CASE 1: Publication
- CASE 2: No publication

Requirements

- CryoEM facility user and main lab user must be registered in EMPIAR
Both must know their EMPIAR tokens

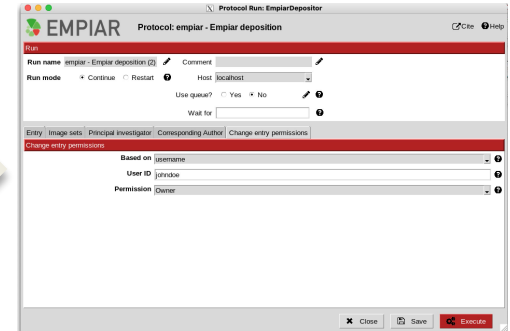
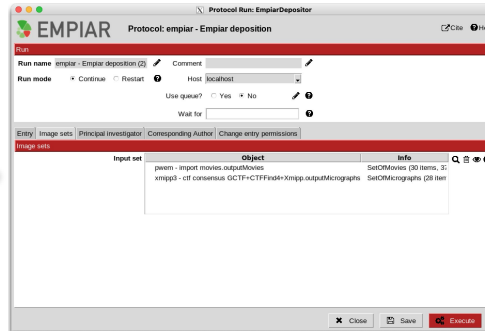
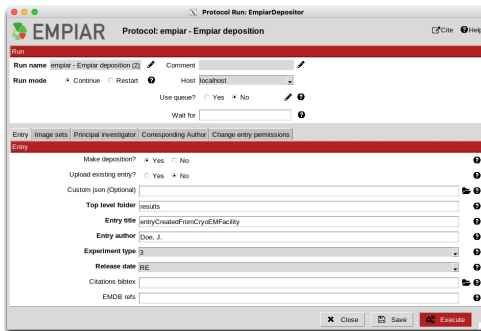


- The CryoEM facility acquires the movies and preprocess them on streaming mode with Scipion



- Data is sent to EMPIAR
 - Raw (movies) and workflow
 - EMPIAR entry ownership is changed to main lab user (no need of sharing credentials or EMPIAR tokens)
 - Remains open for future updates (to be performed by the main lab user)

Use Case Description

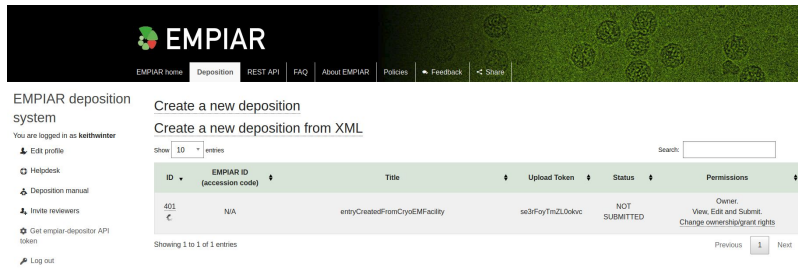


* Raw movies

* Changing EMPIAR entry ownership to lab user

Use Case Description

From CryoEM facility



EMPIAR deposition system

You are logged in as keithwinter

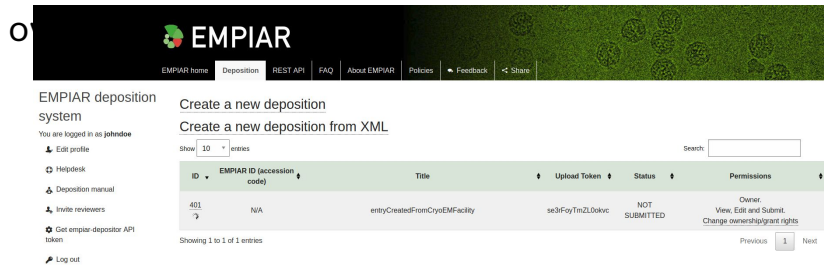
Create a new deposition

Create a new deposition from XML

ID	EMPIAR ID (accession code)	Title	Upload Token	Status	Permissions
401	N/A	entryCreatedFromCryoEMFacility	sa3FoyTmZL0dvvc	NOT SUBMITTED	Owner: View, Edit and Submit. Change ownership/grant rights

Showing 1 to 1 of 1 entries

* CryoEM facility user is still the EMPIAR entry



EMPIAR deposition system

You are logged in as johndoe

Create a new deposition

Create a new deposition from XML

ID	EMPIAR ID (accession code)	Title	Upload Token	Status	Permissions
401	N/A	entryCreatedFromCryoEMFacility	sa3FoyTmZL0dvvc	NOT SUBMITTED	Owner: View, Edit and Submit. Change ownership/grant rights

Showing 1 to 1 of 1 entries

* Main lab user is now the EMPIAR entry owner and CryoEM facility user can't see anymore the entry



EMPIAR deposition ID 401 change of ownership confirmation Recibidos x

empdep-help-testdesk@ebi.ac.uk 19:43 (hace 4 minutos) ☆ ↶ ⋮
para mi

inglés > español Traducir mensaje Desactivar para: inglés x

Dear John Doe,

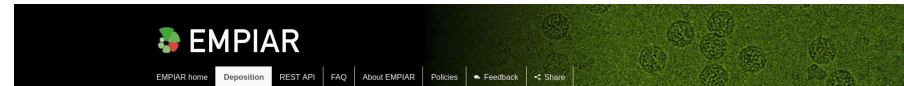
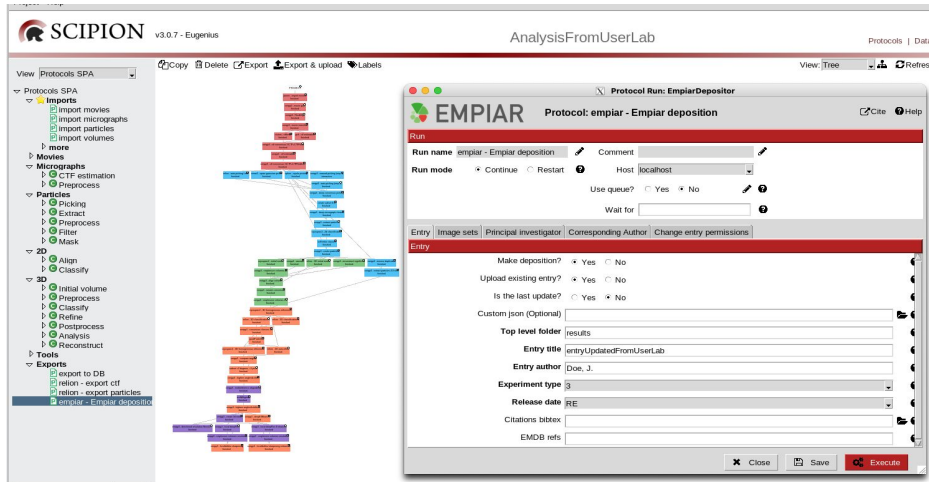
Keith Winter would like to grant you ownership rights over the EMPIAR deposition ID 401. To accept the change of ownership, click this link within 48 hours https://www.dev.ebi.ac.uk/rdbe/emdb/external_test/master/empiar/deposition/grant_rights/confirm/0462144c350e4345b3d1980e7b2c59bd10c8a654

Best wishes,
EMPIAR annotation team

Responder Reenviar

* Main user lab is asked to accept the change of ownership

Use Case Description



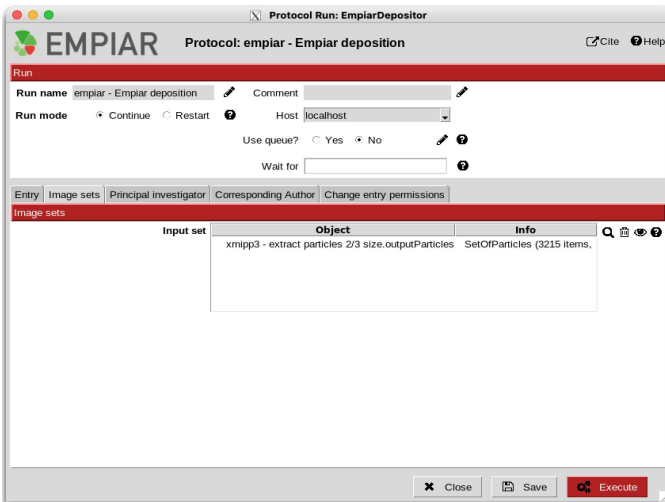
EMPIAR deposition system
 You are logged in as johndoe
 Edit profile
 Helpdesk
 Deposition manual
 Invite reviewers
 Get empiar-depositor API token
 Log out

Create a new deposition
 Create a new deposition from XML

Show 10 entries Search:

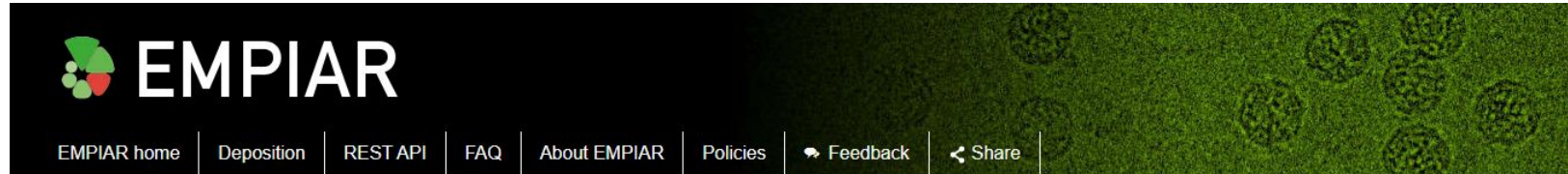
ID	EMPIAR ID (accession code)	Title	Upload Token	Status	Permissions
401	N/A	entryUpdatedFromUserLab	se3FoyTmZL0okvc	NOT SUBMITTED	Owner: View, Edit and Submit. Change ownership/grant rights

Showing 1 to 1 of 1 entries Previous 1 Next



* EMPIAR entry updated

* Lab user continues processing and eventually updates the workflow and intermediate data



EMPIAR-10516

Cryo electron microscopy of SARS-CoV-2 spike in prefusion state

Publication: Continuous flexibility analysis of SARS-CoV-2 Spike prefusion structures
 Melero R [id](#), Sorzano CO [id](#), Foster B, Vilas JL [id](#), Marabini R [id](#), Ramirez-Portela E [id](#), Sanchez-Garcia R [id](#), Herreros D, del Cano L, Losana P, Fonseca-Reyna Y, Conesa P [id](#), Wrapp D [id](#), Chacon P [id](#), McLellan J, Tagare H, Carazo J [id](#)
International Union of Crystallography Journal (2020)
 DOI: [10.1101/2020.07.08.191072](https://doi.org/10.1101/2020.07.08.191072)

Related PDB entries: [6zow](#), [6zp5](#), [6zp7](#)

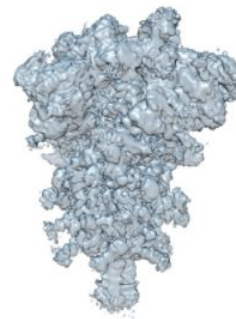
Related EMD entries: [EMD-11328](#), [EMD-11336](#), [EMD-11337](#)

Deposited: 2020-09-22
Released: 2020-10-12
Last modified: 2020-10-12
Dataset size: 2.1 TB
Dataset DOI: [10.6019/EMPIAR-10516](https://doi.org/10.6019/EMPIAR-10516)

Experimental metadata: [Download xml](#)
SCIPION workflow: [Open in workflow viewer](#)

Image set
 — 1. 2 outputMovies

Contains:
 micrographs



Quick links

- [EMDB](#)

- [PDBe](#)

- [Biolmage Archive](#)

- [EMPIAR Quick tour](#)

- [Statistics](#)

- [Re-use case study](#)

- [EMPIAR in the news](#)

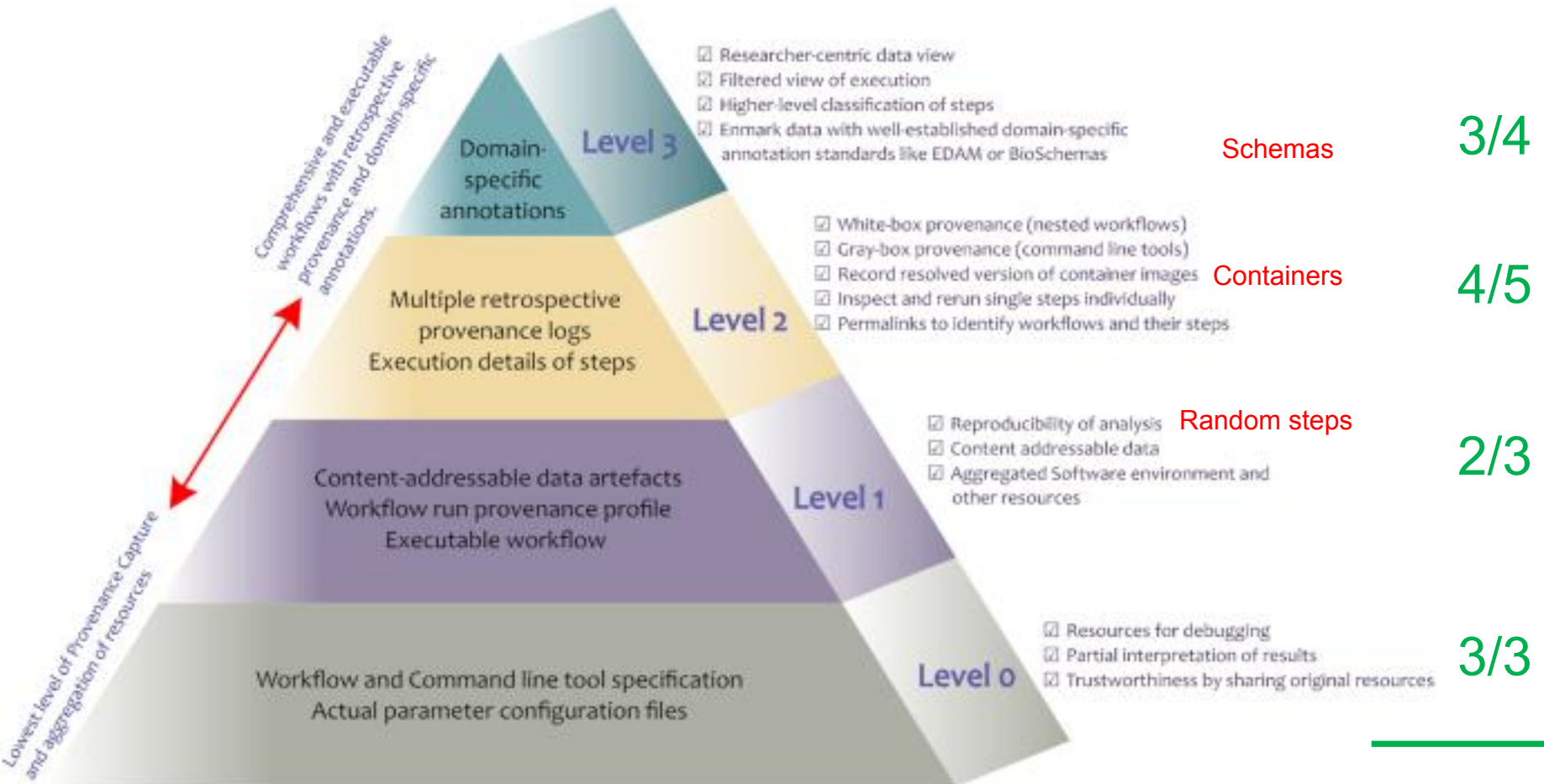
- [Contact us](#)

- [EMPIAR@PDBj](#)

EMPIAR citations

[Auto3DCryoMap: an automated particle alignment approach for 3D cryo-EM density map reconstruction.](#)
 Al-Azzawi A, Ouadou A, Duan Y, Cheng J. (2020)
[Cryo-EM structures and functional characterization of homo- and heteropolymers of human ferritin](#)

CWL Provenance



Khan, et al. Sharing interoperable workflow provenance: A review of best practices and their practical application in CWLProv. Gigascience, 2019, 8(11)

12/15

Functionality, File format

- Metadata
 - CWL output
 - Data and workflow ontology
 - Workflow hub
 - RO-crate

Cryo Electron Microscopy

Last uploaded: July 28, 2020



- Summary
- Classes**
- Properties
- Notes
- Mappings
- Widgets

Details

Acronym	CRYOEM
Visibility	Public
Description	Ontology that describes data types and image processing operations in Cryo Electron Microscopy of Single Particles
Status	Alpha
Format	OWL
Contact	Carlos Oscar Sorzano, coss@cnb.csic.es
Categories	Imaging

Submissions

Version	Released	Uploaded	Downloads
unknown <small>(Parsed, Indexed, Metrics, Annotator)</small>	07/23/2020	07/28/2020	OWL CSV RDF/XML Diff
unknown <small>(Archived)</small>	07/23/2020	07/28/2020	OWL Diff
unknown <small>(Archived)</small>	07/23/2020	07/23/2020	OBO

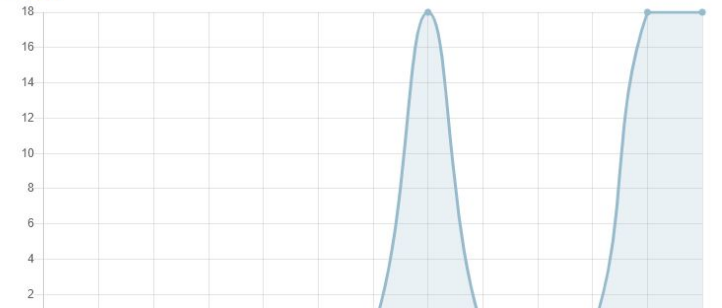
Views of CRYOEM +

No views of CRYOEM available

Metrics ?

Classes	111
Individuals	0
Properties	0
Maximum depth	6
Maximum number of children	11
Average number of children	3
Classes with a single child	9
Classes with more than 25 children	0
Classes with no definition	34

Visits ↓



Summary



I2PC



Laura del Caño



Irene Sánchez