

CNB-CSIC Pilot Node

Providing to the structural biology community essential data and services to assess the quality of cryo-electron Microscopy data

FACTSHEET FOR: Structural biology community: researches, pharmaceutical companies, cryo-EM facilities, etc.

Pilot Node Profile

The CNB-CSIC Pilot Node responds to the challenges and possibilities of the Structural Biology community related to data validation in terms of quality by offering the cryo-EM Validation Report Service (VRS), a modular and open validation grading system that qualifies structure maps at six different levels depending on the information available to assess it.



Pilot Core Services

- **AAI**
{in progress}

Pilot Exchange Services

- **Cryo-EM Validation Report Service (VRS)**

EOSC Beyond Core Innovation Sandbox

A pre-production environment where a large range of users, from researchers to node operators, can test the latest developments of the EOSC core.

It acts as a Federator Node offering Core Federating Capabilities for the Pilot Nodes.

User story at-a-glance

Throughout the cryo-EM data cycle, numerous steps involve data generation, beginning with sample preparation and acquisition at the cryo-EM facilities and culminating in the reconstruction of the volume map and atomic models that represent the nature of a macromolecule target. As the number of maps deposited in public databases determined by cryo-EM is quickly growing, it becomes crucial to complement cryo-EM data with quality-related data at the latest stage of the cryo-EM data cycle. Indeed, not all data have the same quality, although it is not easily discernible.

In this context, the cryo-EM Validation Report Service (VRS) will be offered to the structural biology community.

Users could upload and validate their data via an open-access website, where an automated Scipion workflow will handle the data analysis.

This service eliminates the need for users to download datasets, install software or set up the environment. A comprehensive PDF report summarising the evaluation will be available for download.

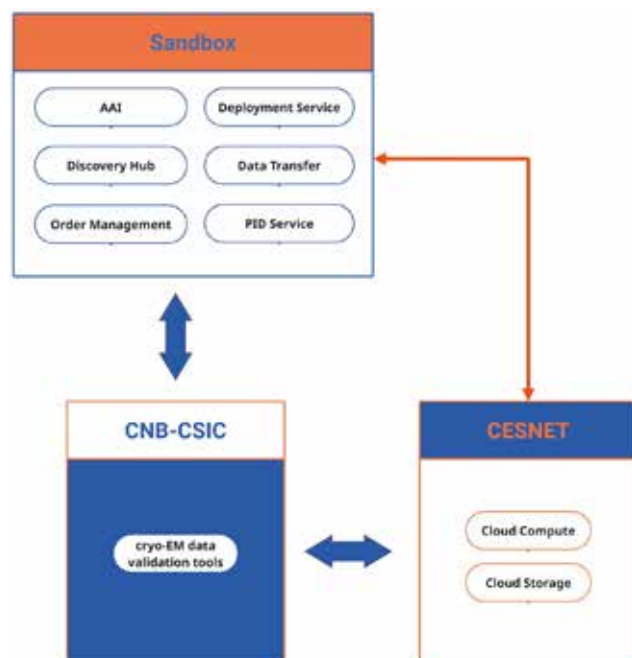
CNB-CSIC Node integrations with the Core Innovation Sandbox and other Pilot Nodes

Integrated Core Federating Capabilities from the Core Innovation Sandbox

- AAI
- Deployment Service
- User Space (planned)
- Order Management (planned)
- Helpdesk (planned)
- Monitoring (planned)
- Data Transfer (planned)
- PID (planned)

Integrated services from other Pilot Nodes

- Instruct-ERIC AAI



Value of the Node piloting activities

The Cryo-EM Validation Report Service (VRS) can be used in two main ways: to validate private user data or to assess existing public structures deposited in the EMDB and PDB. In the first case, structural biology researchers can gain valuable insights into the quality of their data, along with recommendations on how to improve their results.

This process eliminates the need for users to install any software or have access to high-performance computing resources to perform these validations. In the second case, the service also contributes to greater openness and reproducibility within the structural biology community.

Next steps

In the upcoming months the VRS service will be fully integrated with AAI, User Space and Order Management and later with the Helpdesk, Monitoring and PID core service too.

About EOSC Beyond

www.eosc-beyond.eu

The ambition of EOSC Beyond is to support the growth of the EOSC in terms of integrated providers and active users by providing new Core technical solutions that allow developers of scientific application environments to easily compose a diverse portfolio of EOSC Resources, offering them as integrated capabilities to researchers.

Useful Links

CNB-CSIC Pilot Node:

<https://www.eosc-beyond.eu/pilot/cnb-csic>

(cryo-EM) Validation Report Service:

<https://biocomp.cnb.csic.es/EMValidationService/>