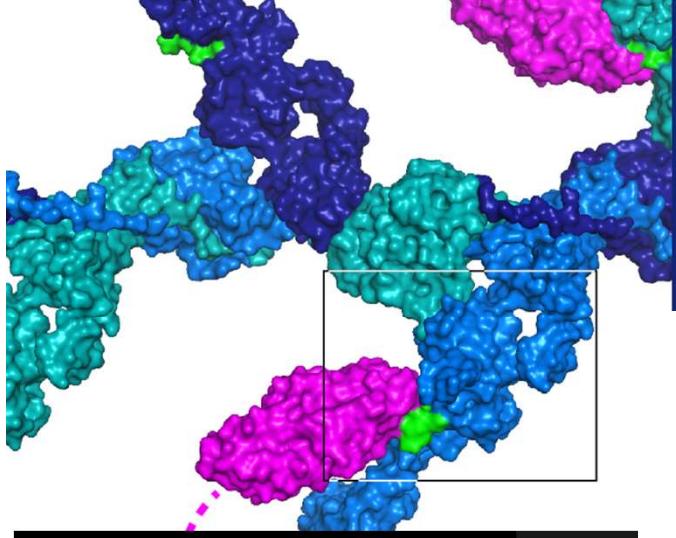


Nexus/HDF5 at ESRF



**Andy Götz,
Wout de Nolf + Thomas Vincent
+ Laurent Claustre**



10-03-2022

A team led by Karolinska Ir (Sweden) has combined Artificial Intelligence (AI) with structural biology at the ESRF and SciLifeLab to predict the structures of two similar proteins that prevent bacterial infection.

Human Organ Atlas

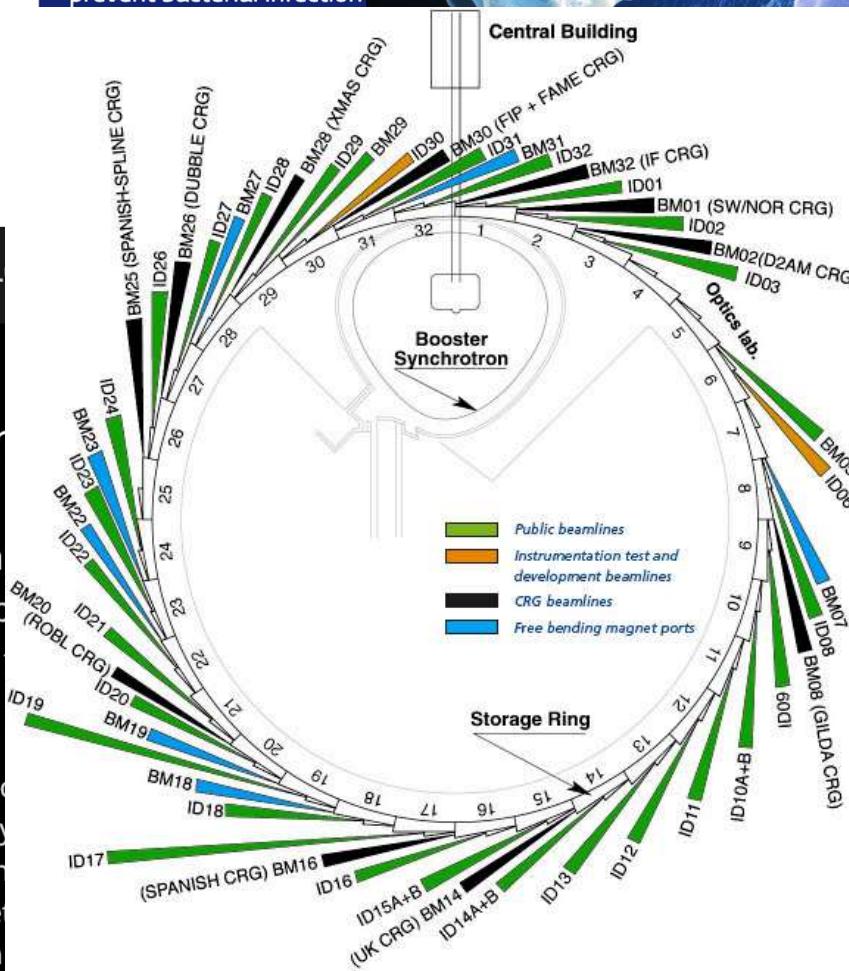
[EXPLORER](#)

Welcome to the Human Organ Atlas

The Human Organ Atlas uses **Hierarchical Tomography** to span a previously unprecedented range of anatomical understanding of human anatomy, from the organ scale down to the cellular scale.

Histology using optical and electron microscopy can resolve structures with sub-micron accuracy but only at the level of a single organ, while clinical CT and MRI scans can only resolve structures with resolution only down to just below a millimetre. By contrast, HiP-CT can do 3D, imaging intact organs with ca. 20 micron resolution across several microns.

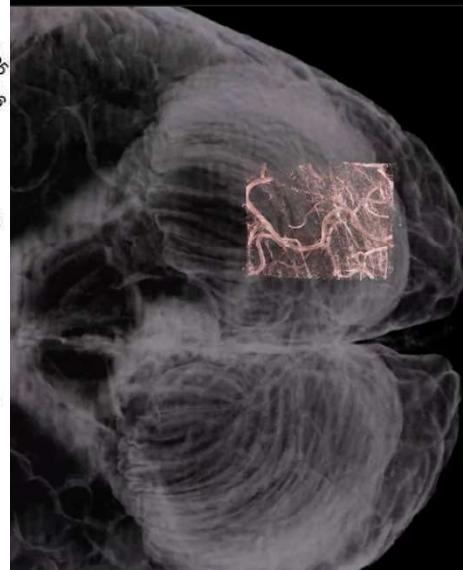
We hope this open access Atlas, enabled by the ESRF-EBS, will act as a reference to provide new insights into our biological makeup in health and disease. To stay up to date, follow [@HiP-CT](#)



07-03-2022

Proteins are not rigid structures: they move, breathe and adapt to their environment in order to optimise their shapes and functions. Cutting-edge work in NMR spectroscopy and at the ESRF's X-ray crystallography beamlines maps the structural details of "breathing motions" in the core of a protein.

Share



HiP-CT imaging and 3D reconstruction of a [complete brain](#) from the body donor LADAF-2020-31. More videos can be viewed on the [HiP-CT YouTube channel](#).

- **Tools – libraries**

- [libhdf5](#) – used mostly from C++ by the detector acquisition software (Lima)
- [h5py](#) – “workhorse” library used for all python programs (ESRF is also contributor)
- [hdf5plugin](#) – Python module to easily manage compression filters
- [Silx-kit](#) – Python library for reading + writing hdf5 (main module is Fabio)

- **Viewers**

- [Silx view](#) – a [Qt](#) application for exploring hdf5 files; provides widgets to ease writing applications using hdf5 : hdf5 browser tree, dialogs to open dataset/group inside hdf5 file
- [H5web](#) – based on [WebGL](#) it is a library and a web application (used in data portal, Braggy for displaying diffraction images, ESRF Jupyter-lab, daiquiri, ...)

- **Applications**

- [Lima](#) – Detector acquisition library, using direct chunking for writing (most detectors)
- [BLISS/NexusWriter](#) – Tango device server for writing scan data (1/2 ESRF beamlines)
- [NXTomoMill](#) – used to create NXTomo definitions for data processing
- [Nxtoascii](#) – program to export data in user defined ascii format
- [Ewoks](#) – ESRF workflow system persists data in Nexus/HDF5

- **Nexus definitions**

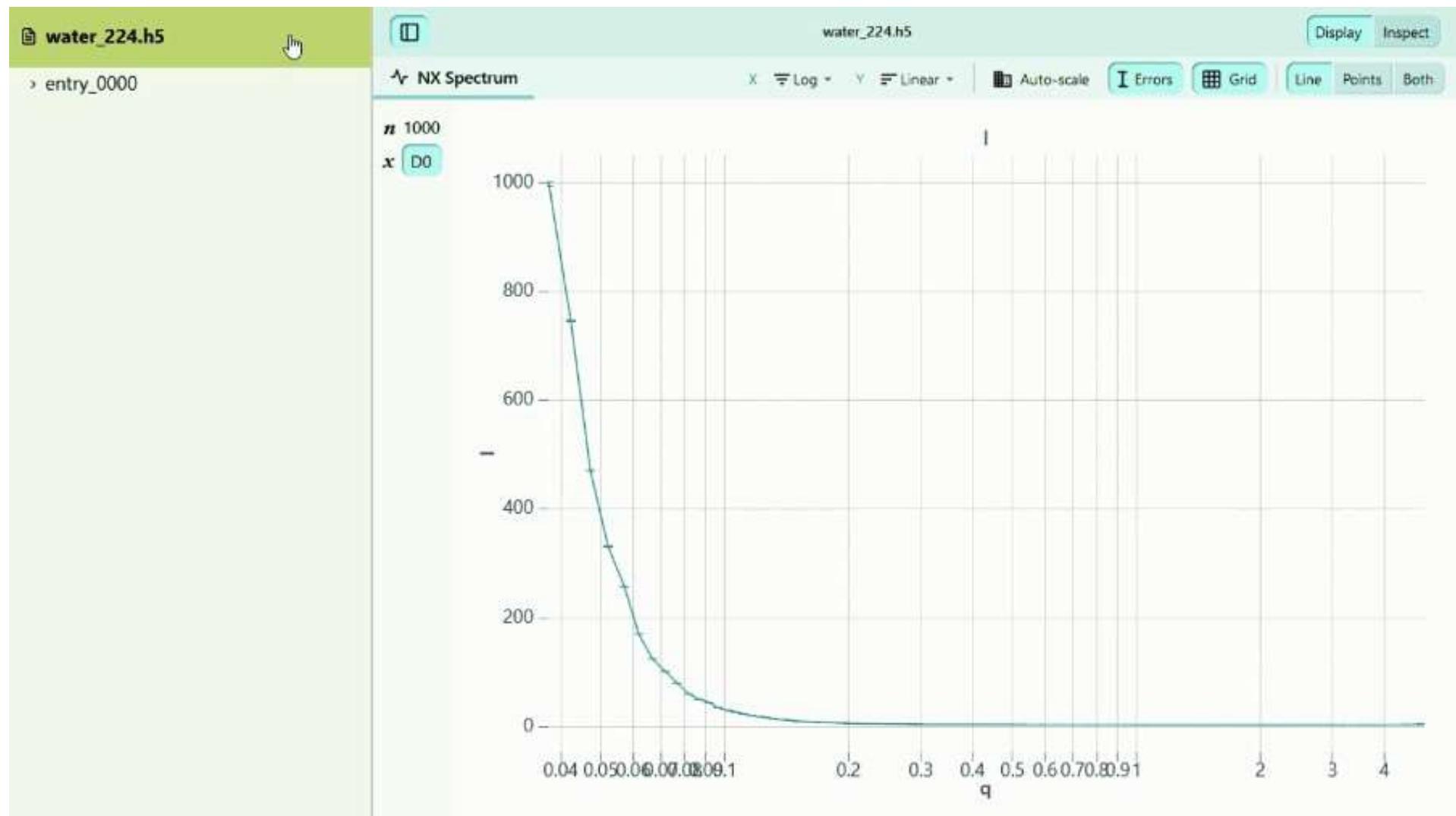
- [Nexus](#) - used for generic scan data files, single master file, metadata in data portal
- [NXTomo](#) – used by tomography + imaging beamlines

ESRF DEVELOPED APPLICATIONS WITH HDF5 SUPPORT

- PyMCA
- pyFAI
- Nabu
- PyHST
- PyNX
- BLISS
- LIMA & LIMA2
- silx
- Fabio
- h5web
- jupyterlab-h5web
- Data analysis programs (mostly Python) + jupyter notebooks

- **Silx kit – generic viewer + widgets for Nexus/HDF5**
- <https://github.com/silx-kit/silx> (<https://doi.org/10.5281/zenodo.591709>)
- **BLISS – organization of Nexus/HDF5 files**
- https://bliss.gitlab-pages.esrf.fr/bliss/master/data/data_nexus.html
- **H5web – web viewer and graphics library for Nexus/HDF5**
- <https://github.com/silx-kit/h5web>
- **Jupyterlab – Nexus/HDF5 viewer plugin for Jupyterlab**
- <https://github.com/silx-kit/jupyterlab-h5web>
- **Nxtoascii – convert Nexus/HDF5 to ascii**
- <https://gitlab.esrf.fr/denolf/nxtoascii>
- **EWOKS – ESRF workflow system**
- <https://gitlab.esrf.fr/workflow/ewoks/ewoks>
- **ESRF Nexus/HDF5 master file configuration**
- <https://gitlab.esrf.fr/icat/hdf5-master-config>

H5WEB – NEXUS/HDF5 WEB VIEWER + LIBRARY



<https://h5web.panosc.eu> , integrated in data portal, braggy, daiquiri, ...

BLISS – EXAMPLE OF HDF5 FILE ORGANISATION

Name	Description	Type	Shape	Link
stresstest_1.h5		NXroot		
1.1	(T) "sequence_of_scans"	NXentry		
2.1	(T) "ct 1e-06 1"	NXentry		
end_time	(V) "2021-04-14T10:20:04.240355+00:00"	string	scalar	
instrument		NXinstrument		
measurement		NXcollection		
elapsed_time	(V) 0	float64	scalar	Soft
epoch	(V) 1.61839e+09	float64	scalar	Soft
thermo_sample	(V) 0	float64	scalar	Soft
start_time	(V) "2021-04-14T10:20:03.749071+00:00"	string	scalar	
title	(V) "ct 1e-06 1"	string	scalar	
3.1	(T) "ascan robz 0.5 1.5 10 1e-06"	NXentry		
end_time	(V) "2021-04-14T10:20:05.717945+00:00"	string	scalar	
instrument		NXinstrument		
att1		NXcollection		
beamstop		NXcollection		
elapsed_time		NXdetector		
~ data	(V) Compressed 1D data	float64	11	
epoch		NXdetector		
lima_simulator2		NXdetector		
acq_parameters		NXcollection		
ctrl_parameters		NXcollection		
data	(V) 3D data	uint16	11 × 1024 × 1024	Virtual
type	(V) "lima"	string	scalar	
lima_simulator2_roi1		NXdetector		
~ avg	(V) Compressed 1D data	float64	11	
~ data	(V) Compressed 1D data	float64	11	
~ max	(V) Compressed 1D data	float64	11	
~ min	(V) Compressed 1D data	float64	11	
selection		NXcollection		
~ std	(V) Compressed 1D data	float64	11	
type	(V) "lima"	string	scalar	

2022 EUROPEAN HDF5 USERS MEETING @ ITER

- **2022 European HDF5 Users Group (HUG)**, happening in-person and virtually on **May 31-June 2, 2022 at ITER** in Saint Paul-lez-Durance, France
- **Registration @ <https://www.hdfgroup.org/hug/europeanhug22/>**

