
ESS Guidelines for Scientific Data

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1. PURPOSE

These guidelines provide implementation guidance to accompany the Policy for Scientific Data [ESS-2506519], which governs the handling of data generated by ESS.

2. GOOD PRACTICE

The proposal team (PT) is encouraged to ensure that experiments' metadata are as complete as possible, as this will enhance the possibility for the PT and others to search for, retrieve and interpret scientific research data.

The PT is strongly encouraged to provide a complete log of the protocol carried out and what happened during the experiment. The logs must be entered in the electronic logbook if ESS provides one and it has not been done automatically. In the absence of a facility electronic logbook, the experimental team must use other means and link a read-only copy of the logbook to the scientific research data.

The PT should be careful to not include personal information, like the phone numbers of team members or collaborators, that cannot be openly shared due to the restrictions outlined in the General Data Protection Regulation (GDPR).

ESS undertakes to provide means for the capture of such metadata items that are not automatically captured by an instrument, in order to facilitate recording the fullest possible description of the raw data.

Researchers who aim to carry out analyses of open data and metadata are encouraged to contact the original PI to inform them and suggest a collaboration, if appropriate. Researchers must acknowledge the source of the data and cite its unique identifier and any publications linked to the same raw data.

PIs and researchers who carry out analyses of raw data and metadata are encouraged to link the software used to obtain the results of these analyses with the raw data / metadata using the mechanisms provided by the metadata catalogue, if this is not done automatically. Furthermore, they are encouraged to make such software and results openly accessible.

Researchers are strongly encouraged to follow best practices adopted by many journals concerning citing the software used and developed for the data analysis.

For each publication using facility data, authors are strongly encouraged to make available the analysis procedure description, scripts, software and software environments that completely describe the process of data analysis from the raw and metadata to the published results, and which allow others to reproduce that analysis.

Authors are encouraged to deposit these files at ESS as auxiliary data associated with the dataset at the time of the submission of the manuscript, and to make them available as open access after the publication date.

Where a software tool cannot be made available, for example for licensing reasons, the analysis procedure description should explain which tool and version has been used, and how the analysis could be repeated if that tool was available.

3. GLOSSARY

| Term | Definition |
|-----------------------------|---|
| Auxiliary Data | Data that provide contextual information regarding the experiment and its datasets but which are collected outside the context of the experiment conducted at ESS, such as information about the sample images, provenance and preparation, data processing scripts and processing environment information such as software tools and versions used. |
| Embargo Period | The period during which the proposal team (PT) have exclusive access to the data. |
| Instrument(s) | Any and all instruments, including beamline instruments, used at ESS during the execution of experiments. |
| Metadata | Information related to datasets that characterise and identify a raw data dataset. This includes, but is not limited to, a reference to the proposal number, a data set identifier, time, duration and location of the data collection and sample name as well as aggregate information about the raw data, like total number of counts, minimum, maximum or average values for other parameters. |
| Metadata Catalogue | The metadata index of scientific research held by ESS. |
| Principal Investigator (PI) | Main proposer identified on the experiment proposal. |
| Processed Data | Data obtained by processing raw data. |
| Proposal Team (PT) | Everyone designated by the PI with the right of access by way of notification on the original experimental proposal or via written communication to the Scientific Coordination and User Office (SCUO). |
| Raw Data | Experimental information collected during an experiment at ESS, including, but not limited to, neutron event data, neutron images, sample environment information, the setup and parameters of the instrument. |
| Scientific Research Data | Raw data, metadata, processed data and auxiliary data. |

DOCUMENT REVISION HISTORY

| Revision | Reason for and description of change | Author | Date |
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