



*Citation for published version:*

Patel, M, Coles, S & Lyon, E 2009, 'Curation and Preservation of Crystallography Data', The 5th International Digital Curation Conference - Moving to Multi-Scale Science: Managing Complexity and Diversity, London, UK United Kingdom, 2/12/09 - 4/12/09.

*Publication date:*  
2009

*Document Version*  
Early version, also known as pre-print

[Link to publication](#)

*Publisher Rights*  
CC BY

**University of Bath**

## **Alternative formats**

If you require this document in an alternative format, please contact:  
[openaccess@bath.ac.uk](mailto:openaccess@bath.ac.uk)

### **General rights**

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

### **Take down policy**

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

# Curation & Preservation of Crystallography Data

Manjula Patel<sup>1</sup>, Simon Coles<sup>2</sup>, Liz Lyon<sup>1</sup>,

m.patel@ukoln.ac.uk,<sup>1</sup>UKOLN & DCC, University of Bath; <sup>2</sup>EPSRC NCS, University of Southampton

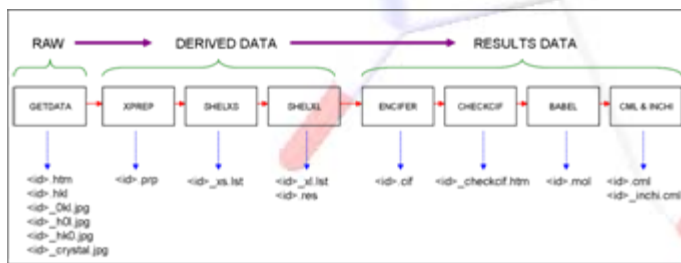
5<sup>th</sup> International Digital Curation Conference, December 2009, London, UK

## Project Aims

The eCrystals Federation project aims to enhance the management of crystallography data at the institution level, incorporating data generated in departments, laboratories and by individual researchers or practitioners. The work described is concerned with the development of approaches to the preservation and curation of crystallography data in open repositories.

## Crystallography Data

Crystallography is the sub-discipline of chemistry concerned with determining the structure of a molecule and its 3D orientation with respect to other molecules in a crystal through the analysis of diffraction patterns obtained from X-ray scattering experiments. This normally involves several stages:



## Preservation Planning

Repository managers are under increasing pressure to provide expertise in IT skills, domain knowledge and preservation issues [1].

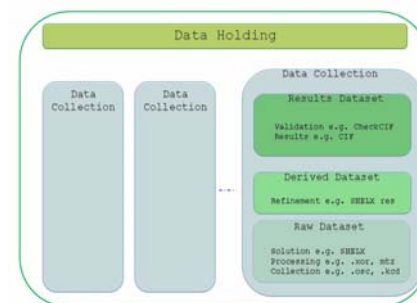


## References

- [1] Manjula Patel, Preservation Planning for Crystallography Data, WP4, eCrystals Federation Project, 25th June 2009
- [2] Manjula Patel, Preservation Metadata for Crystallography Data, WP4, eCrystals Federation Project, 3rd September 2009
- [3] Manjula Patel, Representation Information for Crystallography Data, WP4, eCrystals Federation Project, 19th May 2009

## Preservation Metadata

Preservation metadata is information that supports and documents digital preservation processes; it includes information relating to provenance, authenticity, preservation activity, technical environment and rights issues. This strand is concerned with on-going community consensus work relating to the development of a Metadata Application Profile for crystallography data [2].



## OAIS Representation Information

According to the Reference Model for an Open Archival Information System (OAIS), Representation Information (RI) is any information required to render, process, interpret, use and understand data.

The work here relates to an investigation of RI for Crystallography data and its role in the curation, maintenance and management of such data [3].

