

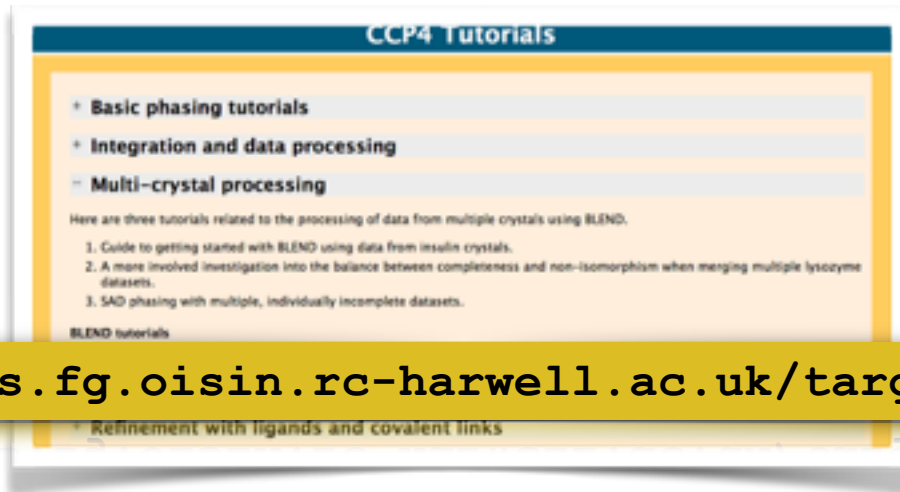
# BLEND TUTORIALS

James Foadi & Pierre Aller

**CCP4-DLS Workshop**  
**December 2015**



# Locations on the Web



CCP4 Tutorials

- Basic phasing tutorials
- Integration and data processing
- Multi-crystal processing

Here are three tutorials related to the processing of data from multiple crystals using BLEND.

- Guide to getting started with BLEND using data from insulin crystals.
- A more involved investigation into the balance between completeness and non-isomorphism when merging multiple lysozyme datasets.
- SAD phasing with multiple, individually incomplete datasets.

BLEND tutorials

- Refinement with ligands and covalent links

<http://tutorials.fg.oisin.rc-harwell.ac.uk/targets/standard/>



BLEND: managing, scaling and merging multiple datasets

John Flack<sup>1</sup> and Peter Main<sup>2</sup>  
<sup>1</sup>Harwell Oxford, [john.flack@diamond.ac.uk](mailto:john.flack@diamond.ac.uk), <sup>2</sup>Harwell Oxford, [peter.main@diamond.ac.uk](mailto:peter.main@diamond.ac.uk)

Most use of the software is in programs equipped with the program BLEND (Gard<sup>1</sup> et al., 2012) and to-date how it can be used effectively to merge complete and individual data sets out of several partial or complete ones. The user manual is a long and detailed document of using data from multiple crystals and with the software (Gard<sup>1</sup> et al., 2012; Gard<sup>1</sup> et al., 2012; Main<sup>2</sup> et al., 2012; Main<sup>2</sup> et al., 2012).

**WARNING:** All merging routines included in this tutorial have been validated using PROWLERS and SHELXL. These CCP4 programs are periodically subjected to small changes. It is therefore possible that some of the merging routines contained in this tutorial appear slightly different from what the user observes with their version of CCP4. These differences are very minimal and should be considered in primary due to different numerical or algorithmic approximations.

**CONTENTS**

- Getting started with BLEND
- Integration and data processing
- Multi-crystal processing
- Refinement with ligands and covalent links

**DATA SETS INCLUDED WITH THIS TUTORIALS**

INSULIN DATA SETS OF CRYSTALLOGRAPHY IN CRYSTALS

[http://www.jfoadi.me.uk/BLEND\\_documentation/BLEND\\_tutorial.html](http://www.jfoadi.me.uk/BLEND_documentation/BLEND_tutorial.html)

# Purpose of the tutorials

To get you started with **multi-crystal data management**

To help you assembling **complete datasets**

To judge the **type and quality** of your complete datasets

# Datasets

**14** crystals of insulin

**28** sweeps of lysozyme

**12** crystals of lysozyme soaked in sodium bromide

**Focus especially on ...**

**Tutorial 2: combination and graphics**

**Tutorial 4: automated filtering of datasets**

**Updated version of BLEND:**  
**[module load blend/dev\\_jf](#)**

**Enjoy these tutorials!**