

File naming convention:

0. The Tutorial Descriptions

The tutorial texts are provided as pdf files with the following naming convention:

exp\$_protein_experiment_tutorial.pdf

The place holders for protein and experiment are explained in Table 1.

1. Data Collection

The diffraction images are named according to the following scheme:

exp\$_protein_experiment_qualifier_###.img

The place holders for protein, experiment and qualifier are explained in Table 1.

2. Data Processing

The input file for the data processing program XDS (Kabsch, 1993, 2010a,b) is simply called XDS.INP and is supplied as such. All other files are named as they were named by the processing procedure.

3. Structure Solution

All files created during the structure solution process are archived in a tar file, which was downloaded from the respective Auto-Rickshaw run:

exp\$_protein_experiment_autorickshaw.tar

The files in the archive can be retrieved using the command tar xvf file.tar

4. Structure Refinement

For the structure refinement part, the following three files are supplied:

exp\$_protein_experiment_refine.def	command file for running REFMAC5
exp\$_protein_experiment_refine.log	log file from REFMAC5-run
exp\$_protein_experiment_refine.pdb	final refined coordinate file
exp\$_protein_experiment_refine.mtz	final refined structure factor file

Table 1. File naming convention.

Experiment No.	Protein	Experiment type	Qualifier
exp1	ins	ssad	-
exp2	thau	mad	peak
			infl
			hrem
			lrem
exp3	lyso	molrep	-
exp4	lyso	ions	-
exp5	lyso	ligands	-
exp6	lyso	siras	native
			deriv
exp7	thau	rip	before
			after

Directory Structure of the Tutorial

The whole tutorial is organized according to the following directory structure, which consists of either three or four levels.

<u>Level</u>			
<u>1</u>	<u>2</u>	<u>3</u>	<u>4</u>
exp\$	contains the tutorial itself		exp\$_protein_experiment_tutorial.pdf
	data	contains all images, unless more than one data set is present	
		xds	contains all processing files

In the cases an experiment consists of more than one data set, an additional layer is inserted in between data and xds:

	qualifier1	image directory
	xds	processing directory
	qualifier2	
	xds	
	
struct_sol	contains the archive file provided for the structure solution path	
struct_ref	contains all files provided for structure refinement	

alternative representation:

Level 1	Level 2	Level 3	Level 4
exp\$	contains the tutorial file itself exp\$_protein_experiment_tutorial.pdf		
	data	contains all images, unless more than one data set is present	
		xds	contains all processing files
In the cases an experiment consists of more than one data set, an additional layer is inserted in between data and xds:			
		qualifier1	image directory
		xds	processing directory
		qualifier2	
		xds	
		...	
	struct_sol	contains the Auto-Rickshaw archive file with all files provided for the structure solution path	
	struct_ref	contains all files provided for structure refinement	