

Crystallography Service Sample Database Administrator's Guide

J.P.Hagon
Computer Systems Support
School of Chemistry

March 4, 2012

Introduction

This guide is intended for staff who administer the Newcastle University Crystallography Service Sample Database. It includes both a general description of the web interface and associated administration procedures along with a more technical description of the software interface and the database itself so that administrators can recover from situations such as a forgotten administrator password.

1 General Description of the System

1.1 Introduction

The system consists of a *front-end* which is used by users and administrators to submit sample requests and upload analysis data. This front-end is implemented using the ruby programming language and version 3 of Ruby on Rails. The front-end is hosted on an *Apache* server running on an *Ubuntu* linux system. Technical details will be described elsewhere.

The *back-end* consists of a set of ruby programming libraries and a SQL database — in this case SQLite3. More technical aspects of the back-end will be described elsewhere.

1.2 Users

The system has a relatively simple user setup with just one basic user type. However, there are three levels of authority that a user can have:

Standard Most users of the system will have a standard account which allows them to submit sample requests and view their own sample data.

Group Leader These users have the additional privilege of being able to see all of the sample data for their own group in addition to their own samples. A group of users may have more than one designated group leader.

Administrator An administrator, in addition to standard user privileges, can do many administration tasks. These include adding/deleting users, changing user privileges, submitting/updating/deleting samples, editing public web pages on the server and uploading files to the server.

Users can either self-register or be added by an administrator. An administrator can also disable a user account without actually deleting it. Only the most basic information about a user is stored in the database, namely first name, last name and email address. the email address serves as a login id. The user can set his own password. If the user forgets his password, the system can email him a secure link to the server via which the password can be reset.

1.3 Groups

All users must be associated with a group. Typically this will be a research group associated with a particular person. When a user self-registers, he must select an appropriate group. If such a group does not exist, an administrator must set one up for him. Usually one or more users will be designated *group leaders* and will have access to information about all the group's samples.

1.4 Samples

The primary purpose of the system is to track and keep a record of samples submitted to the crystallography service. A typical workflow is shown in Figure 1. Emails are sent automatically by the system when a sample status is updated by an administrator.

1.5 Public Pages

Most information on the server can be viewed only by registered users. However, there are some pages which are more generally accessible. Such pages include the home page, general information pages and the sample queue. Public pages can be created and edited by an administrator using tools provided by the server software. rather than write pure HTML, an administrator can use a text-based markup language called Textile which can produce sophisticated web pages with all the usual constructs such as headings, paragraphs, floating elements, tables and images.

2 The Database

The core of the system is the database which holds information about users, samples etc. In this section we describe the whole database structure (or *schema* in database parlance).

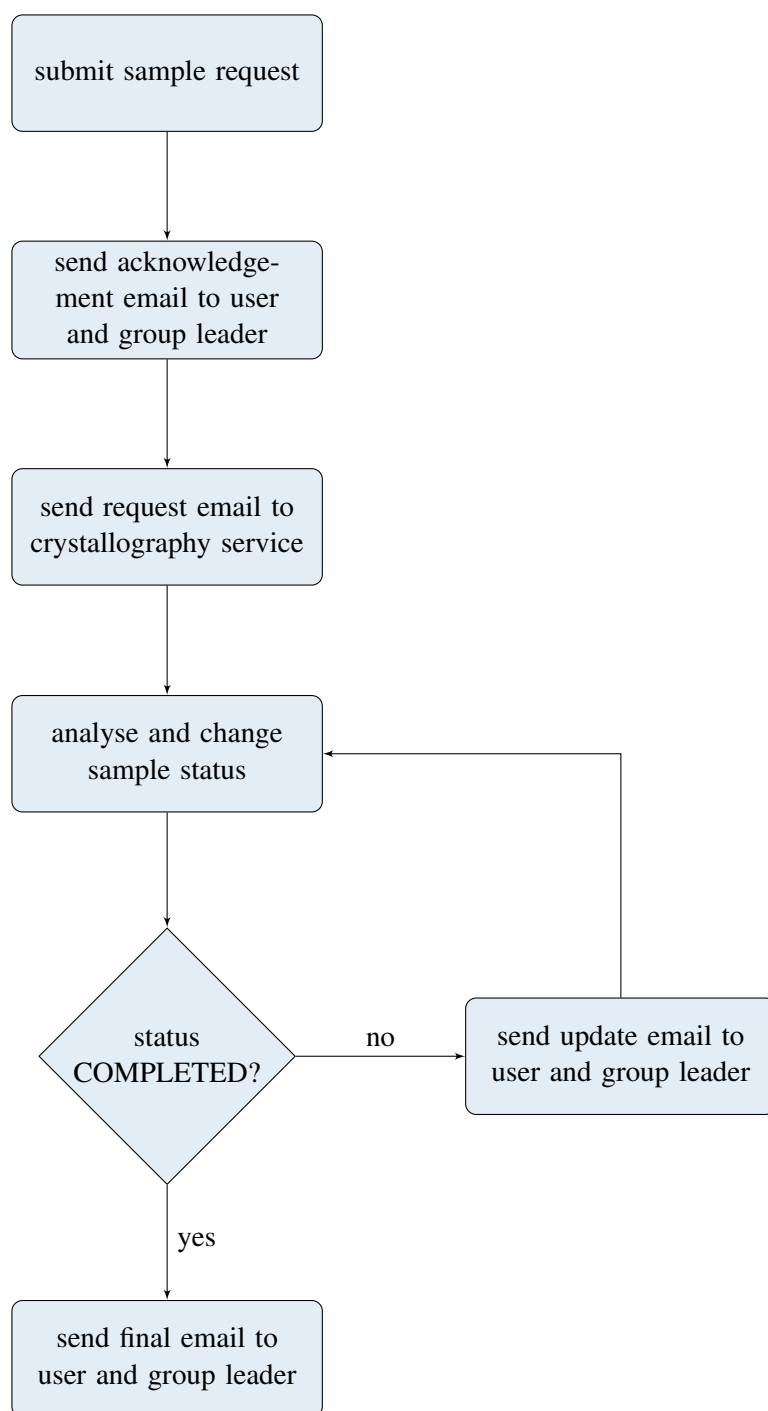


Figure 1: Typical workflow for sample processing cycle. Emails are sent automatically by the system whenever the status of a sample is updated.

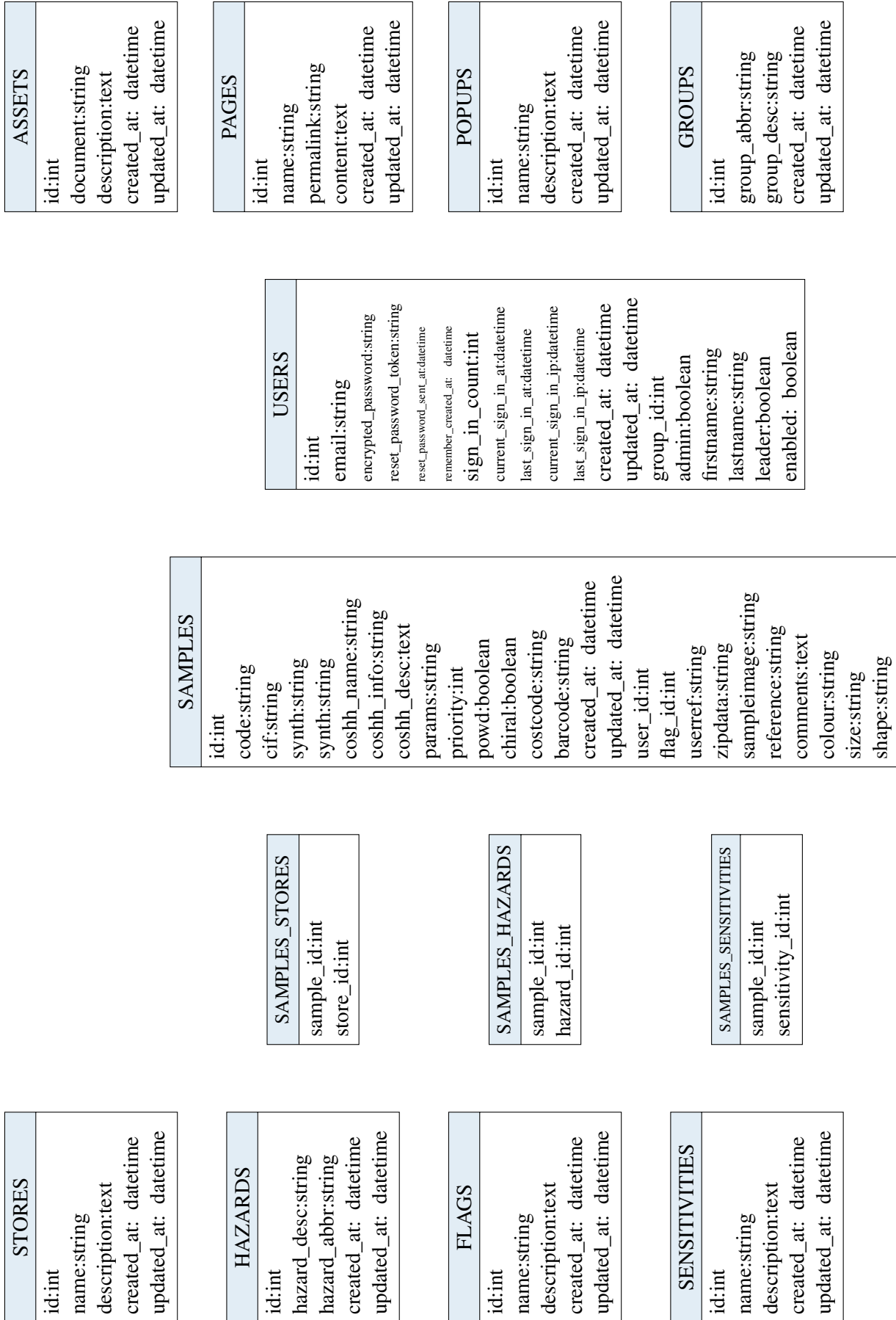


Figure 2: The overall database schema.

Contents

1	General Description of the System	1
1.1	Introduction	1
1.2	Users	1
1.3	Groups	2
1.4	Samples	2
1.5	Public Pages	2
2	The Database	2