Crystallography Service
SamTrack
Administrator's Guide

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Introduction

This guide is intended for staff who administer the Newcastle University Crystallography Service *SamTrack* 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.

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1 General Description of the System

1.1 Introduction

SamTrack is a software application for tracking samples submitted to the Newcastle University Crystallography Service. The system consists of a *front-end* which is used by users and administrators to submit sample requests, upload analysis data, edit sample status etc. This front-end is implemented using the ruby[1,3] programming language and version 3 of *Ruby on Rails*.[2,4] The front-end is hosted on an *Apache*[5] server running on an *Ubuntu*[6] 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*.[7] 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, — 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 work-flow is shown in Figure 1. Emails are sent automatically by the system when a sample status is updated by an administrator.

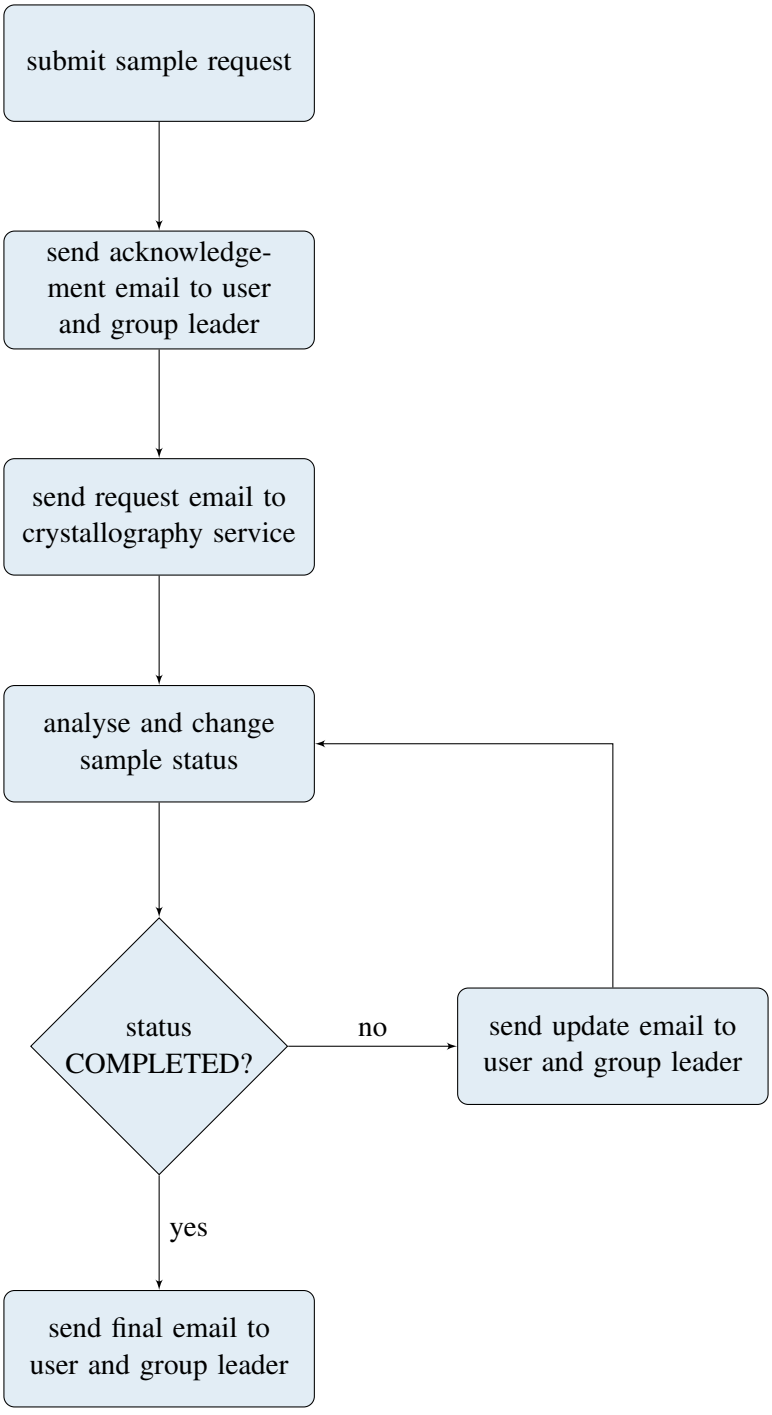


Figure 1: Typical work-flow for sample processing cycle. Emails are sent automatically by the system whenever the status of a sample is updated.

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*[8] which can produce sophisticated web pages with all the usual constructs such as headings, paragraphs, floating elements, tables and images.

2 Web Management Guide

2.1 Introduction

In this section we describe the web management interface to the sample tracking database. Before going through the basics of the web interface there is one important point to make regarding the use of *Microsoft Internet Explorer*:

> There is a current issue with delete operations[a] when using Internet Explorer. Basically, the delete operation will appear to work but actually doesn't delete anything. All other operations which change the database (create, edit) work fine but the delete operation does not. For this reason, it is recommended that administrators use another browser such as Firefox or Chrome when doing system management tasks.
>
> [a] This seems to affect all Rails3 applications.

When a manager is logged-in, the home page of the system looks similar to that shown in Figure 2

There are three parts to this browser view:

(i) a main display showing the contents of a page of information;

(ii) a menu on the left side of the browser window;

(iii) login information and a `sign_out` link above the main display on the right.

The left side menu consists of three sections:

Information These links point to *static* pages which can be created by an administrator. the administrator can also add extra links to the information section. We describe how to do this in §2.2.

User Tools These tools allow a user to view his sample list, submit a new sample and view his profile information. Additionally, if a user is also a group leader, he will have access to the *My Group Samples* link for listing all samples in the user's group.

Admin Tools This is the main set of web-based tools for administrators. We will describe each of these in the next section.

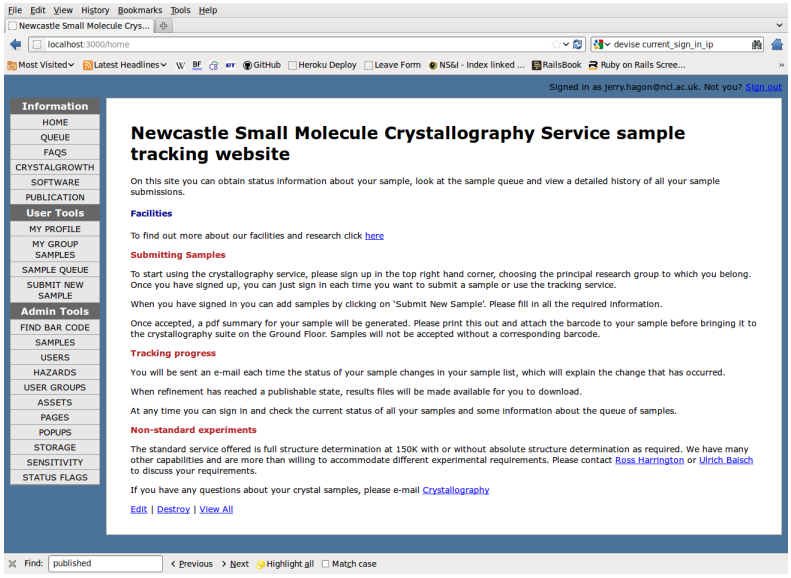


Figure 2: Administrator's view of home page.

2.2 Adding Static Pages

Clicking the *PAGES* link in the *Admin Tools* sub-menu produces the pages index shown in Figure 4. This shows a list of pages. For each of these pages is a set of buttons allowing the administrator to show, edit or delete the page as shown in Figure 3. These buttons are used throughout the database editing pages on the web server. At the bottom of the list is a link to create a new page.

Figure 3: The *show*, *edit* and *delete* buttons.

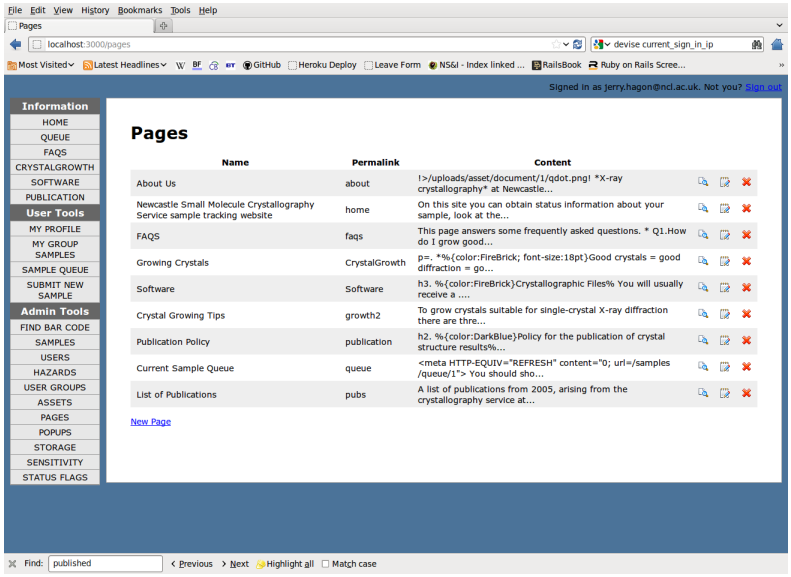


Figure 4: The pages index view.

Figure 5 shows the page editor — a very simple form for entering/changing text. This example shows the home page data. the content is entered in a markup language called Textile*. You can also specify the name of the page (this will be used to set the HTML title attribute and a permalink†. At the bottom are links to the Textile Reference Manual, the page view and the pages index. the page can be referred to via the URL:

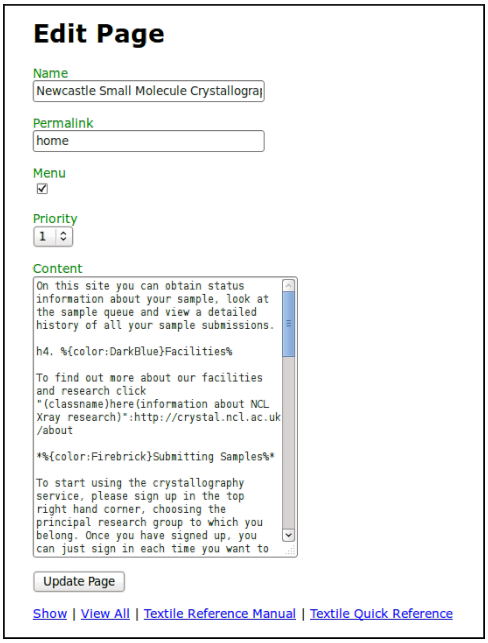


Figure 5: The page edit view.

```
<server name>/permalink
```

thus making static page addressing very simple. An alternative URL which can be generally used for any page is:

```
<server name>/pages/<id>
```

but the permalink-based URL is what you'd almost always use in practice. If, for some reason, you want to use the id-based URL, but don't know what the id is, then just click the 'show' icon in the pages index for the page you're interested in and look at the URL in the web browser window.

Note that there is also a checkbox labelled *Menu*. If this is checked then the page is added to the left hand *Information* menu of static pages. The *Priority* parameter is an integer that determines the order of the page in the menu. If two pages have the same priority their order is determined alphabetically. A good practice is to initially assign priorities in units of, say, 10. Subsequently, if a new page is created, there are then plenty of 'spare' priority numbers which can be used to add menu links in between existing links — otherwise existing priority numbers may need to be tweaked.

2.3 Uploading General Files to the Server

You can upload arbitrary files to the server. These files are referred to as 'assets' and can be uploaded via the *ASSETS* link in the *Admin Tools* menu. Clicking on this link will take you to the assets index page which looks very similar to the pages index described in the previous section. each index entry tells you the pathname of the file on the server, together with a description of what the file contains. Often these files will be images or documents (e.g. PDF files) that you want to link to on one of the static web pages created as described in the previous section.

At the bottom of the asset index list is a link to create a new asset. Clicking this takes you to a simple menu where you can browse for a file to upload to the server. Clicking the *Create Asset* button will then upload the file to the server. It will then be listed in the asset index with an entry under the *Document* column pointing to its location in the file system. This location has the general form:

```
/uploads/asset/document/<id>/<filename>
```

*You are allowed to mix HTML and Textile together.

†A tag which is used as a basis for a concise URL.

Here, `<filename>` is the actual name of the uploaded file as it was when it was uploaded. `<id>` is the database id the document has in the `assets` table described in detail in §4. The actual URL of the document is then:

`<servername>/uploads/asset/document/<id>/<filename>`

2.4 Creating Users and Groups

A user must belong to a group, so it is advisable to create a group for a user before the user is created. Creating a user group is straightforward via the *USER GROUPS* link in the *Admin Tools* menu. As usual, this will take you to an index of existing groups, with a link to create a new group at the bottom. Creating a new group merely requires that you enter two fields:

(i) a 3-letter group abbreviation (it *must* be three letters);

(ii) a longer group description.

Users can be created in two ways; they can self-register by clicking on the link top-right on the home page or they can be created by an administrator. In either case the form used to create and register a new user is the same.

2.5 Sample Management

In this section we give a complete description of the sample management work-flow.

(i) First, a user fills out a sample submission form online. This form is shown in Figure 6. This figure shows the submission form from the point of view of both a non-administrative user and an administrator.

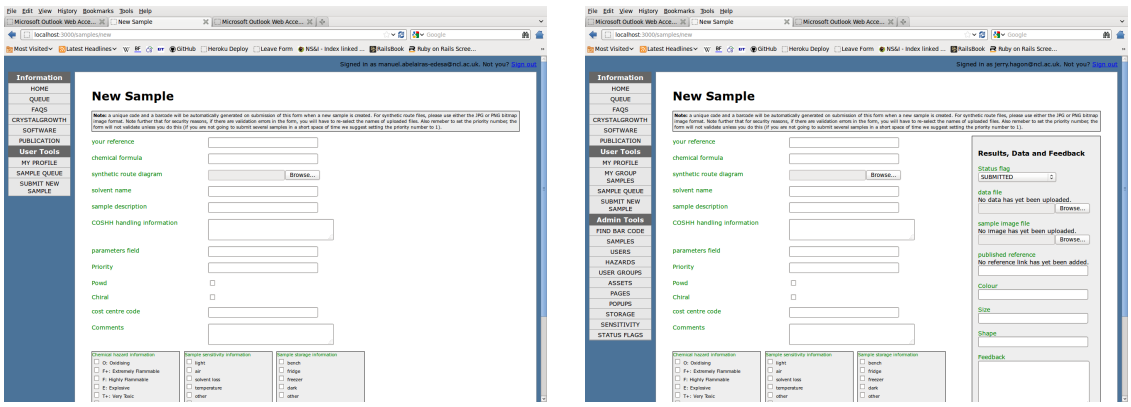


Figure 6: User's view (left) and administrator's view (right) of the sample submission form.

The bits that an ordinary user doesn't see are those parts of the sample fields that are subsequently filled in by an administrator in the course of sample processing.

There is a lot of validation built into the form making it very unlikely that a form will be submitted with incomplete information. Table 1 gives a complete list of validation checks. If a validation check fails on submission of the form, the user will be presented with the *Invalid Fields* box which will tell him which fields have not been entered correctly and

!htb

Field	Description	Validation
cif	chemical formula	can't be blank
synth	synthetic route diagram	must be supplied
coshh_name	name of solvent	can't be blank
coshh_info	COSHH handling information	can't be blank
coshh_desc	sample description	can't be blank
params	unit cell parameters or CSD/Newcastle code	can't be blank
priority	user sample priority number	integer, range 1–9
userref	user reference	alphanumeric without spaces
costcode	cost centre code	can't be blank

Table 1: List of sample validation requirements.

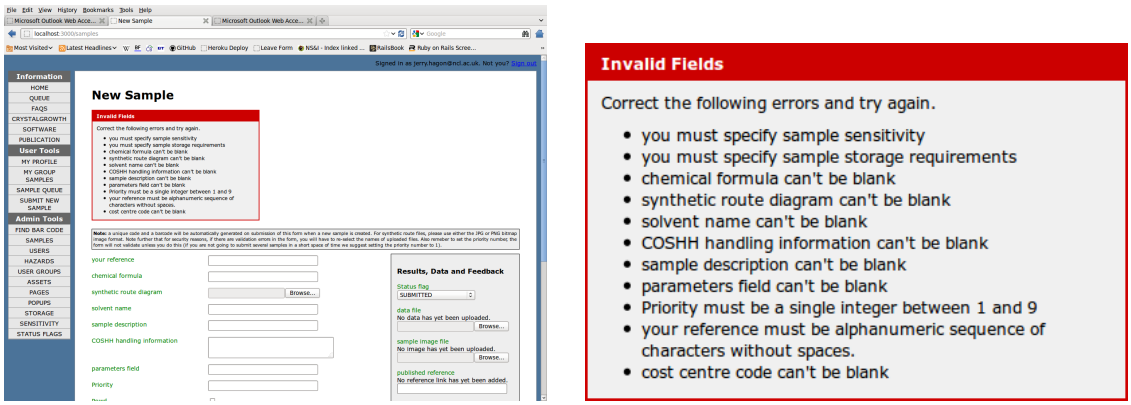


Figure 7: Illustrating what happens when an invalid form is submitted. The user sees an *Invalid Fields* box (shown enlarged on the right). In this case, an administrative user has failed to fill in any of the fields — hopefully a very rare occurrence!

what is required. An extreme example of this is shown in Figure 7 which shows what happens when none of the fields in the form are filled-in.

(ii) On successful submission of the sample form, the user (and group leaders if the user is not a group leader himself*) will receive a confirmation email containing a link to the *Sample Receipt* — a PDF file containing the user input information as well as a unique code identifying the user, user group and sample and a unique bar code. The email has the following general form with the tags in angle brackets filled-in automatically:

```
Dear User

New Sample Submission Code: <SAMPLE CODE> (your ref <SAMPLE USERREF>)
Submitted By: <USER FULL NAME>


your sample analysis request has been received. Please download a
receipt using the link below. Please quote the sample code in any
```

*If there is more than one group leader then the other group leaders will also receive an email.

```
correspondence.

There is a tear-off slip at the bottom
of the receipt which you should attach to your sample.
You will be informed via email of any
changes in the status of your sample.

<LINK TO SAMPLE RECEIPT>

Copies of this email are sent to both sample submitters and their
research group leaders (where different).

Newcastle Crystallography Service
```

A tear-off slip at the bottom of the sample receipt containing the bar code, sample code and provided user reference as well as essential COSHH information can be attached to the actual sample itself. Figure 8 shows a typical sample receipt.

The receipt is generated on-the-fly from the supplied sample information. To perform the generation of the PDF, the well-known Prawn ruby library is used. Once the sample has been submitted, a user can regenerate the sample receipt at any time via a PDF link button in the sample list on his profile page shown in Figure 9.

(iii) Next, the user brings his sample (with attached slip) for analysis and at this point he should also see it in the sample queue.

(iv) Initially the sample will have a status of `SUBMITTED`. At various points in the analysis, this status will be changed by crystallography staff. Whenever the status is changed, an email is sent to both the user and group leaders informing them of the change. The text of the email looks similar to this:

```
Dear User

This is to inform you that the status of sample
<SAMPLE CODE> (your ref <SAMPLE USERREF>) submitted by
<USER FULL NAME>
has changed as follows:

New Status: <NEW STATUS FLAG> <NEW STATUS FLAG DESCRIPTION>

Old Status: <OLD STATUS FLAG> <OLD STATUS FLAG DESCRIPTION>

<LINK TO FULL SAMPLE INFORMATION>

Copies of this email are sent to both sample submitters and their
research group leaders (where different).

Newcastle Crystallography Service
```

(v) When crystallography staff have uploaded all results files (docx, res and sample image) to the server and added any additional text feedback for the sample, they will flag the sample as `COMPLETED` and the process will end. The sample data will continue to be available to users (and administrators) indefinitely after that.

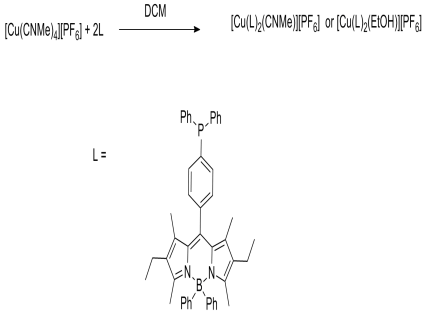
Newcastle Crystallography Service

Bedson Building ✦ Newcastle University ✦ NE1 7RU

Sample Code: LJH-LD-12-0002 Your Ref: LD261

Please check the details on this receipt. Changes can be made only by Crystallography staff. Please use the tear-off slip at the bottom of the page and attach it to your sample. You will be automatically informed via e-mail of any changes to your sample status.

Proposed Structure and Synthetic Route



Sample Details and Requirements

Chemical Formula: C96H95B2CuF6N5P3 OR C96H98B2CuF6N4OP3
Powder Diffraction Required? No
Chiral Structure? No
Your Priority Number: 2

User Details

Submission Date: 2012-03-02 15:29:54 UTC
Submitted By: Laura Davies
Research Group: Lee Higham Research Group
Contact E-Mail: l.h.davies@ncl.ac.uk
Cost Centre Code: n/a
Assigned Bar Code: FQYSY1J7L15

Supplied COSHH Information

Name of Solvent: Ethanol/Pentane
Description of Sample: Copper Bodipy phosphine complex
Handling Procedures: Flammable, Irritant
User Comments: Structure should be similar to LD260. As the crystals were grown in ethanol, the bound MeCN ligand may exchange with the ethanol.

Hazards:	Storage:	Sensitivity:
Highly Flammable (F) Harmful (Xn) Irritant (Xi)	bench dark	light

LJH-LD-12-0002(LD261)

F Q Y S Y 1 J 7 L 1 5

Supplied COSHH Information

Name of Solvent: Ethanol/Pentane
Description of Sample: Copper Bodipy phosphine complex
Handling Procedures: Flammable, Irritant
User Comments: Structure should be similar to LD260. As the crystals were grown in ethanol, the bound MeCN ligand may exchange with the ethanol.

Hazards:	Storage:	Sensitivity:
Highly Flammable (F) Harmful (Xn) Irritant (Xi)	bench dark	light

School of Chemistry Crystallography Service, Newcastle University

Figure 8: Example of a sample receipt (the actual size is A4). Note the tear-off slip at the bottom. The receipt is generated on-the-fly from the supplied sample information. The green border is not part of the PDF rendering, it is used here merely to show the A4 page border.

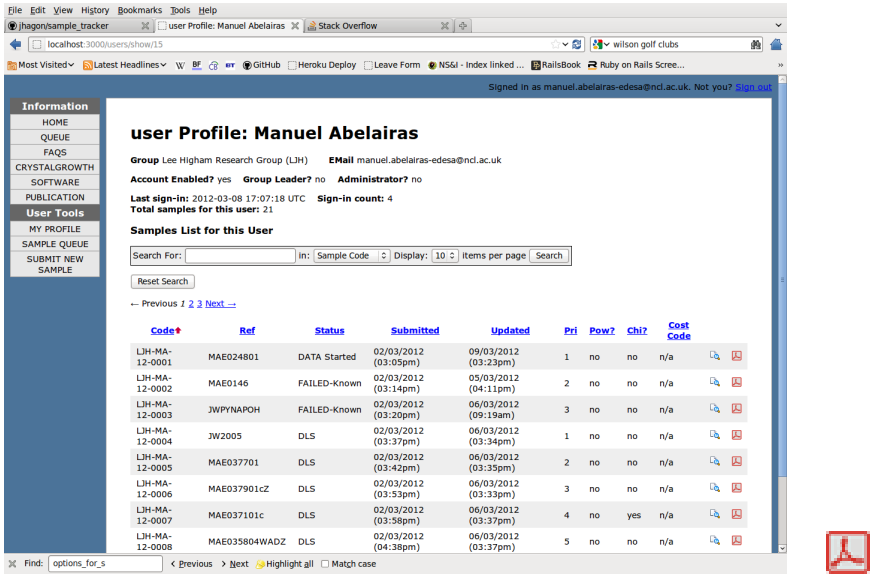


Figure 9: User profile page showing sample list with PDF icon (shown enlarged bottom right).

Results files (docx and res) will usually be made available in a single zip file, with the sample image in a separate file. The files are uploaded by administrators using the sample edit form shown in Figure 10. Note that only administrators have access to the sample edit form. Users will see the information in a slightly different way, not as a form but as a standard 'show' page. This view is shown in Figure 10.Note that if administrators do not fill in the feedback section, then a default message 'No feedback given.' is seen on the relevant part of the sample show page. This is also illustrated in Figure 11.

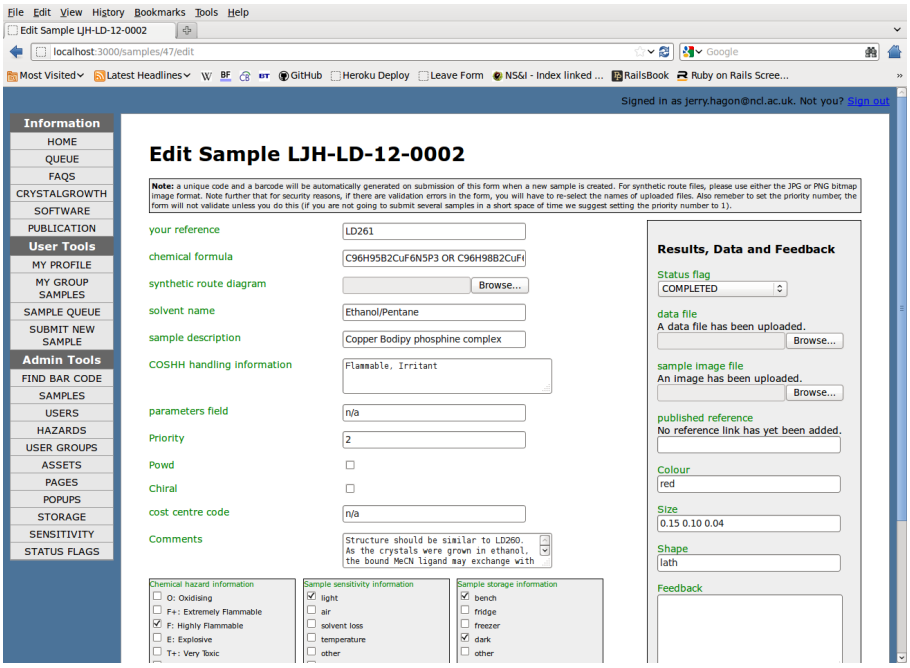


Figure 10: A fully complete sample edit form.

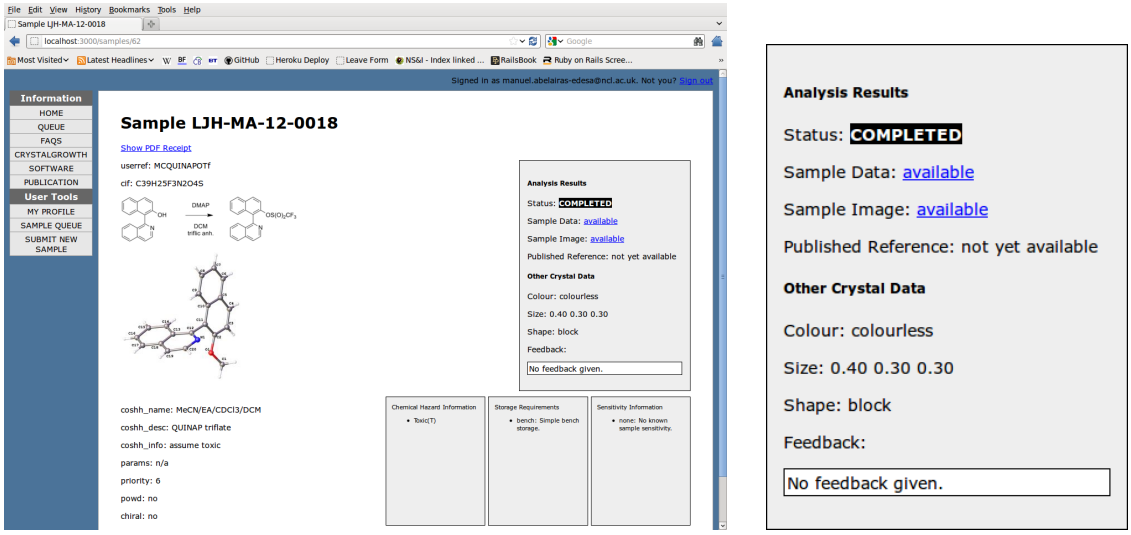


Figure 11: The user's view of a completed sample (left). On the right is an enlarged view of the results section. Note also that a thumbnail image of the sample is displayed. This thumbnail, when clicked, will show the full-size image which can then be downloaded if desired.

2.6 Sample Search and Display Tools

It is important that both administrators, group leaders and users can find information about a particular sample or group of samples. In this section we describe the tools that are available to quickly find the sample data you need.

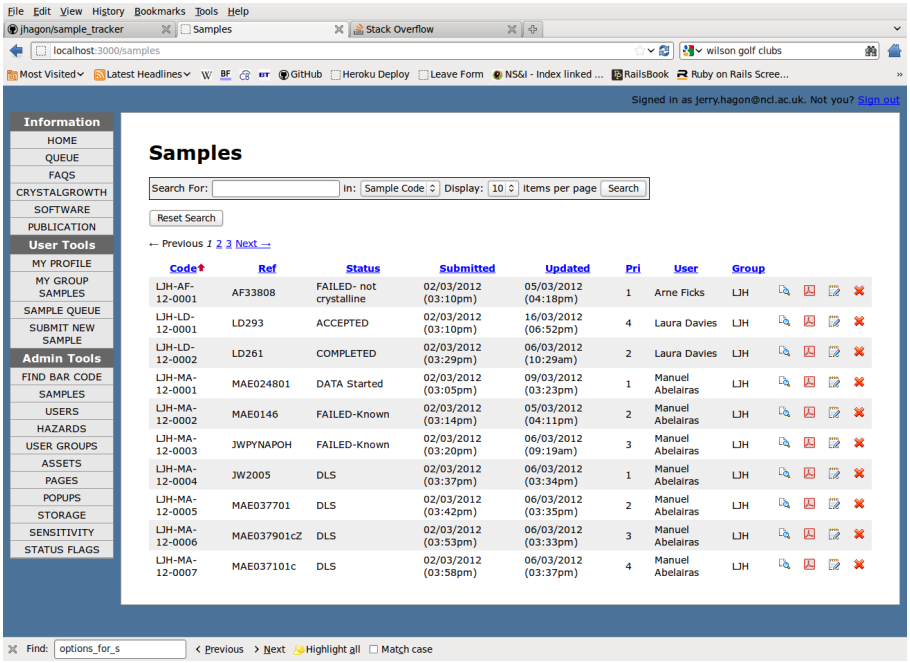


Figure 12: An administrator's view of the full sample index. In this case the red arrow next to the header in the *Code* column indicates that the list has been sorted by sample code in ascending order (the default sorting).

For administrators, the usual starting point will be the main sample index page shown in Figure 12. By default, this index is sorted by sample code in *ascending* order. This is indicated by a small red arrow pointing upwards next to the header text in the *Sample Code* column. Clicking the header text of the *Sample Code* column will reverse the order — i.e. it will now be *descending* order. This is indicated by a blue arrow pointing downwards. The list can be sorted on any other of the displayed columns simply by clicking the column header. repeated clicking on the same column header will toggle the sort order between ascending/descending.

The number of samples displayed per page can also be controlled by the user. By default, this number is set by a global variable, `ITEMS_PER_PAGE` defined in the `config/environment.rb` file*. However, it can be easily changed by selecting the desired value from a drop-down list in the search form above the sample list. The first entry in this list is always the value in the `ITEMS_PER_PAGE` variable. After the choice is made, the list will be re-paginated according to the selected value. Note that for a full samples listing, the search box itself must be empty when you do this.

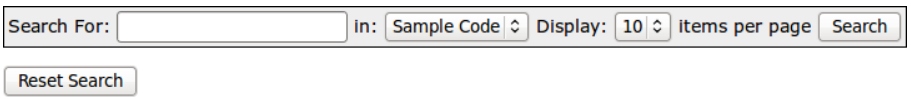


Figure 13: The sample index search form. This is usually found above the list of samples in most of the sample index pages.

To narrow down the list of samples you need to type something into the search box in the search form above the sample list. This search form is common to most of the sample listing pages and is shown in Figure 13. Currently You can search on three fields: the sample code, the user reference or the status. When you perform a search, the results will be paginated according to the setting of the pagination parameter described above. Note that search results can be sorted as before by clicking the header text of the column that you wish to sort by. Below the search form is a reset button which resets all the search parameters (but not the pagination) to their default values.

You can also use the standard SQL % and _ symbols as 'wildcard' characters. The percent symbol maps to one or more characters in afield, whereas the underscore maps to exactly one character.

For example if you want to search for all user references which contain the letter sequence ABC followed by any set of characters followed by 123, then you should enter ABC%XYZ. The following strings would all match this search:

```
ABC-XYZ  ABC123XYZ ABC1-2-3-XYZ ABCDXYZ
```

However, only the first and last of the above strings would match if ABC_XYZ was entered instead. You can use any combination of these wildcard characters in a string search.

> Note that searches are *not* cumulative — they are always made with respect to the full set of samples. In other words if you perform a second search after an initial search, the results of the second search will be exactly the same as if it had been performed first.

*See the *System Management* section for further details.

2.6.1 Bar Code Scanning

Figure 14: A Zebex scanner.

As mentioned earlier, each sample has associated with it a unique bar code and it may sometimes be convenient to scan a sample bar code and have the associated sample record displayed to the screen. To this end, the system has a very simple interface which allows a simple low-cost USB scanner such as the *Zebex* scanner shown in Figure 14 to be used to extract a bar code. The approach taken to facilitate this is brute force.

In the *Admin Tools* menu is a link called *Find Bar Code*. Clicking this takes the user to a very simple form with just a single entry field for a bar code. Now, assuming that the scanner is plugged in to the same PC, if the mouse is clicked in the search box, then when the scanner scans the bar code (usually a button needs to be pressed on the scanner) the actual code will magically appear in the box. Pressing the search button on the form should then produce the matching sample (see Figure 15. For this to work correctly, the bar code scanner needs to be put in *keyboard emulation* mode. Most scanners are capable of doing this, including the Zebex. Of course, you can also type in the bar code by hand if you don't have access to a scanner.

Sample Bar Code Search

IMJX8B0VU5D Search

-->

Code	Ref	Status	Submitted	Updated	Priority	User	Group				
LJH-AF-12-0001	AF33808	FAILED- not crystalline	02/03/2012 (03:10pm)	05/03/2012 (04:18pm)	1	Arne Ficks	Lee Higham Research Group	Show	PDF	Edit	Destroy

Figure 15: A successful search using the *Find Bar Code* form.

3 System Management and Internals

3.1 Introduction

In this section we will explain lower-level aspects of the system and its management. This includes the operating system, command shell, web server, database, ruby language, ruby gems, and the rails3 system which is used to do most of the programming.

3.2 Basic Components of the System

To begin with, we will describe the components of the system from the operating system right up to the *Rails3* software which is used to write the web interface to the sample database. Figure 16 summarises the main components and their relationships.

Let's now look at each of these components individually:

Operating System The system runs on a computer running the Ubuntu version of the linux operating system. The specific release used at present is *Ubuntu 10.04.3 LTS*. Release 10.04 is also known via the code name 'lucid'. LTS stands for 'Long Term Support'. Extended support for this version will last until 2014.

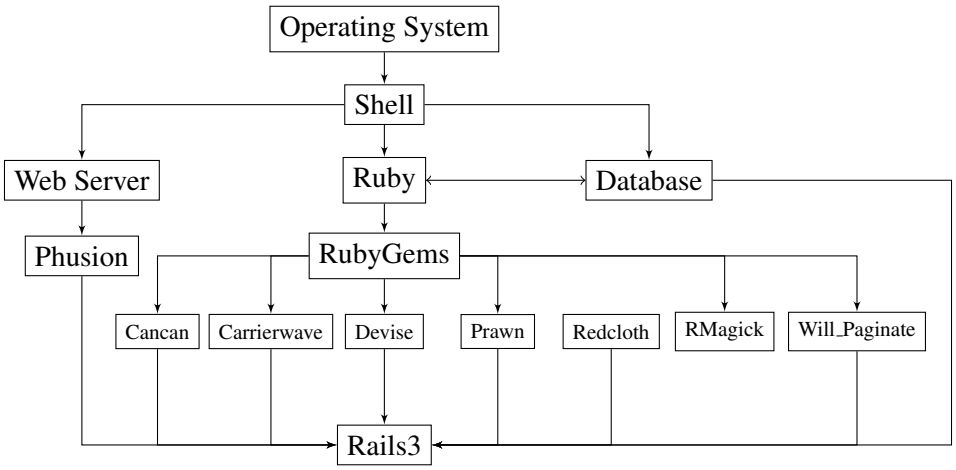


Figure 16: The main components of the sample tracking system and their relationships. This diagram takes a 'top-down' view starting with the operating system and moving through the various software layers down to the rails3 system itself on which the sample tracking software is based.

Shell Access to most software on linux is vis a command shell. There are many different shells available, the default being the *bash* shell. We will assume the use of bash throughout this guide, but other shells can be also be used with little, if any modification to the software itself.

Running under the shell are the three principal components of the system: a web server, database and the ruby programming language environment.

Web Server The web server we use is the ubiquitous *Apache*, specifically version 2.2.14.

Ruby The version of ruby that comes with Ubuntu 10.04.3 is 1.8.7. Unfortunately, this version is not recent enough to run a rails3 application. So, we use the *Ruby Version Manager* to run a more recent version of ruby (1.9.2).

Database Rails 3 requires a database application to store and retrieve sample data. We are using the *SQLite3* database. This is a 'lightweight' database which requires very little separate maintenance. In particular, it does not require a separate authentication process for access, nor does it need to run a separate process in the background as with other database software such as *mysql*.

There are two other components of the system which sit between the web server, ruby and database layer:

Phusion Passenger is an Apache module – a 'plugin' – which interfaces a rails3 application to the Apache web server. It also supplies some debugging and error logging information which can be useful when things go wrong.

Ruby Gems are extension libraries to ruby. Some of them are specific to rails3, but most have wider applicability and can be used in more general applications. The ruby gems used in the sample tracking application are described in the next section.

3.2.1 Ruby Gems

The following Ruby Gems are used in the application:

cancan[9] written by well-known Rails programmer Ryan Bates is used for authorisation. By this we mean controlling which parts of the application can be accessed by users. For example, some parts of the application can be accessed only by administrative users and others can be accessed by anyone — even those who have not registered to use the system.

carrierwave[10] is used to manage the upload of various files to the application including data files, image files and general asset files.

devise[11] is an authentication plugin to Rails which handles user data and user authentication. It provides related functionality such as forgotten password recovery (via email), user login statistics and more.

prawn[12] is a ruby library for producing PDF files. It is used to auto-generate the sample receipts.

redcloth[13] is a Ruby library used for parsing and display of Textile input.

rmagick[14] is a well-known software application consisting of both libraries and utility programs for manipulation of bitmap graphic files. This gem interfaces the ImageMagick libraries to Ruby allowing ImageMagick routines to be called from within a Ruby program.

will_paginate[15] is used to set up pagination of sample listings (and other things).

3.3 Files and Directories

In this section we describe the overall file and directory structure of the application. Some of the files contain parameters which can be changed to affect the behaviour of the application or the appearance of the views. The overall directory structure is shown in Figure 17.

The application root directory contains the following files:

```
config.ru Gemfile Gemfile.lock README.markdown
```

`README.markdown` is a brief summary of the application, written in *markdown*, a simple markup language similar to Textile. The contents of this file are automatically displayed when viewing the home page of the application on GitHub.

`config.ru` is a file used to initialise the application via a special software interface called *Rack**.

`Gemfile` contains a list of gems required to run the application. `Gemfile.lock` contains a list of all gems and their dependencies and is used to update or install additional gems for the application. In practice, only the `Gemfile` is actually edited.

There are 12 directories directly under the application root:

*Rack is part of the interface between a rails application and a web server.

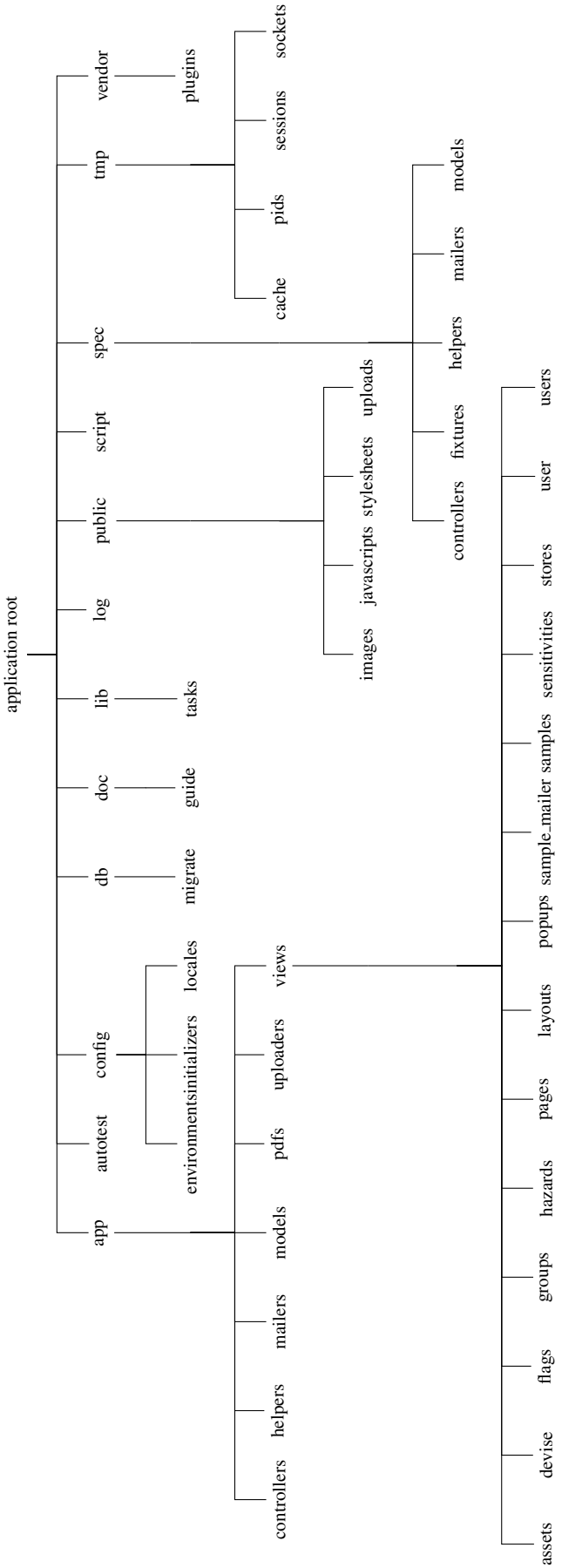


Figure 17: The application directory structure. Only directories are shown here. See text for a detailed explanation.

3.3.1 The app Directory

This directory contains the bulk of the application code and templates for most of the page views. It contains the following subdirectories:

controllers as its name implies contains code which *controls* the interface between the database and the browser. Each table in the database has its own controller code stored in a file in this directory. So, for example, the controller code for access to the samples table is contained in the file `samples_controller.rb`. The `.rb` extension indicates that this file contains ruby code.

helpers contains so-called 'helper' functions (again written in ruby) which are used to produce page views. Generally, there is a file of helper routines corresponding to each database table, for example the helper code containing routines to aid the display of sample data is stored in the file `samples_helper.rb`. Other files, such as `application_helper.rb` are more general-purpose and can be accessed more widely, not just to facilitate page display for particular database table items.

mailers contains code used by the Rails mail subsystem. In the sample tracking application, when samples are updated, an email is sent to relevant users. The file `sample_mailer.rb` contains the ruby code which sends the email.

models is one of the most important directories because it contains the code which interacts with the database. In Rails, each database table defines a 'model' and the code to access this model is contained in a file in the `models` directory. In the case of the samples model for example, this file is called `sample.rb`.

pdfs contains code to generate PDF versions of model data. Only sample data is rendered to PDF form in this application. The rendering code (using the Prawn library) is contained in the file `sample_pdf.rb`.

uploaders contains code for uploading files to the server. For each upload type, there is a file containing the appropriate code for that file type (although often the code will be almost identical in many cases). The standard naming convention for these files is `<uploader_name>_uploader.rb`. For example, in the case of an *asset* upload, the code to do this is stored in the file `document_uploader.rb` because the *asset* model has a field value called *document* which has been declared in its model code as an uploader called *document**. Other uploader file types include zip data files, sample images and synthetic route diagrams.

views contains template HTML code for displaying page views of data from the database. As can be seen from Figure 17, the views directory itself contains lots of subdirectories. each subdirectory corresponds to a model from the sample database and contains the view templates for various different types of view associated with that model. Let us look at the central model in the system, the *sample* model. A listing of the `sample` subdirectory shows the following files:

```
edit.html.erb          groupindex.html.erb  queue.html.erb
findbarcode.html.erb   index.html.erb       show.html.erb
_form.html.erb         new.html.erb         userindex.html.erb
```

*Note here that it is the uploader name which determines the name of the file containing the uploader code, not the field name. In this case the two are equal, but they don't have to be.

These files all contain a mixture of traditional HTML and embedded ruby — hence the `.html.erb` extension. Some of the files are specific to the sample model but others are common to other models. In particular, the files (omitting the extension) `new`, `show` and `edit` are templates for the *create*, *read* and *edit* operations. Additionally, `_form` is a form template for editing or entering model data. This form template is actually included by the new and edit templates. To get an idea of how this works, here is the edit template contained in the file `edit.html.erb`:

```
<% title "Edit Sample #{@sample.code}" %>

<%= render 'form' %>

<p>
  <%= link_to "Show", @sample %> |
  <%= link_to "View All", samples_path %>
</p>
```

Note that there are familiar HTML elements such as the paragraph tags and . Text within the <% and %> tags is ruby code. Note in particular the `render 'form'` directive. This reads in the content of the file `_form.html.erb`.

Also contained in the `views` directory are the email templates used when sending confirmation/update notifications to users. These templates are contained in the `sample_mailer` subdirectory. There are four template files:

```
sample_receipt.html.erb  sample_update.html.erb
sample_receipt.text.erb  sample_update.text.erb
```

The files contain templates for both simple text and HTML formatted emails corresponding to emails sent on sample submission (a receipt email) and emails sent when a sample status is updated (an update email). Here is a listing of the template for a receipt email with HTML formatting:

```
<p>
Dear User
</p>

<p>
New Sample Submission Code: <%=@sample.code%> (your ref <%=@sample.userref%>)<br />
Submitted By: <%="#{@sample.user.firstname} #{@sample.user.lastname}"%>
</p>

<p>
your sample analysis request has been received. Please download a
receipt using the link below. Please quote the sample code in any
correspondence.
</p>

<p>
There is a tear-off slip at the bottom
of the receipt which you should attach to your sample.
You will be informed via email of any
changes in the status of your sample.
</p>

<p>
<%= link_to "Analysis Request Receipt", "#{sample_url(@sample, :host => MAIL_HOST)}.pdf" %>
</p>

<p>
Copies of this email are sent to both sample submitters and their
research group leaders (where different).
</p>

<p>
Newcastle Crystallography Service
</p>
```

Note the HTML formatting elements, and as well as some embedded ruby (between the <% and %> tags). The text version is similar, but without the HTML formatting tags.

> You can edit the view templates without needing to restart the application. However, large-scale changes to views should be incorporated into the official source code repository on GitHub (see section 3.6).

3.3.2 The public Directory

This directory contains files that can be *directly* viewed by a web browser. For example, if you create a file called `info.html` in this directory then (provided its permissions are suitable) you will be able to view its contents simply by entering the following URL into your web browser:

```
http://crystal.ncl.ac.uk/info.html
```

The public directory contains things such as stylesheets, error pages corresponding to the standard HTTP error codes* 404, 422 and 500, generic images (e.g. icons for buttons and logos), javascript files and any files which are uploaded to the server.

This last category includes all file uploads to do with samples and assets. These files are all placed in a directory called `uploads` within the public directory. Uploaded files are further organised depending on whether they are to do with samples or whether they are a generic asset. An example will best illustrate this. Suppose that a zip file of sample analysis data is uploaded by an administrator. He is free to give the zip file any name. Suppose he calls the file `results.zip`. Then, when the file is uploaded via the sample edit form, it will be placed in the following location:

```
public/uploads/sample/zipdata/62/results.zip
```

Similarly, a synthetic route image file called `synthroute.png` uploaded by a user when submitting a sample analysis request, will be placed in the file:

```
public/uploads/sample/synth/<sample_id>/synthroute.png
```

where `<sample_id>` is the id automatically assigned by the database engine to that particular sample†. To summarise, the general form of the file path for uploaded files is:

```
<application root>/public/uploads/<model>/<uploader>/<id>/<file name>
```

*404 and 500 refer to 'file not found' and 'internal server error' respectively. A 500 error often arises when a program script malfunctions or there is a database problem.

†In fact another file will be automatically created in the same directory, this file is a thumbnail version of the user's file and will be given a similar name to that which the user submitted except prefixed by the string `thumb_`.

3.3.3 The config Directory

This directory contains configuration and initialization files for the rails application. You will rarely, if ever need to edit most of these. However, there is one file, `environment.rb`, which contains some parameters that you may want to change occasionally. Here is a listing of this file (linefeeds have been added for clarity but do not appear in any of the string variables):

```
# Load the rails application
require File.expand_path('../application', __FILE__)

# Initialize the rails application
SampleTracker::Application.initialize!
ITEMS_PER_PAGE = 10 # default num items per page for will_paginate

###################  SPECIFIC GLOBAL VARS ###################
TEXTILE_REF_URL = "http://redcloth.org/textile/"
CRYS_EMAIL = "xray.cryst@ncl.ac.uk"
LOCAL_ADMIN_EMAIL = "crysadmin@milkyway.ncl.ac.uk"
TEXTILE_QUICK_REF_URL = "http://en.wikipedia.org/wiki/Textile_%28markup_language%29"
SAMPLE_INTRO_TEXT = "a unique code and a barcode will be
automatically generated on submission of this form when a new sample
is created. For synthetic route files, please use either the JPG or PNG
bitmap image format.
Note further that for security reasons, if there are validation errors
in the form, you will have to re-select the names of uploaded files.
Also remeber to set the priority number, the form will not validate unless
you do this (if you are not going to submit several samples in a short
space of time we suggest setting the priority number to 1)."
QUEUE_INTRO_TEXT = "The following gives an appoximate wait time before your
sample will be analysed. The actual time will vary depending on sample
quality and priority number."
DLS_VISIT_DATE = "31/06/2012"
DLS_QUEUE_INTRO_TEXT = "The following samples are awaiting analysis at the
Diamond Light Source (DLS). The next visit to DLS is
scheduled for #{DLS_VISIT_DATE}."
```

There are several constants (those parameters in capitals) which define parameters which affect the way the application runs:

ITEMS_PER_PAGE is the parameter that controls the *default* pagination of lists as mentioned elsewhere. Lists will use this parameter as a default, but in most cases users can change the pagination on-the-fly.

TEXTILE_REF_URL contains a URL pointing to a complete Textile reference — currently it refers to the RedCloth web site.

CRYS_EMAIL is the email account to which sample submission requests are sent.

LOCAL_ADMIN_EMAIL this is set to the email address which appears in the *From* part of all emails which are automatically sent to users by the sample tracking system.

TEXTILE_QUICK_REF_URL contains a URL to a Textile quick reference page. This is currently set to the Wikipedia entry for Textile and is used on the page edit screen to help administrators edit static pages as shown in Figure 5.

SAMPLE_INTRO_TEXT contains the text that appears at the beginning of the sample submission form — see for example Figure 10.

QUEUE_INTRO_TEXT contains the text that appears in a box at the beginning of the sample queue page.

DLS_VISIT_DATE contains the date of the next visit to the *Diamond Light Source*. This parameter will often be referenced in other global variables and view files. For example, the DLS_QUEUE_INTRO_TEXT variable in the listing above refers to this variable.

DLS_QUEUE_INTRO_TEXT contains the text that appears at the beginning of the DLS sample queue page.

> Note that if any of these parameters are changed, the server will need to be restarted before the changes will take effect. You should also make a note of such changes in the case of a system upgrade because the source code on GitHub will not necessarily have these parameters set to the same values.

3.3.4 The db Directory

This directory contains the actual database used in the application. The production database is stored in a single file, `production.sqlite3`. There may also be a development database, `development.sqlite3` used for development work. The latter file is never used in a production environment however. One other important file is `schema.rb`. This is a file containing ruby code which can be used to re-generate the entire blank database schema.

There is also a directory called `migrate`. This contains all of the *migrations* which have been applied to the database since it was first initialised. A migration is simply an adjustment to the database schema. For example, you may create an initial table in the database but later realise that you want to change some characteristic of the table such as adding an extra field or changing the datatype of an existing field. You can do this by setting up a migration — basically a bit of ruby code which will perform the necessary changes. The file `schema.rb` mentioned earlier can be thought of as an accumulation of all the migrations that have been applied to the database to get it to its current state.

3.3.5 Other Directories

There are several other directories:

tmp holds temporary files created by *SamTrack*. This directory has subdirectories for storing cache contents, session information and sockets. These files are automatically cleaned up from time-to-time although an occasional manual clean-out may be necessary if things go wrong.

doc contains documentation of various sorts. The subdirectory `guide` contains this administrator's guide as well as the LaTeX source file and included figures needed to create it. There are also several markdown formatted files which contain informally-written information about the development of the application.

spec is not used at present. It is intended as the location for a complete testing suite for the application. The test suite has not yet been written, but may be in the future.

autotest is intended to hold files related to automatic testing. It is not used at present.

lib contains code that doesn't neatly fit anywhere else. Within this directory is a file called `development_mail_interceptor.rb` which is used to set up an email environment in development mode, where you don't want emails to be sent to actual users. The code in this file redirects all email to a specific developer's email address. There is also a `tasks` directory used to put code for any Rake* tasks which have been written by developers. No custom Rake tasks have been written for this application so the directory is currently empty.

log contains special development log information.

vendor is the place where third-party code can be stored. It has a subdirectory, `plugins` where extensions to rails are stored. Plugins extend core rails functionality. We don't use any rails plugins in this application at the moment so the directory is empty. The `vendor` directory can also be used to store rails and all of its dependencies rather than relying on the operating system to provide them. At present we don't use this feature, but in future, when the application is stable, this is probably where we will install an independent copy of rails and its dependent software (e.g. gems) in order that the whole application is autonomous and not reliant on what the operating system provides.

3.4 Web Server Management

Most of the time, you should need only two commands when managing the web server — the commands to switch it on and off. To do this use:

```
sudo apache2ctl start|stop
```

You would typically stop the server to do some maintenance such as editing a stylesheet or a major upgrade to the software. Occasionally you may need to change some server parameters in the web server configuration files. The main configuration file is `/etc/apache2/apache2.conf`. You will rarely, if ever, need to change anything here unless you want to tweak the server performance (in which case you'll definitely need to know what you're doing). This file does contain some parameters for the apache *Phusion Passenger* module which is needed to interface Rails with the apache server:

```
LoadModule passenger_module /usr/local/rvm/gems/ruby-1.9.2-p290/
gems/passenger-3.0.9/ext/apache2/mod_passenger.so
   PassengerRoot /usr/local/rvm/gems/ruby-1.9.2-p290/gems/passenger-3.0.9
   PassengerRuby /usr/local/rvm/wrappers/ruby-1.9.2-p290/ruby
```

These configuration lines are added as part of the installation of *Phusion Passenger* and tell it where the ruby interpreter and passenger software reside in the file system.

The `apache2.conf` file also contains a line which refers to some other configuration files:

```
Include /etc/apache2/sites-enabled/
```

*Rake is a *build tool* which is used by developers to automate certain tasks. It is also used within rails to perform database migrations.

The above line tells the server to get some further configuration details from the contents of the directory `/etc/apache2/sites-enabled`. `sites-enabled` contains a file called `000-default` which contains the descriptions of all the *virtual hosts**. The most important virtual host entry is the one for the host `crystal.ncl.ac.uk`. Here is the entry in full:

```
<VirtualHost *:80>
      ServerName crystal.ncl.ac.uk
      DocumentRoot /usr/local/share/sample_tracker/public
      <Directory "/usr/local/share/sample_tracker/public">
         AllowOverride all
         Options -MultiViews
      </Directory>
        ErrorLog /var/log/apache2/error-crystal.log
</VirtualHost>
```

For virtual hosting to work, any name given to a virtual host (e.g. in this case `crystal.ncl.ac.uk`) must be an official alias for the actual apache web server (in this case `milkyway.ncl.ac.uk`). We will now describe in detail what these directives mean.

The first line is a tag which defines the beginning of a virtual host definition. It has the form `<VirtualHost *:80>`. The number 80 is the *port number*†. The last line is a closing tag, `</VirtualHost>`. the lines in-between contain the directives which control the configuration of this host.

ServerName This directive sets the name of the virtual host, in this case `crystal.ncl.ac.uk`.

DocumentRoot Sets the absolute path of the directory on the server which contains all static documents which can be *directly* viewable on a web browser. No documents outside this directory can be viewed directly or downloaded. In this case, the document root is `/usr/local/share/sample_tracker/public` i.e. the `public` directory within the root *SamTrack* directory. This is a standard rails convention.

ErrorLog Specifies the absolute path of the error log file for this virtual host. Here, it is set as `/var/log/apache2/error-crystal.log`.

There is also a `Directory` section in the virtual host definition. This has the form of an opening and closing tag with directives in-between. The opening tag has an argument which is the full path of the particular directory to which the directives apply. Note that the argument is in quotes. In this case the argument is the same directory as the document root. Note further that there may be more than one `Directory` section. The directives are as follows:

AllowOverride This directive controls whether directives contained in a file (conventionally called `.htaccess` contained in a particular directory can override earlier configuration directives at the server configuration level. The argument refers to which type of directive can be overridden — in this case `all`.

Options This sets a number of options when viewing files contained in the relevant directory. here, we have set the `-MultiViews` option which allows a single document to be displayed in different ways dependent on browser capabilities.

*A single Apache web server can support multiple so-called virtual hosts which behave as separate web sites.

†A port number defines a communications channel between computers on the Internet. Port 80 is usually used by the HTTP protocol for communication between web servers and browsers although other port numbers can be used.

Root Directory Location of *SamTrack*
It should be clear from the above that if you want to change the root directory of *SamTrack* you must edit the virtual host directive file and change the `DocumentRoot` directive and `Directory` section argument appropriately.

We end this section on web management with a brief discussion about file permissions. Once you have uploaded the application and all its files to a suitable location you must make sure that the file permissions are correct. The correct permissions for all files are to set group ownership to `root` and user ownership to `nobody`*. This can be done with a simple one-line command:

```
sudo chown -R nobody.root <application document root>
```

3.5 Raw Database Management

Hopefully, you won't often need to refer to this section because *SamTrack* will handle all of the database operations for you. Sometimes however, the database becomes broken in some way and needs to be edited in its 'raw' form. For example, you may be logged in as an administrator and inadvertently remove your own administration rights. If you were the only administrator then you now have a problem because only an administrator can change a user's rights! We will look at how to solve this particular problem later in this section. We consider specifically SQLite3 database manipulation here since that is the database used in the application. In this section we describe two utilities for manipulating SQLite3 databases, the command-line linux program *sqlite3* and the web browser plugin *sqlite-manager*.[16]

3.5.1 Database Management with sqlite3

sqlite3 is available on all systems where the SQLite3 database is installed. Here, we briefly describe how to use it to manipulate the sample database and give one example of its use in a practical situation. A simple command gets you started:

```
sqlite3 <sqlite3 database file>
```

which produces some informational output followed by a prompt:

```
SQLite version 3.6.22
Enter ".help" for instructions
Enter SQL statements terminated with a ";"
sqlite>
```

All commands in sqlite3 begin with a full stop. Assuming, we're looking at the sample tracking database, typing `.tables` will give a list of tables in the database:

```
sqlite> .tables
assets                  pages                   schema_migrations
flags                   popups                  sensitivities
groups                  samples                 stores
```

*`nobody` is a special user account available on most linux systems.

```
hazards                 samples_sensitivities  uploads
hazards_samples         samples_stores         users
sqlite>
```

The `.schema` command can be used to check the schema of either individual tables or, without an argument, *all* tables:

```
sqlite> .schema samples
CREATE TABLE "samples" ("id" INTEGER PRIMARY KEY AUTOINCREMENT NOT NULL, "code"
varchar(255), "cif" varchar(255), "synth" varchar(255), "coshh_name" varchar(255
), "coshh_desc" varchar(255), "coshh_info" text, "params" varchar(255), "priorit
y" integer, "powd" boolean, "chiral" boolean, "cost_code" varchar(255), "barcode
" varchar(255), "created_at" datetime, "updated_at" datetime, "user_id" integer,
 "flag_id" integer DEFAULT 1 NOT NULL, "userref" varchar(255), "zipdata" varchar
(255), "sampleimage" varchar(255), "reference" varchar(255), "comments" text, "c
olour" text, "size" text, "shape" text, "feedback" text);
sqlite>
```

What is displayed here is the SQL command sequence needed to create the table (in this case the samples table). You can deduce from this the whole table schema — field names, data types, whether a particular field is allowed to be NULL or if it has a default value etc.

If you want to actually enter data into or edit a database, you need to understand the database query language SQL. A good, quick introduction is available on the *w3schools* web site.[17] Now, as an example, let's return to the problem of giving a user administration rights when there are no other such users*. In this case we'll use sqlite3 to give a particular user administration rights. We'll assume that the user's last name is 'Hagon'. First, we need to find the user. Here's the SQL to do that†:

```
sqlite> select * from users where lastname = 'Hagon';
2|jerry.hagon@ncl.ac.uk|$2a$10$V2eSY1MD2dWkIESZ/3mtGe8hYvVDVkDTDEd4NKqZOQJ3t9wg9
8iFq|hkTD7hHWzEu5ErjSFh2y|2012-02-16 10:19:43.792239||190|2012-04-06 07:43:02.65
2582|2012-04-04 13:58:26.642714|127.0.0.1|127.0.0.1|2011-11-06 15:18:43.971379|2
012-04-06 07:43:02.653005|19|f|Jerry|Hagon|t|t
sqlite>
```

Now, what does all this mean? First, each field in the output is separated by a vertical bar (|). The order of the fields is determined by the schema, so let's find this out:

```
sqlite> .schema users
CREATE TABLE "users" ("id" INTEGER PRIMARY KEY AUTOINCREMENT NOT NULL, "email" v
archar(255) DEFAULT '' NOT NULL, "encrypted_password" varchar(128) DEFAULT '' NO
T NULL, "reset_password_token" varchar(255), "reset_password_sent_at" datetime,
"remember_created_at" datetime, "sign_in_count" integer DEFAULT 0, "current_sign
_in_at" datetime, "last_sign_in_at" datetime, "current_sign_in_ip" varchar(255),
 "last_sign_in_ip" varchar(255), "created_at" datetime, "updated_at" datetime, "
group_id" integer, "admin" boolean DEFAULT 'f', "firstname" varchar(255), "lastn
ame" varchar(255), "leader" boolean DEFAULT 'f', "enabled" boolean DEFAULT 't');
CREATE UNIQUE INDEX "index_users_on_email" ON "users" ("email");
CREATE UNIQUE INDEX "index_users_on_reset_password_token" ON "users" ("reset_pas
sword_token");
sqlite>
```

*If you think about it, this will always be the case initially!

†Note that SQL commands must be terminated by a semi-colon.

Ignoring the `CREATE UNIQUE INDEX` which don't relate to the order of the fields, we see that in the `CREATE TABLE` entry (which ends with the semi-colon before the firts line beginning with `CREATE UNIQUE INDEX`) the last five fields are `admin`, `firstname`, `lastname` `leader` and `enabled`. `admin` is the key field — it's a *boolean* field having only two values, true or false (labelled as either `'t'` or `'f'` in the above output.

The last five entries for the user were listed as `f|Jerry|Hagon|t|t` which means that he is not an administrative user. To give this user administrative rights we must change the `admin` field (5th from last). Here is the SQL to do that:

```
sqlite> update users set admin='t' where id=2;
sqlite> select * from users where lastname = 'Hagon';
2|jerry.hagon@ncl.ac.uk|$2a$10$V2eSY1MD2dWkIESZ/3mtGe8hYvVDVkDTDEd4NKqZOQJ3t9wg9
8iFq|hkTD7hHWzEu5ErjSFh2y|2012-02-16 10:19:43.792239||190|2012-04-06 07:43:02.65
2582|2012-04-04 13:58:26.642714|127.0.0.1|127.0.0.1|2011-11-06 15:18:43.971379|2
012-04-06 07:43:02.653005|19|t|Jerry|Hagon|t|t
sqlite>
```

And we can see from the `select` command that the change has been applied. Note that we have used the SQL *update* command and applied it to the user whose `id` field is 2. Now, the `id` field is the first one in the list and we have used that to refer to the user. We could also have used any other field, but the `id` field is unique and so is guaranteed to refer to only one user. A command such as:

```
update users set admin='t' where lastname='Hagon';
```

would also work but if there were, say, two users with that same last name, the change would be applied to both of them.

3.5.2 Database Management with sqlite-manager

sqlite-manager provides a graphical user interface to SQLite3 database management. It is a web browser plugin available for the Firefox web browser and can be easily installed via a simple one-click link.[16] The plugin is accessed via the Firefox *Tools* menu as shown in Figure 18.

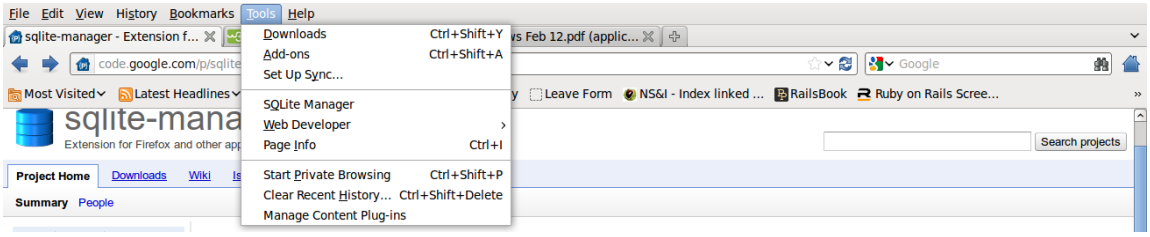


Figure 18: Firefox *Tools* menu showing the link to the installed *sqlite-manager* plugin (4th from top in the menu).

When sqlite-manager starts up, you first see the main window shown in Figure 19. To read in a database, select *Connect Database* from the *Database* menu. A file browser window will appear, but by default it shows only those files with extension `.sqlite`. At the bottom right of this window is a drop-down select box which allows you to view 'All Files'. After selecting this option you will be able to see any file in the window. After browsing to the appropriate

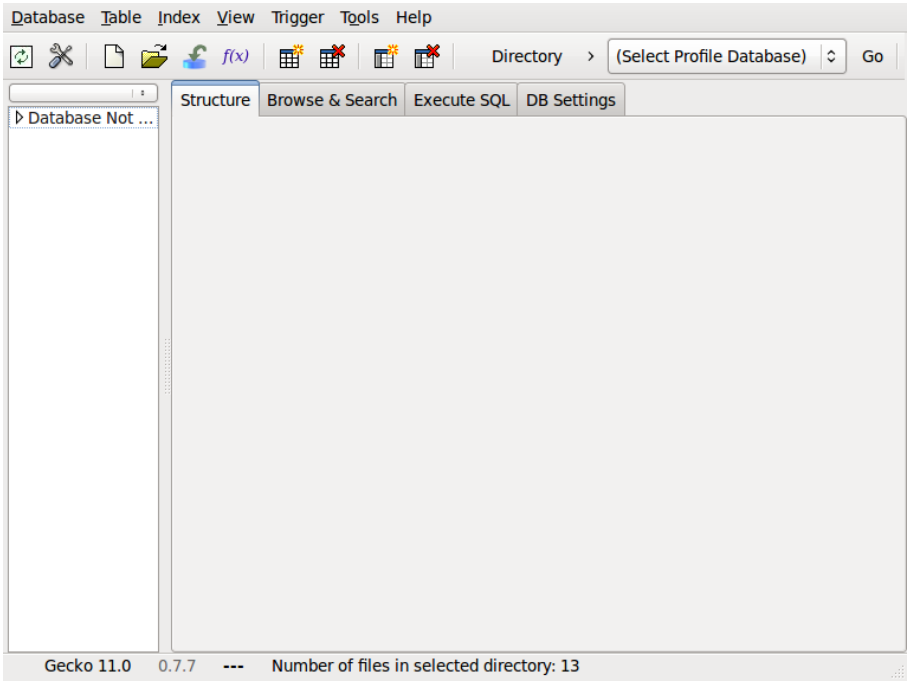


Figure 19: Initially the user is presented with the main sqlite-manager window.

directory and selecting the database file you want (we will use a sample tracking database file in the description to follow), the main window should show the database as shown in Figure 20.

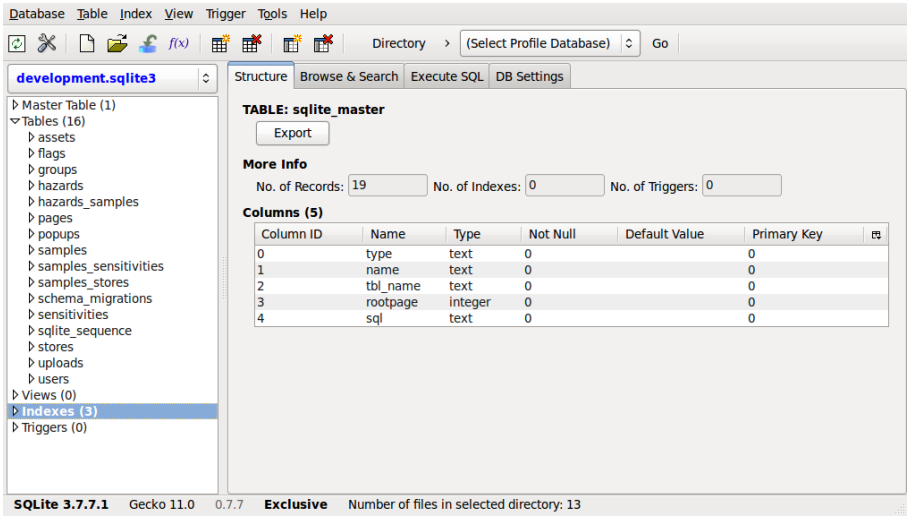


Figure 20: The main sqlite-manager window after loading a sample tracking database file. Note the list of tables in the left hand panel.

We will now try to do the same update that was performed using the command-line utility *sqlite3* previously. To begin, select the *users* table from the list in the left hand panel then select the *Browse & Search* tab in the main panel. You should see a list of users (you can use the mouse to adjust the width of the field columns). This is shown in Figure 21.

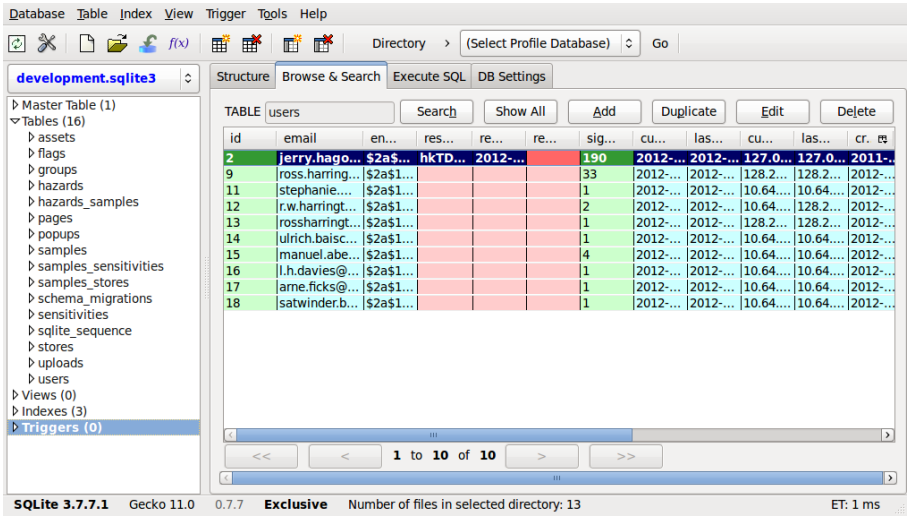


Figure 21: The *users* table listing in the *Browse & Search* tab in the main panel.

Editing an entry is easy, just double-click on the row that you want to edit — in this case the first one. The *Edit Record* box will pop up. Scroll down until you reach the admin field, change its value accordingly and then click the *OK* button (Figure 22.

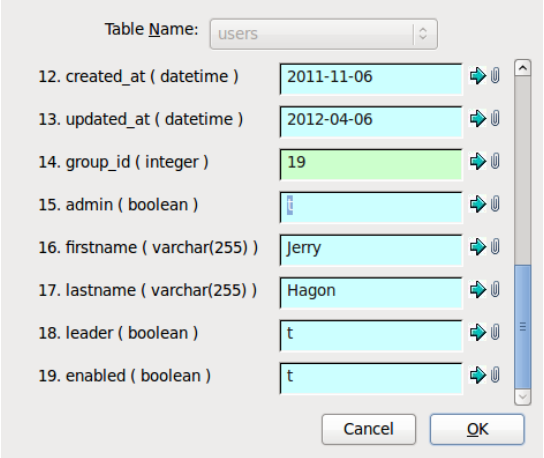


Figure 22: The sqlite-manager *Edit Record* window. Each field in the record can be edited.

The sqlite-manager plugin is very powerful and well-worth experimenting with (using a test database of course!). It can perform arbitrary SQL commands via an SQL command panel and has simple short-cuts for doing most update/create operations. There are also easy-to-use search and sort facilities.

There are other tools which can be used to manipulate SQLite3 databases. The two we have described are freely available. Other free alternatives are also available as well as commercial tools. Some of these are described on the SQLite web site.

3.6 Software Updates and GitHub

The *SamTrack* application is stored on GitHub,[18] a a web-based hosting service for projects that use the *Git* revision control system. This means that the source code is safe and new versions of the software can be quickly downloaded and installed. Anyone can view the *SamTrack* repository. The URL is `https://github.com/jhagon/sample_tracker`. Typing this URL into your browser produces a page something like that shown in Figure 23.

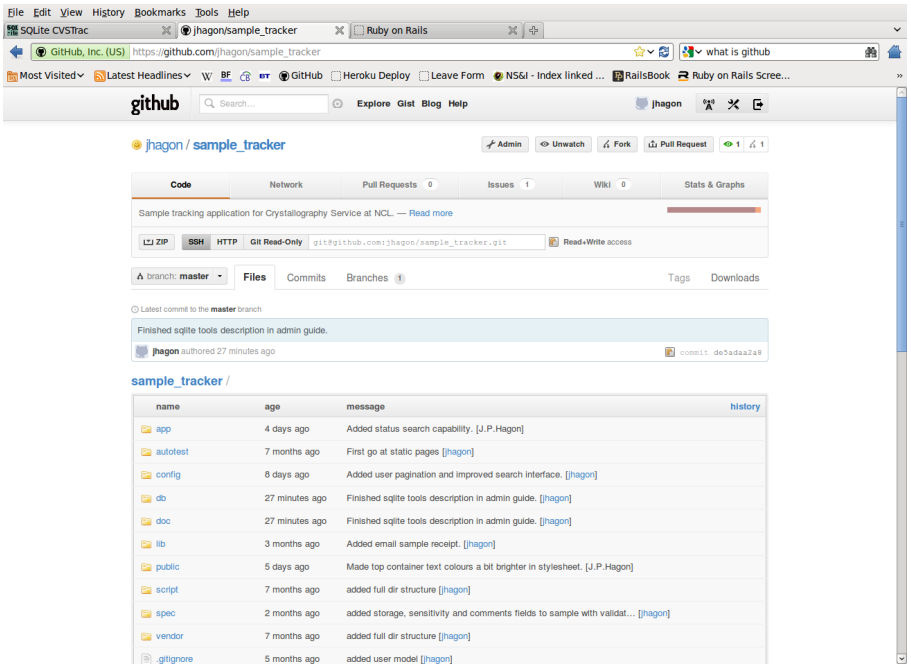


Figure 23: The *SamTrack* GitHub repository.

The GitHub repository contains a wealth of information about the development of the software and its current status. You can browse the entire file structure of the system, downloading individual files or the entire repository. Any development work on the system will be mirrored on GitHub so that the latest version of the software can be downloaded at any time. It is also possible to download any previous version of the software if needed.

To download the current version of *SamTrack*, simply click on the *ZIP icon* near the top of the file browser panel on the left hand side. This will pack the whole of the source into a compressed ZIP file. If you require a specific version, then first click the *history* link on the top right of the main file browser panel. This will take you to the *Commit History* page. If you click on the descriptive text for a particular revision, you will be taken to the summary page for that particular revision. Near the top right is a *Browse code* button which when clicked will take you to a file browser panel for that revision. Again, you will see a *ZIP icon*, on the top-left of the file browser panel which you can click to get a ZIP file of that version.

You can also submit bug reports via the GitHub page although you must be registered to do so. Current issues can be viewed via the link at the top of the main repository page. Also, there are statistics and charts which provide detailed information about the application.

3.7 Backup and Upgrade Procedures

It is essential of course to make sure that the system is adequately backed-up. As we have seen, a copy of the software itself (both current and previous versions) is safely stored on GitHub. However, GitHub does not store sample data — you must take steps to make sure the sample data is safe. As a general rule, if you back up the whole of the application root directory then that is sufficient. As mentioned in section 3.3.3 you should also make a note of any global parameters that you change because these will not necessarily be reflected in the GitHub source if you perform a full upgrade of *SamTrack*.

Volatile sample data is stored in two places:

(i) The SQLite3 database file `<application root>/db/production.sqlite3`;

(ii) The public directory `<application root>/public` and everything underneath it.

3.7.1 System Upgrade Procedure

There are two circumstances where you will need to do a full system upgrade:

- after major updates to the software;
- whenever the database schema has changed (no matter how small the change may be).

Database Schema Changes
Schema changes can be very minor, e.g. a renaming of a field, a change in data type, a change in default value etc. or they can be more complex, such as the addition of one or more fields or even whole new tables. However, a schema change *no matter how small* necessitates a full system upgrade in the manner described below.

We will go through the steps needed to perform a full software upgrade. This procedure is also described in the file `<application root>/doc/UPGRADE.markdown`*

1. login using the `crysadmin` account and switch to a root shell:

   ```
   sudo bash
   ```

2. Stop the web server:

   ```
   apache2ctl stop
   ```

3. Change to the directory which contains the *SamTrack* application (usually `/usr/local/share`) and move the application root directory to a different place thus retaining a complete copy of the old system — we don't want to scrub it just in case!

   ```
   cd /usr/local/share
   mv sample_tracker sample_tracker.old
   ```

*If you view this file (and any other markdown-formatted file) on GitHub, it will be nicely formatted according to the markdown specifications.

4. Go to the GitHub repository where the latest copy of the application is stored and download a copy using the procedure described in section 3.6. Put the downloaded ZIP file in a temporary directory such as `/tmp`. The ZIP file will have a name similar to `jhagon-sample_tracker-b493e1b.zip` with the `b493e1b` part indicating the revision:

   ```
   mv jhagon-sample_tracker-b493e1b.zip /tmp
   ```

5. Now, unzip the file in the temporary directory (at the moment, it doesn't matter where you do this):

   ```
   unzip jhagon-sample_tracker-b493e1b.zip
   ```

   You should have a directory called something like:

   ```
   jhagon-sample_tracker-b493e1b
   ```

   tem Move the above directory to the live application location:

   ```
   mv jhagon-sample_tracker-b493e1b /usr/local/share
   ```

   then change to the `/usr/local/share` directory and rename the `jhagon-sample_tracker-b493e1b` directory to `sample_tracker`:

   ```
   cd /usr/local/share
   mv jhagon-sample_tracker-b493e1b sample_tracker
   ```

6. Change to the `sample_tracker` directory and remove the production database (if it exists) and also the `public` directory:

   ```
   rm db/production.sqlite3
   rm -rf public
   ```

7. Now we must import the live production database and `public` directory from the saved copy of the previous application:

   ```
   cp <previous sample_tracker dir>/db/production.sqlite3 db
   cp -r <previous sample_tracker dir>/public .
   ```

   where the above commands are assuming we're in the new application root directory (`/usr/local/share/sample_tracker`). If the database schema has not changed, go to step 10. Otherwise:

8. We must now migrate the database to its new schema. First we must make sure we are running the latest ruby. The server's default version of ruby is too old so we must instead use a special version which we can access by typing:

   ```
   source /etc/profile.d/rvm.sh
   ```

   to check this, if you type 'ruby -v' you should get something similar to this — the important part is the version number of ruby, it should be 1.9.x:

```
ruby 1.9.2p290 (2011-07-09 revision 32553) [i686-linux]
```

9. Now perform a database schema migration by typing the following:

   ```
   export RAILS_ENV=production
   rake db:migrate
   ```

   Note that you may see a couple of warnings during the rake command, but this is OK.

10. We are almost done. Next change the ownership of the entire `sample_tracker` directory structure to user `nobody`. Before doing this we change directory to that which holds the application root directory:

    ```
    cd /usr/local/share
    chown -R nobody.root sample_tracker
    ```

11. Now all that is left is to start the web server (and hope!):

    ```
    apache2ctl start
    ```

At this point you should perform a few checks on the new system. If there are problems, you can stop the web server, scrub the new version and copy the previous saved version back to the correct location. then restart the web server.

4 Database Schema Description

4.1 Introduction

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) at the time of writing. The easiest way to get an overall view of the database schema is to study Figure 24. This shows all the tables, fields and relationships in a single diagram. We now give a brief description of each table.

Note that all tables except join tables have an auto-incremented integer field called `id` which servers as the unique primary key for each record in the table. The `id` field will not be listed explicitly in the description of each table. All non-join tables also have two other fields, `created_at` and `updated_at` in a datetime format. Again, we will not explicitly list these fields in the description of the tables which follows.

4.2 The Samples Table

The samples and users tables are the key parts of the database as is evident from Figure 24. They are related to each other via a *one-to-many* relationship, i.e. *one* user can have *many* samples but a single sample is associated with just *one* user. The samples table consists of the following fields:

code a string, automatically generated by the system having the general form `AAA-AA-YY-1111` where the `AAA` and `AA` represent 3-letter codes for group and submitter respectively; the `YY` represents the year and the `1111` represents a number which is incremented for that group but reset to zero at the start of each calendar year.

cif a string representing the chemical formula of the sample in cif format.

synth a string representing the file name of an image file specifying the details of the synthesis.

coshh_name a string representing the name of the solvent (if any).

coshh_info another string describing any procedures in case of contact with the sample.

coshh_desc a text field providing a brief description of the sample (e.g. organic amide).

params a string representing unit cell parameters or CSD/Newcastle code for possible by-products or previously obtained, unpublished results.

priority an integer between 1 and 9 to give an indication of priority.

powd a boolean parameter indicating if the sample requires powder diffraction (y/n).

chiral another boolean indicating whether the molecule is chiral (y/n).

costcode a string providing a cost centre code for charging if relevant.

barcode a string field for an automatically generated Code39 standard bar code.

user_id this integer holds the `id` field of the user who requested the sample analysis.

flag_id an integer holding the `id` field of the status flag of the sample.

userref a string for a user-defined reference. This is required to be an alphanumeric sequence of characters *without spaces*.

zipdata a string holding the name of a zip file containing the results of the analysis.

sampleimage a string holding the name of an image file of the sample molecule after it has been identified by the analysis.

reference a text field for a published reference (typically in the form of a DOI).

comments a text field for any general comments the user wishes to make about the sample.

colour a string holding information about the colour of a sample after analysis.

size a string holding information about the size of a sample after analysis.

shape a string holding information about the shape of a sample after analysis.

feedback a text field containing any additional comments on the sample by crystallography staff.

4.3 The Users Table

The users table, in addition to maintaining a record of users and their samples, also serves as a key part of the authentication and authorisation system which will be described later. the users table is related to the samples table via a *one-to-many* relationship, i.e. *one* user has *many* samples.

email a string holding the email address of the user. This serves also as the user login id.

encrypted_password a string holding the user's password in an encrypted form.

reset_password_token a string containing a special token used if the user has forgotten his password and needs to reset it.

reset_password_sent_at a datetime field recording the time a token enabling a user to reset his password was sent.

remember_created_at a datetime field specifying the time at which a user requested that his login id be remembered by the browser so he need not type in his credentials.

sign_in_count an integer holding the number of times a user has logged-in.

current_sign_in_at a datetime field holding the sign-in time for the current session.

last_sign_in_at a datetime field holding the last sign-in time for the user.

current_sign_in_ip a datetime field holding the user's ip address for the current session.

last_sign_in_ip a datetime field holding the previous login ip address for the user.

group_id an integer representing the `id` field of the group to which the user belongs.

admin a boolean field indicating whether the user is an administrator (y/n).

firstname a string holding the user's first name.

lastname a string holding the user's last name.

leader a boolean field indicating whether the user is a group leader (y/n).

enabled a boolean field indicating if the account is enabled (y/n).

4.4 The Stores, Hazards and Sensitivities Tables

These tables are each very similar and have the same basic structure. They are used to specify storage, hazard and sensitivity properties for a sample. They all have a *many-to-many* relationship with the samples table. This is because a sample can have, for example, *many* storage requirements, but also a single storage requirement can be associated with *many* samples. All these tables have essentially the same fields:

name a string defining a short name for the property.

description a text field describing the property at greater length.

For historical reasons, the hazards table uses the names `hazard_abbr` and `hazard_desc` for the `name` and `description` fields. Also the `hazard\_desc` field is a text field rather than a string.

Associated with these tables are three further *join tables* which facilitate the many-to-many relationship between a sample and its properties. These join tables are called `samples_stores`, `samples_hazards` and `samples_sensitivities`. They all contain two fields corresponding to the sample `id` field and the associated property `id` field. For example, `samples_stores` contains the fields `sample_id` and `store_id`. Both these fields are integers of course.

4.5 The Groups Table

This table represents groups of users, normally research groups but also perhaps external companies etc. It is a simple table, but important in the way the whole system works. It contains the following fields:

group_abbr a 3-letter string as an abbreviation for the group. Amongst other things this is used to form part of the sample code string mentioned earlier.

group_desc a string giving a more complete description of the group.

4.6 Other Tables

There are several other tables which are less important than the ones discussed so far in the sense that they are strictly not necessary for a working sample tracking system. However, they do assist in making the system much easier to manage and also help making the system much friendlier for users. These tables are the `assets`, `pages` and `popups` tables.

4.6.1 The Pages Table

The purpose of this table is to provide a means by which administrators can add 'static' content to the sample tracking web site. Each static page has its content stored in this table. The fields are:

name a string storing a name for the page. This is typically used to provide a title for the page in a web browser window.

permalink another string used to provide a short, quick URL for the page.

content a text field which contains the page content. This is expected to be written in Textile markup language (although a mixture of pure HTML and Textile can be used.

menu a boolean specifying whether this page should appear on the *Information Menu*.

priority an integer specifying a priority for ordering the page on the *Information Menu*.

4.6.2 The Assets Table

The assets table keeps a record of general files which have been uploaded to the server. These files are typically graphical images, pdf documents etc. and will usually be referenced in one of the static pages created by administrators which are stored in the `pages` table. An 'asset' is simply one of these uploaded documents and the `assets` table keeps a record of it. The fields are:

document the full path name of an uploaded document. This path name is ultimately assigned using the carrierwave file uploading plugin to ruby on rails.

description a text field giving a brief description of the document.

4.6.3 The Popups Table

This table stores descriptive information about the primary fields in the samples table. It has two fields:

name this string should have the same name as one of the sample fields for which a detailed description is required.

description a text field giving a detailed description of the associated sample field in the corresponding `name` field.

The `popups` table, as its name implies, provides descriptive text in popup boxes whenever a user hovers the mouse over the appropriate field in the sample submission form.

4.6.4 The Flags Table

This table stores a set of status flags together with a more verbose description of what the flag means.

name a string containing the name of the status flag, e.g. `SUBMITTED`, `COMPLETED` etc. There can be any number of flags but the aforementioned flags must be present because when the sample is originally submitted it is, by default, given the status `SUBMITTED`. Also, when analysis is finished, the sample queue list will omit all samples which have had the `COMPLETED` flag set or have a status flag which begins with the string `FAILED`.

description a text field giving a detailed description of the associated flag name.

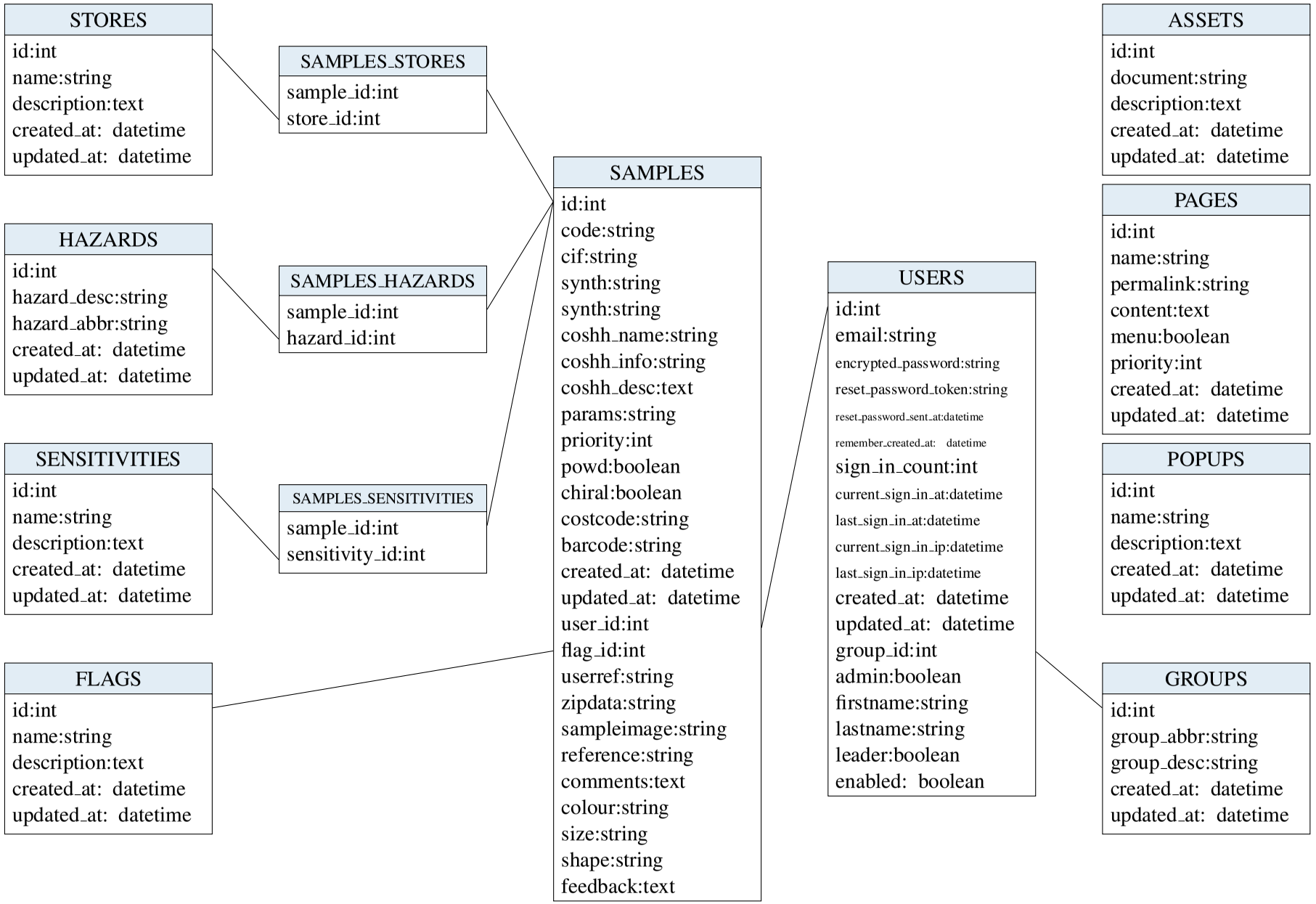


Figure 24: The overall database schema. Relationships between tables are indicated with lines joining the relevant fields. Note that the tables `SAMPLES_STORES`, `SAMPLES_HAZARDS` and `SAMPLES_SENSITIVITIES` are *join tables* which serve only to facilitate a many-to-many relationship between the tables they link.

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