# The SeqHound Manual

## Part II: Sections 4-7

## For Administrators and Developers

## Release 3.3

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* not available at time of writing

## About this manual.

This manual contains everything that has been documented about SeqHound. It is distributed in two Parts (Part I: For Users and Part II: For Administrators and Developers).
If you can't find the answer here then please contact us. This manual was written and reviewed by the persons listed under "Who is SeqHound". Any errors should be reported to *seqhound@blueprint.org*.
You can find out more about the general architecture of SeqHound by reading the *SeqHound paper* that is freely available from BioMed Central. This paper is included in the supplementary material distributed with this manual. See:
Michalickova K, Bader GD, Dumontier M, Lieu H, Betel D, Isserlin R, Hogue CW. *SeqHound: biological sequence and structure database as a platform for bioinformatics research.* **BMC Bioinformatics.** 2002 Oct 25;3(1):32.
PMID: 12401134

**The SeqHound Manual (Part I: Sections 1-3) For Users.**
*Section1 and Section 2* is a one page description that tells you what to read first to get started depending on what kind of user you are.
*Section 3* is of interest to programmers who want to use the remote API to access information in the SeqHound database maintained by the Blueprint Initiative.

**The SeqHound Manual (Part II: Sections 4-7) For Administrators and Developers**
*Section 4* is of interest to programmers and system administrators who want to set up SeqHound themselves so they can use the local API.
*Section 5* is an in-depth description of everything that's in the SeqHound database and how it gets there (table by table). This section will be of interest to all users.
*Section 6* describes how programmers can add to SeqHound. This section also describes our internal development process at Blueprint.
*Section 7* includes Appendices of background and reference material.

## Conventions

The following section describes the conventions used in this manual.
*Italic*
is used for filenames, file extensions, URLs, and email addresses.
`Constant Width`
is used for code examples, function names and system output.
**`Constant Bold`**
is used in examples for user input.
***`Constant Italic`***
is used in examples to show variables for which a context-specific substitution should be made.

## How to contact us.

General enquiries or comments can be posted to the SeqHound usergroup mailing list *seqhound.usergroup@blueprint.org*. You may also subscribe to this list to receive regular updates about SeqHound developments by going to *http://lists.blueprint.org/mailman/listinfo/seqhound.usergroup* .

Private enquiries, bug reports from external users, questions about SeqHound or errors found in this manual may be sent to *seqhound@blueprint.org*.

## Who is SeqHound?

Chronologically ordered according to when the person first started work on SeqHound.

Chris Hogue
Katerina Michalickova
Gary Bader
Ian Donaldson
Ruth Isserlin
Michel Dumontier
Hao Lieu
Marc Dumontier
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Victor Gu
Rachel Farrall
Michael Matan
Elizabeth Burgess
Kai Zheng

# 4. Setting up SeqHound locally.

## 4.1 Overview.

This section describes how one can set up the SeqHound system on your own hardware using freely available SeqHound executables. These executables will allow you to build and update the SeqHound database as well as run a web-interface and a remote API server.
*Section 4.2* should be reviewed first for system requirements before attempting to install the SeqHound system.
*Section 4.3* tells you how to download executables from the SeqHound ftp site for your platform and operating system. SeqHound code may also be downloaded from this site.
*Section 4.4* describes how SeqHound code may be compiled on your own hardware using the freely available code available on the SeqHound ftp site. This step is only required if SeqHound executables are not available for your platform or if you want to make use of the local programming API. If you obtain SeqHound executables from the ftp site and want to build your local SeqHound database, you still need to go through Steps 8, 9, 10, 11 and 13 in this section which describe how to install the MySQL server and ODBC driver.
*Section 4.5* contains detailed instructions for using the executables to build the SeqHound data tables and for setting up the SeqHound web-interface and remote API server.

## 4.2 SeqHound system requirements.

Before attempting to set up SeqHound yourself, you should review the system requirements listed below. The SeqHound system is able to run on a number of operating systems (we recommend and can best support a UNIX operating system like Sun Solaris or Red Hat Linux). Setting up SeqHound will require approximately 700 GB of disk space (see below).
Questions about system requirements, compilation, setup and maintenance can be addressed to *seqhound@blueprint.org*. We will do our best to address all inquiries but resources may not allow us to solve all problems arising on all possible set ups.

**OS and hardware architecture**

SeqHound code is compiled on the following platforms based on release version code. Blueprint production SeqHound is compiled and run on Sun-Fire-880 - Sun Solaris (version 9). We have also compiled and tested SeqHound on the Fedora Core 2.0 and the MacOS X operating systems.

Release versions of SeqHound executables are available for.

| | |
|---|---|
| x86 architecture | (Fedora Core 2.0) |
| Sun-Fire-880 | Sun Solaris (version 9) |
| PowerPC architecture | MacOS X |

We have also successfully built executables on the following platforms.

| | |
|---|---|
| x86 architecture | FreeBSD |
| x86 architecture | QNX |
| x86 architecture | Windows NT |
| PowerPC architecture | PPC Linux |
| SGI | Irix 6 |
| Alpha architecture | Compaq Alpha OS |
| HPPA 2.0 architecture | HPUX 11.0 |
| HPPA 1.1 architecture | PA-RISC Linux |

**Memory (RAM)**

We recommend a minimum of **1 GB** of RAM to run the SeqHound executables.

**Hard Disk**

**Source code and executables**

| Component | Image Size |
|---|---|
| SeqHound Source and compiled | 220.0 MB |
| NCBI Toolkit | 560.0 MB |
| NCBI C++ Toolkit | 12GB |
| bzip2 Library | 4.5 MB |
| slri lib | 7.3MB |
| slri lib_cxx | 9.4 MB |
| **Source code and executables (total)** | 13GB approx |

**Database**

| Component | Image Size |
|---|---|
| data tables | 300 GB |
| data tables backup | 300 GB |
| **Database (total)** | 700 GB* |

*700GB includes 300 GB for a single copy of the SeqHound data tables. The SeqHound system includes a second copy of the data tables used for back up and updating. We suggest a minimum of **700 GB** for SeqHound installation. This allows for yearly growth of the data tables as well as for a RAID5 disk configuration.
We are using the MySQL database storage engine InnoDB, which provides transaction support and automatic recovery in the event of database server outage. There is no need to keep a separate instance of the database when the InnoDB storage engine is used. To prevent deadlock during data insertion and update, you should not run SeqHound parsers in parallel against the InnoDB database server. As a result, it takes up to three extra days for the initial build of SeqHound database using the InnoDB storage engine. If you wish to use the MyISM storage engine, you can run parallel parsers to speed up the initial build of SeqHound. However, you will need to keep a separate database instance for database update and backup as the storage engine MyISM does not support transaction and automatic recovery.

**Other Software**

| | |
|---|---|
| Apache Webserver(version 1.3) | See *http://www.apache.org/* for software installation for you platform. |
| Apache Jakarta Tocat JSP/Servlet Container (version 4.1) | See *http://jakarta.apache.org/tomcat/* for software installation for you platform. |
| Perl (version 5.8.3) | See *http://www.cpan.org/* for installation for your platform. Requiredmodules include *Net/FTP.pm*, *sun4-solaris-64/DBI.pm* |

**Compiling SeqHound Code yourself.**

It is not necessary to compile SeqHound executables yourself; the system may be set up using the executables provided on the ftp site for selected Operating Systems. However, if you wish to make use of the local API then you must compile SeqHound yourself.

**ODBC compliant database engines**

Blueprint uses the ODBC compliant MySQL database engine. We are using version 4.1.10 in production; this version supports nested SQL queries and internationalization. We have not tested SeqHound on other ODBC compliant RDBMS such as Oracle, DB2 and PostgreSQL.

**Library dependencies**

| **Library** | **Source** |
|---|---|
| NCBI Toolkit | from *ftp://ftp.ncbi.nih.gov/toolbox/ncbi_tools/* |
| NCBI C++ Toolkit (optional*) | from *ftp://ftp.ncbi.nih.gov/toolbox/ncbi_tools/* |
| bzip2 Library | from *http://sourceforge.net/projects/slritools/* |
| slri lib | from *http://sourceforge.net/projects/slritools/* |
| slri lib_cxx (optional*) | from *http://sourceforge.net/projects/slritools/* |

* This library is only required if you plan to use the SeqHound remote C++ API.

## 4.3 Obtaining precompiled SeqHound executables.

It is not necessary to compile SeqHound executables yourself; the system may be set up using the precompiled executables provided on the ftp site for selected Operating Systems. If you choose to compile the executables yourself, skip to step 4.3.1.

You will require about 220 MB of disk space to store the SeqHound compiled executables. These instructions assume you are logged in as user "seqhound" on a UNIX system running the bash shell and you have perl installed on your system.

1. Decide the location to install the SeqHound binary executables. For example, if you want to install in the directory /home/seqhound/execs, do the following:

   **`mkdir execs`**

   **`cd execs`**

2. Download the SeqHound installation utility script installseqhound.pl from the FTP site: ftp.blueprint.org

   **`ftp`** *`ftp.blueprint.org`*

   When prompted for a name enter

   **`anonymous`**

   When prompted for a password type your email address:

   ***`myemail@home.com`***

   **`cd pub/SeqHound/script`**

   **`get`** ***`installseqhound.pl`***

   Close the ftp session by typing:

   **`bye`**

3. Run the perl script to download and install SeqHound executables. The perl script will download SeqHound binary executables based on the specified platform (linux or solaris), unpack the tar ball, modify the configurations files .odbc.ini and .intrezrc (for ODBC database access) and deploy the configuration files. It requires two commandline arguments: platform (linux or solaris) and installation path (e.g. /home/seqhound/execs). Enter the path to the ODBC driver (e.g.

/usr/lib/libmyodbc3.so, please refer to step 10 in section 4.4 for ODBC driver path), database server name, port number, user id, password and database instance name when prompted by the perl script.

```
./installseqhound.pl [linux OR solaris] [/home/seqhound/execs]
```

Upon successful execution of the perl script, you should see the following directories in the directory execs:

*build*
*config*
*example*
*include*
*lib*
*sql*
*test*
*updates*
*www*

The configuration file .odbc.ini can be found in the home directory (e.g. /home/seqhound).

### 4.3.1 Obtaining SeqHound Source Code.

Follow the instructions below to download SeqHound source code . If you downloaded and unpacked the executables, you can skip section 4.3.1 and 4.4 and continue with *section 4.5*.

1. In your home directory, make a new directory where you will store the new SeqHound code.

   **`mkdir compile`**

   Move into this directory and set an environment variable called `COMPILE` to point to this directory.

   **`cd compile`**
   **`export COMPILE=`pwd``**
   (where (`) is a single back-quote)

2. Download the perl utility seqhoundsrcdownload from the SeqHound ftp site

   Note: We no longer support SeqHound download from the Sourceforge FTP site. Please download SeqHound from ftp://ftp.blueprint.org/pub/SeqHound/

   From the *compile* directory, type:

   **`ftp ftp.blueprint.org`**

   When prompted for a name enter

   **`anonymous`**

   When prompted for a password type your email address:

```
myemail@home.com
cd pub/SeqHound/script
get seqhoundsrcdownload.pl
```

Close the ftp session by typing:

```
bye
```

3. Download SeqHound source code by running the perl script seqhoundsrcdownload.pl. The script will download the source code tar file and unpack the tar file into two directories **slri** and **bzip2**. You will also see a release note file Release_notes_x.x.txt in the same directory **compile**.

```
./seqhoundsrcdownload.pl
```

4. Set the `SLRI` environment variable

   Move to the *slri* directory and set the environment variable "`SLRI`" to point to this directory.

```
cd $COMPILE/slri
export SLRI=`pwd`
```

## 4.4 Compiling SeqHound executables on Solaris

These instructions describe how to compile SeqHound running on the Solaris platform. They may be used as a guide for compiling SeqHound code on other platforms. Instructions are similar for Linux and differences are noted.

**Using these instructions**

These instructions assume that:

You have downloaded the SeqHound code from the ftp server and you have set environment variables called `COMPILE` and `SLRI`. See *section 4.3.1*

You are using the bash shell.

Note: On Linux platforms, to compile SeqHound libs with ODBC support you also need unixODBC-devel package which contains the *sql.h* + other libs/headers required to compile SeqHound libs with ODBC support. This is not needed to run SeqHound, just to compile it.

These instructions were tested on a Sun-Fire-880 architecture running a Sun Solaris OS (version 9). The system information for the test-box (results of a "`uname -a`" call) were:

```
SunOS machine_name 5.9 Generic_117171-15 sun4u sparc
SUNW,Sun-Fire-880
```

1. Download the NCBI toolkit

   SeqHound is dependent on code in the NCBI toolkit

   Move to the *compile* directory and ftp to the NCBI ftp site:

   **`cd $COMPILE`**
   **`ftp ftp.ncbi.nlm.nih.gov`**

   When prompted for a name enter **`anonymous`**

   When prompted for a password type ***`myemail@home.com`***

   **`cd toolbox/CURRENT`**

   Make a note of the *FAQ.html* and the *readme.htm* files.

   Change your transfer type to binary and get the zipped directory called *ncbi.tar.gz*

   **`bin`**

   **`get ncbi.tar.gz`**

   Close the ftp session by typing:

   **`bye`**

Uncompress the toolkit.

```
gunzip ncbi.tar.gz
tar xvf ncbi.tar
```

2. Edit the platform make file.

   Go to the platform directory and locate the file with a "*.mk*" extension that applies to your platform. For 64-bit Solaris system the file is "*solaris64.ncbi.mk*" and in Linux the file is *linux-x86.ncbi.mk*.

   ```
   cd $COMPILE/ncbi
   cd platform
   ```

   In Linux *linux-x86.ncbi.mk* replace the line `/home/coremake/ncbi` with `${NCBI}`

   Use the following line (a Perl command) to replace the string in the Solaris file `/netopt/ncbi_tools/ncbi64/ncbi` with the string `${NCBI}`

   in the *solaris64.ncbi.mk* file:

   ```
   perl -p -i.bak -e 's|/netopt/ncbi_tools/
   ncbi64/ncbi|\${NCBI}|g' solaris64.ncbi.mk
   ```

   so for instance, the line

   `NCBI_INCDIR = /netopt/ncbi_tools/ncbi64/ncbi/include`

   Will become:

   `NCBI_INCDIR = ${NCBI}/include`

   You could also edit this file in hand using a text editor if you don't have Perl installed.

   Copy the file up one level to the *ncbi* directory and rename it "*ncbi.mk*"

   ```
   cp solaris64.ncbi.mk ../ncbi.mk
   ```

3. Set environment variables in preparation for the toolkit build.

   Move back to the ncbi directory and set the environment variable `NCBI` to point to that directory

   ```
   cd $COMPILE/ncbi
   export NCBI=`pwd`
   ```

   check this by typing

   ```
   echo $NCBI
   ```

   the value shown will replace `${NCBI}` in the "*solaris64.ncbi.mk*" file that you modified in the above step when the make file is run.

Note: The make file in the NCBI toolkit will use the C compiler from Sun instead of the compiler gcc. We do not recommend using gcc as it generates seqhound parsers that lead to segmentation fault at run time.

Finally, paths to the compiler and the archive executable *ar* should be added to your PATH variable:

```
export
PATH=/usr/local/bin:/opt/SUNWspro/prod/bin:/usr/ccs/bin:$
PATH
```

You can check all of your environment variables by typing

```
set | sort
```

At this point, the relevant environment variables should be something like this:

```
COMPILE=/export/home/your_user_name/compile
NCBI=/export/home/your_user_name/compile/ncbi
OSTYPE=solaris2.9
PATH=/opt/SUNWspro/prod/bin:/usr/local/bin:/usr/ccs/bin:/
usr/bin:/usr/ucb:/etc:.
```

If you want, you can read the readme file in the *make* directory.

```
cd make
more readme.unx
```

---

Note: For the Solaris UNIX OS only, the SeqHound API functions `SHoundGetGenBankff` and `SHoundGetGenBankffList` breaks due to a bug in the NCBI library file *ncbistr.c* (in directory *ncbi/corelib* and *ncbi/build*). To fix the problem, replace all the code inside the function `Nlm_TrimSpacesAroundString()` in the file *ncbistr.c* with the following text

```
    char *ptr, *dst, *revPtr;
    int spaceCounter = 0;
    ptr = dst = revPtr = str;

    if ( !str || str[0] == '\0' )
        return str;

    while ( *revPtr != '\0' )
        if ( *revPtr++ <= ' ' )
            spaceCounter++;

    if ( (revPtr - str) <= spaceCounter )
    {
        *str = '\0';
        return str;
    }

    while ( revPtr > str && *revPtr <= ' ' )
revPtr--;
    while ( ptr < revPtr && *ptr <= ' ' ) ptr++;
    while ( ptr <= revPtr ) *dst++ = *ptr++;
    *dst = '\0';

    return str;
```

---

4. Build the NCBI toolkit

   Move back up to the *compile* directory and run the make command.

   ```
   cd $COMPILE
   ./ncbi/make/makedis.csh |& tee out.makedis.txt
   ```

   Note: to build Solaris 64 bit binaries add the following to the command line:

   ```
   SOLARIS_MODE=64 ./ncbi/make/makedis.csh
   ```

   This runs a c-shell script to make the toolkit and tees the output to the screen and a log file "*out.makedis.txt*". It is safe to ignore the multiple error messages that you may see.

   At the end of a successful build you will see

   ```
   ************************************************************
   *The new binaries are located in ./ncbi/build/ directory*
   ************************************************************
   ```

The *ncbi.tar* file can be removed from the "*compile*" directory after the successful build process has been completed.

5. Make the bzip2 library

   The bzip2 code was downloaded as part of the seqhound code in step 4.3.1 above. Move to the *bzip2* directory and run the make file.

   ```
   cd $COMPILE/bzip2
   make –f make.bzlib
   ```

6. Set the `BZDIR` environment variable.

   ```
   cd $COMPILE/bzip2
   export BZDIR=`pwd`
   ```

7. In your home directory, add the following environment parameters to the appropriate configuration file such as *.bashrc* or *.bash_profile*. Text in italics should be changed to the correct path on your machine that points to directory having DBI.pm:

   ```
   export NCBI=$COMPILE/ncbi
   export BZDIR=$COMPILE/bzip2
   export SLRI=$COMPILE/slri

   export VIBLIBS="-L/usr/X11R6/lib -lXm -lXpm -lXmu -lXp -
   lXt -X11 -lXext"
   ```

```
export
PERL5LIB=/usr/local/lib/perl5/site_perl/5.8.3/sun4-
solaris-64
```

8. Install MySQL server and create database “seqhound”.

   SeqHound is built and tested in MySQL version 4.1.10. You can download MySQL from *http://dev.mysql.com/downloads/mysql/4.1.html* and follow the manual at *http://dev.mysql.com/doc/mysql/en/index.html* to install MySQL on your server. The data directory where the MySQL server points to should have 700 GB for a full SeqHound database. After MySQL is installed, you need to log into MySQL and create database “seqhound”:

   ```
   create database seqhound;
   ```

   Note that "`;`" must be used at the end of all MySQL statements.

9. Install ODBC driver:

   Note that for Linux platforms, the unixODBC package needs to be installed prior to the ODBC driver otherwise the following error will occur:

   ```
   error: Failed dependencies:
           libodbcinst.so.1 is needed by MyODBC-3.51.09-1
   ```

   a) Go to web site: *http://dev.mysql.com/doc/connector/odbc/en/faq_2.html*

   b) Find and download RPM distribution of ODBC driver *MyODBC-3.51.07-1.i586.rpm*.

   c) As user "root", install the driver.

      For first time installation

      ```
      rpm -ivh MyODBC-3.51.01.i386-1.rpm
      ```

      For upgrade

      ```
      rpm -Uvh MyODBC-3.51.01.i386-1.rpm
      ```

   d) The library file *libmyodbc3*. will be installed in directory */usr/lib* or */usr/local/lib*.

10. Set up the configuration file for ODBC driver.

    Create a configuration file called *.odbc.ini* in your home directory with the following content:

Edit the file called *.intrezrc* in directory *slri/seqhound/config/*.

```
[mysqlsh]                    ← header must not be used for other sections
Description  = MySQL ODBC 3.51 Driver DSN
Trace        = Off
TraceFile    = stderr
Driver       = /usr/lib/libmyodbc3.so   ↓ your library path
DSN          = mysqlsh       ← same as the header name
SERVER       = my_server
PORT         = my_port
USER         = my_id
PASSWORD     = my_pwd
DATABASE     = seqhound      ← database name
```

Text in ***italics*** should be changed. Text ***/usr*** in the value of variable Driver should be changed to the path where unixodbc resides. Text ***my_server*** should be changed to the IP address or the server name of the MySQL server. Text ***my_port*** should be changed to port number of the MySQL instance. Text ***my_id*** and ***my_pwd*** should be replaced by your user id and password to the MySQL database.

---

Note that the values for the headers such as DSN, USER, PASSWORD and DATABASE must be less than 9 characters.

---

11. Set up ODBC related variables:

    **export ODBC=*path_to_unixodbc***

    Where ***path_to_unixodbc*** should be replaced by the path of the UnixODBC driver on your machine.

    In your home directory, add parameter "LD_LIBRARY_PATH" to the appropriate configuration file such as *.bashrc* or *.bash_profile*:

    **export LD_LIBRARY_PATH = /usr/local/unixodbc/lib:/usr/local/unixodbc/odbc/lib:/usr/local/mysql/lib/mysql:/usr/local/mysql/lib/mysql/lib**

    The value of variable "LD_LIBRARY_PATH" should have all the paths that have the library files *libodbc*, libmyodbc*,* and *libmysqlclient**

12. Build the SeqHound executables

    Move to the compile directory and list all the files in the directory:

    **cd $COMPILE**

    **ls**

    You should see:

    ```
    > ls
    bzip2
    ncbi
    slri
    out.makedis.txt
    ```

Before proceeding you should check your environment variables

```
set | sort
```

to ensure that correct paths have been specified for each of the following variables:

```
NCBI
SLRI
ODBC
BZDIR
```

Compile the SLRI libraries using the following commands:

```
cd $SLRI/lib
make -f make.slrilib
make -f make.slrilib odbc
```

The above commands will build the SLRI libraries needed by SeqHound.

The make files which you are about to invoke call on these variables therefore the paths must be correct. Move to the make directory for SeqHound and run the *makeall* script. The script requires two command line arguments. The first parameter indicates what database backend is to be used for the build (currently the only valid target is `odbc`). The second parameter indicates what SeqHound programs are to be made (a choice of `all, cgi, domains, examples, genomes, go, locuslink, parsers,scripts, taxon, updates`). The output of the build script will be captured in the text file out.makeseqhound.txt.

```
cd $SLRI/seqhound
./makeallsh odbc all 2>&1 | tee out.makeseqhound.txt
```

It is safe to ignore the multiple warning messages that you may see.

After this has finished running, move to the directory *slri/seqhound/build/odbc/* where you will find the executables for SeqHound.

```
cd build/odbc
ls -1
```

You will see

```
>ls –1
addgoid
cbmmdb
chrom
clustmask
clustmasklist
comgen
fastadom
gen2fasta
gen2struc
goparser
goquery
```

```
histparser
importtaxdb
isshoundon
llgoa
llparser
llquery
mother
pdbrep
precompute
redund
seqrem
sh_nbhrs
shunittest_odbc_local
shunittest_odbc_rem
shtest
update
vastblst
wwwseekgi
```

13. Set up the SQL files that create tables.

    **`cd $SLRI/seqhound/sql`**

    In each of files *core.sql*, *redund.sql*, *ll.sql*, *taxdb.sql*, *gendb.sql*, *strucdb.sql*, *cddb.sql*, *godb.sql*, *rps.sql*, *nbr.sql*, there is a line close to the beginning of each file:

    ***#use testsql;***

    This line should be changed to

    **`use seqhound;`**

## 4.5 Building the SeqHound system on Solaris

Using these instructions

These instructions show how the SeqHound executables may be used to build the SeqHound system under a Solaris 8 OS. These instructions may also be used as a guide for setting up SeqHound under other operating systems. These instructions assume that:

- You have downloaded the latest release version of the SeqHound code (see step 4.3.3)
- You have successfully installed MySQL
- You have successfully compiled the SeqHound code yourself (*section 4.4*)

  OR

  you have downloaded the SeqHound executables for your platform and operating system (section 4.3.4).
- You have set environment variables called `COMPILE` and `SLRI` (see steps 4.3.1 and 4.3.6).

- You have a default install of an Apache server running. See *http://www.apache.org/* for freely available software and instructions for your platform.
- You have installed Perl. See *http://www.cpan.org/* for freely available software and installation instructions.
- You have at least 300 MB space available in a directory where you can check out code and compile it.
- You have at least **600 GB** available for the SeqHound executables and data tables. See *section 4.2*.

These instructions were tested on a Sun Ultra machine running the Sun-Solaris 8 OS. The system information for the test-box (results of a "`uname –a`" call) were:

```
SunOS machine_name 5.8 Generic_108528-01 sun4u sparc
SUNW,Ultra-4
```

These instructions assume that you are using the c shell. Syntax may differ for some commands in other shells.

Note: These instructions begin with 'step 14'.

14. Prepare to build the SeqHound database.

    Create a new directory where you will set up SeqHound.

    ```
    mkdir seqhound
    ```

    Set the environment variable SEQH to point to this directory.

    ```
    cd seqhound
    setenv SEQH `pwd`
    ```

    Move to this directory and create new directories

    ```
    cd seqhound
    mkdir 1.core.files
    mkdir 2.redund.files
    mkdir 3.taxdb.files
    mkdir 4.godb.files
    mkdir 5.lldb.files
    mkdir 6.comgenome.files
    mkdir 7.mmdb.files
    mkdir 8.hist.files
    mkdir 9.neighbours.files
    mkdir 10.rpsdb.files
    mkdir precompute
    ```

    The numbered directories will hold parsers and files required for the build of the SeqHound data tables. Directory "*precompute*" will hold the precomputed data of the database.

Move to each of the numbered directories and copy all of the scripts and executables required for the build.

```
cd $SEQH/1.core.files
cp $SLRI/seqhound/sql/core.sql .
cp $SLRI/seqhound/scripts/asnftp.pl .
cp $SLRI/seqhound/scripts/seqhound_build.sh .
cp $SLRI/seqhound/build/odbc/mother .
cp $SLRI/seqhound/build/odbc/update .
cp $SLRI/seqhound/config/.intrezrc .

cd $SEQH/2.redund.files
cp $SLRI/seqhound/sql/redund.sql .
cp $SLRI/seqhound/scripts/nrftp.pl .
cp $SLRI/seqhound/build/odbc/redund .

cd $SEQH/3.taxdb.files
cp $SLRI/seqhound/sql/taxdb.sql .
cp $SLRI/seqhound/scripts/taxftp.pl .
cp $SLRI/seqhound/build/odbc/importtaxdb .

cd $SEQH/4.godb.files
cp $SLRI/seqhound/sql/godb.sql .
cp $SLRI/seqhound/scripts/goftp.pl .
cp $SLRI/seqhound/build/odbc/goparser .

cd $SEQH/5.lldb.files
cp $SLRI/seqhound/sql/ll.sql .
cp $SLRI/seqhound/scripts/llftp.pl .
cp $SLRI/seqhound/build/odbc/llparser .
cp $SLRI/seqhound/build/odbc/addgoid .

cd $SEQH/6.comgenomes.files
cp $SLRI/seqhound/sql/gendb.sql .
cp $SLRI/seqhound/scripts/genftp.pl .
cp $SLRI/seqhound/scripts/humoasn.pl .
cp $SLRI/seqhound/scripts/humouse_build.sh .
cp $SLRI/seqhound/scripts/comgencron_odbc.pl .
cp $SLRI/seqhound/scripts/shconfig.pm .
cp $SLRI/seqhound/genomes/gen_cxx .
cp $SLRI/seqhound/genomes/pregen.pl .
```

```
cp $SLRI/seqhound/genomes/gen.pl .
cp $SLRI/seqhound/genomes/ncbi.bacteria.pl .
cp $SLRI/seqhound/build/odbc/chrom .
cp $SLRI/seqhound/build/odbc/comgen .
cp $SLRI/seqhound/build/odbc/mother .

cd $SEQH/7.mmdb.files
cp $SLRI/seqhound/sql/strucdb.sql .
cp $SLRI/seqhound/scripts/mmdbftp.pl .
cp $SLRI/seqhound/config/.mmdbrc .
cp $SLRI/seqhound/config/.ncbirc .
cp $SLRI/seqhound/build/odbc/cbmmdb .

cd $SEQH/8.hist.files
cp $SLRI/seqhound/build/odbc/histparser .
```

Open the *.intrezrc* file with a text editor like pico and edit.

```
cd $SEQH/1.core.files
pico .intrezrc
```

An example *.intrezrc* file follows. Lines preceded by a semi-colon are comments that explain what the settings are used for and their possible values.

Text in ***italics*** must be changed for the *.intrezrc* file to function correctly with your SeqHound set-up. Variables `username`, `password`, `dsn`, `database` in section `[datab]` should have the same values as `USER`, `PASSWORD`, `DSN` and `DATABASE` respectively in the *.odbc.ini* file you set up in Step 10 in section 4.4. For variable `path` and `indexfile` in section `[precompute],` replace the text in ***italics*** with the absolute path of directory "`precompute`" you just created.

> Warning: This file may have wrapped lines. Take care when editing this file that you do not break any of the lines (i.e. introduce any unwanted carriage returns).

```
--------------------------------example .intrezrc begins---------------------------------
[datab]
;seqhound database that you are connecting
username=your_user_name
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=
[config]
;the executable the cgi runs off of.
CGI=wwwseekgi
[precompute]
;precomputed taxonomy queries
MaxQueries = 100
MaxQueryTime = 10
QueryCount = 50
path = /seqhound/precompute/
indexfile = /seqhound/precompute/index
[sections]
;indicated what modules are available in SeqHound
;1 for available, 0 for not available
;gene ontology hierarchy
godb = 1
;locus link functional annotations
lldb = 1
;taxonomy hierarchy
taxdb = 1
;protein sequence neighbours
neigdb = 1
;structural databases
strucdb = 1
;complete genomes tracking
gendb = 1
;redundant protein sequences
redundb = 1
;open reading frame database
;currently not exported to outside users of SeqHound
cddb = 0
;RPS-BLAST domains
rpsdb = 1
;DBXref Database Cross_Reference
dbxref = 0

[crons]
;customizable variables in cron jobs
;NOTE: all paths must end in '/'
pathupdates=./
pathinputfiles=./
pathinputfilescomgen=./
mail=user\@host.org
defaultrelease=141
pathflags=./
--------------------------------example .intrezrc ends---------------------------------
```

This file should be copied to other directories used during the build process:

```
cp .intrezrc $SEQH/2.redund.files/.
cp .intrezrc $SEQH/3.taxdb.files/.
cp .intrezrc $SEQH/4.godb.files/.
cp .intrezrc $SEQH/5.lldb.files/.
cp .intrezrc $SEQH/6.comgenome.files/.
cp .intrezrc $SEQH/7.mmdb.files/.
cp .intrezrc $SEQH/8.hist.files/.
cp .intrezrc $SEQH/9.neighbours.files/.
cp .intrezrc $SEQH/10.rpsdb.files/.
```

15. Build the core module of SeqHound.

    Building the core module (basically all of the sequence data tables) is not optional. The rest of the modules are optional if there is a need to spare resources or administrative efforts but the corresponding API functionality will not be present.

    **`cd $SEQH/1.core.files`**

    Create the core tables in the database

    Make sure file *core.sql* has line use `seqhound` close to the beginning of the file.

    **`mysql –u my_id –p –P my_port –h my_server < core.sql`**

    Where ***`my_id`***, ***`my_port`*** and ***`my_server`*** should be replaced by your userid for the database, the port of the database and the IP address or the server name of the database server respectively. You will be prompted to enter your password.

    This creates core tables accdb, asndb, nucprot, parti, pubseq, sendb, sengi, taxgi, bioentity, bioname, secondrefs, bioentitytype, nametype, rules, fieldtype and histdb.

    If you are building a full-instance of the SeqHound database then run the *asnftp.pl* script while in the *build* directory:

    **`./asnftp.pl`**

    ---

    Note that any command in these instructions can be run as a ‘nohup’ to prevent the process from ending if your connection to the machine should be lost. For example:

    **`nohup ./asnftp.pl &`**

    ---

    If you only want to build a small test version of the database then manually download a single file. For example:

    **`ftp ftp.ncbi.nih.gov`**

    When prompted for a name enter **`anonymous`**

    When prompted for a password type ***`myemail@home.com`***

    **`cd refseq/cumulative`**

    **`bin`**

    **`get rscu.bna.Z`** (do not uncompress this file)

    **`bye`**

The *asnftp.pl* script downloads all of the GenBank sequence records (in binary ASN.1 format) required to make an initial build of the SeqHound core module. This script will take approximately 24 hours to run and will consume 14 GB of disk space.

Note that all scripts are described in detail in section 5.

Two other files are generated by this script:

*asn.list* is a list of the sequence files that the script intends to download.

*asnftp.log* is where the script logs error messages during execution time.

If you open another session with the machine where you are building SeqHound, you can check how far along *asnftp.pl* is by comparing the number of lines in the *asn.list* file

```
grep ".aso.gz" asn.list | wc –l
```

to the number of lines in the build directory (number of files actually downloaded so far)

```
ls *.aso.gz | wc -l
```

Once *asnftp* has finished, these two numbers should be the same.

Run the seqhound build script. Before running this script, make certain that the *.intrezrc* file, in the same directory, and *.odbc.ini,* in your home directory, have correct configuration values. (see steps 10 in section 4.4 and step 14 in the current section). This parser MUST be given a single parameter that represents the release version of GenBank. You can find the release number in the file: *ftp://ftp.ncbi.nih.gov/ncbi-asn1/daily/Last.Release.*

```
./seqhound_build.sh 141
```

*seqhound_build.sh* executes the mother parser over all source files and populates tables accdb, asndb, nucprot, parti, pubseq, sendb, sengi, taxgi, bioentity, bioname, secondrefs, bioentitytype, nametype, rules and fieldtype. This will take about 75 hours. Table histdb is still empty at this stage. It is populated in Step 25.

Parser mother creates a log file for every **.aso* file that it parses. These log files are located in a subdirectory called "*logs*" and are named "*rsnc0506run*" where "rsnc0506" is the name of the file that was being processed.

While *seqhound_build.sh* is running, you can move on to steps 16-18.

Once *seqhound_build.sh* has finished you can test that all of the files were properly processed by showing that the results of

```
cd logs
grep "Done" | wc –l
```

is the same as

```
ls *run | wc –l
```

is the same as

```
cd ..
ls *aso.gz | wc -l
```

The *seqhound_build.sh* script unzips *.aso.gz* files before feeding them as input to the mother program. *seqhound_build.sh* then rezips the file after mother is done with it. If for some reason, the build should crash part way through, you have to

a) recreate core tables using *core.sql* (see above) and

b) search for any unzipped (**.aso* files) in the *build* directory and rezip them

c) restart *seqhound_build.sh*.

Once the *seqhound_build.sh* script has finished, you should move all of the **.aso.gz* files into a directory where they will be out of the way:

```
mkdir asofiles
mv *.aso.gz asofiles/.
```

16. Build the redundb module.

```
cd $SEQH/2.redund.files
```

Create table redund in the database.

Make sure file *redund.sql* has the line `use seqhound` close to the beginning of the file.

```
mysql –u my_id –p –P my_port –h my_server < redund.sql
```

Where "***my_id***", "***my_port***" and "***my_server***" should be replaced by your userid for the database, the port of the database and the IP address or the server name of the database server respectively. You will be prompted to enter your password.

This creates table redund in the database.

Run the *nrftp.pl* script to download the FASTA nr database of proteins (*ftp://ftp.ncbi.nlm.nih.gov/blast/db*).

```
./nrftp.pl
```

*nrftp.pl* generates a log file "*nrftp.log*" that informs you what happened. If everything went ok, the last two lines should read:

```
Getting nr.gz
closing connection
```

A new file should appear in the *build* directory called "*nr.Z*". You will have to unpack this file by typing:

```
gunzip nr.gz
```

Run the redund parser to make the redund table of identical protein sequences.

Before running this script, make certain that the *.intrezrc* file in the same directory and *.odbc.ini* in your home directory have correct configuration values (see step 10 in section 4.4 and step 14 in the current section).

```
./redund -i nr -n F
```

redund generates the log file "*redundlog*". If everything went ok, the only line in this file should be:

```
NOTE: [000.000] {redund.c, line 259} Done.
```

And about 3 millions records will be inserted into table redund.

17. Build the taxdb module

Create tables of the taxdb module in the database.

**`cd $SEQH/3.taxdb.files`**

Make sure file *taxdb.sql* has line `use seqhound` close to the beginning of the file.

**`mysql –u my_id –p –P my_port –h my_server < taxdb.sql`**

Where ***`my_id`***, ***`my_port`*** and ***`my_server`*** should be replaced by your userid for the database, the port of the database and the IP address or the server name of the database server respectively. You will be prompted to enter your password.

This creates tables taxdb, gcodedb, divdb, del, merge in the database.

Run the *taxftp.pl* script to download taxonomy info from the NCBI (*ftp://ftp.ncbi.nih.gov/pub/taxonomy/taxdump.tar.gz*).

**`taxftp.pl`**

*taxftp.pl* generates a log file *taxftp.log* that informs you what happened. If everything went ok, the last two lines should read:

```
Getting taxdump.tar.gz
closing connection
```

A new file should appear in the build directory called *taxdump.tar.gz*. You will have to unpack this file by typing:

**`gzip –d taxdump.tar.gz`**

**`tar -xvf taxdump.tar`**

There will be seven new files:

*delnodes.dmp*

*division.dmp*

*gc.prt*

*gencode.dmp*

*merged.dmp*

*names.dmp*

*nodes.dmp*

Run the importtaxdb parser to make the taxonomy data tables. *Taxdump* must be in the same directory as this parser.

**`./importtaxdb`**

*importtaxdb* has no command line parameters. *importtaxdb* generates the log file *importtaxdb_log.txt*. If everything went ok, the output of this file should be something like:

```
Program start at Thu Sep  4 13:47:51 2003
Number of Tax ID records parsed: 191647
Number of Tax ID Name records parsed: 246263
Number of Division records parsed: 11
Number of Genetic Code records parsed: 18
```

```
Number of Deleted Node records parsed: 25475
Number of Merged Node records parsed: 4607
Program end at Thu Aug  12 13:49:43 2004
```

And records will be inserted into tables taxdb, gcodedb, divdb, del and merge.

18. Build the GODB module

    Create tables of the godb module in the database.

    **`cd $SEQH/4.godb.files`**

    Make sure file *godb.sql* has line `use seqhound` close to the beginning of the file.

    **`mysql –u my_id –p –P my_port –h my_server < godb.sql`**

    Where ***`my_id`***, ***`my_port`*** and ***`my_server`*** should be replaced by your userid for the database, the port of the database and the IP address or the server name of the database server respectively. You will be prompted to enter your password.

    This creates tables go_parent, go_name, go_reference, go_synonym in the database.

    Run the *goftp.pl* script to download the gene ontology files (*ftp://ftp.geneontology.org/pub/go/gene-associations* and *ftp://ftp.geneontology.org/pub/go/ontology*).

    **`goftp.pl`**

    There is a log file for this script called *goftp.log* that indicates that it got all of these files. Three new files should appear in the build directory called

    *component.ontology*

    *function.ontology*

    *process.ontology*

    Two other files also appear called

    *gene_association.Compugen.GenBank.gz*

    *gene_association.Compugen.UnitProt.gz*

    but these are used as input files by addgoid in the next step.

    Run the goparser to make the hierarchical gene ontology data tables. The three input files must be in the same directory as this parser.

    **`./goparser`**

    goparser has no command line parameters. goparser generates the log file *goparserlog*. If everything went ok, the output of this file should have only one NOTE line:

    ```
    NOTE: [000.000] {goparser.c, line 101} Main: Done!
    ```

    And records will be inserted into tables go_parent, go_name, go_reference, go_synonym.

19. Build the LLDB module

    Create tables of the locus link module in the database.

    **`cd $SEQH/5.lldb.files`**

    Make sure file *ll.sql* has line `use seqhound` close to the beginning of the file.

    **`mysql –u my_id –p –P my_port –h my_server < ll.sql`**

Where ***my_id***, ***my_port*** and ***my_server*** should be replaced by your userid for the database, the port of the database and the IP address or the server name of the database server respectively. You will be prompted to enter your password.

This creates tables ll_omim, ll_go, ll_llink, ll_cdd in the database.

Run the *llftp.pl* script to download the locus link template file (*LL_tmpl*) which is the source for function annotation tables (*ftp://ftp.ncbi.nih.gov/refseq/LocusLink/LL_tmpl.gz*).

```
llftp.pl
```

This script generates the *llftp.log* file. If everything executes correctly, the last two lines of the file should read:

```
Getting LL_tmpl.gz
closing connection
```

And a new file should appear in the build directory called *LL_tmpl.gz* which you will have to unpack using the commands

```
gzip –d LL_tmpl.gz
```

Run the llparser to create the set of functional annotation data tables. The input file must be in the same directory as this parser.

```
./llparser
```

llparser has no command line parameters. llparser generates the log file "*llparserlog*". At the time of writing, the output of this file will have thousands of lines like:

```
NOTE: [000.000] {ll_cb.c, line 654} LL_AppendRecord: No
NP id. Record skipped.
```

(these lines are expected since many LocusLink records are not linked to specific sequence records)

followed by the last line of the file:

```
NOTE: [000.000] {llparser.c, line 90} Main: Done!
```

Records will be inserted into tables ll_omim, ll_go, ll_llink and ll_cdd. Run the addgoid parser to populate the go annotation table. This parser uses input files that were downloaded in the previous step 13. Copy those files to this directory:

```
cp ../4.godb.files/gene_association.Compugen.GenBank.gz
./
cp ../4.godb.files/gene_association.Compugen.UniProt.gz
./
```

The files need to be unpacked.

```
gunzip gene_association.Compugen.GenBank.gz
gunzip gene_association.Compugen.UnitProt.gz
```

The input files must be in the same directory as addgoid

```
./addgoid –i gene_association.Compugen.GenBank
```

after this parser has finished, use it to parse the other input file

```
./addgoid –i gene_association.Compugen.UniProt
```

At the time of writing, this second input file is not parsed since cross references between Swissprot and GenBank ids are not available. This is being corrected by the dbxref module project.

---

addgoid MUST BE EXECUTED AFTER ALL CORE TABLES AND LLDB TABLES HAVE BEEN BUILT; the llparser makes the ll_go table into which the addgoid script writes. This program is dependent on tables asndb, parti, accdb and nucprot..

---

addgoid generates the log file *addgoidlog*. The output of this file will look like:

```
=========[ Sep 5, 2003 10:28 AM ]======================
ERROR: [000.000] {addgoid.c, line 235} No GI from 100K_RAT.
ERROR: [000.000] {addgoid.c, line 235} No GI from 100K_RAT.
ERROR: [000.000] {addgoid.c, line 235} No GI from 100K_RAT.
ERROR: [000.000] {addgoid.c, line 235} No GI from 100K_RAT.
```

This is normal. These errors are caused by the inability to find GI's for names of proteins/loci that are annotated in the GO input file. This problem is being addressed by the dbxref module.dir

This program writes to the existing ll_go table that was generated by llparser.

20. Build the GENDB module

Change directories to the Complete Genomes directory (*comgenomes*).

**`cd $SEQH/6.comgenomes.files`**

Create tables of the GENDB module in the database.

Make sure file *gendb.sql* has line `use seqhound` close to the beginning of the file.

**`mysql –u my_id –p –P my_port –h my_server < gendb.sql`**

Where ***`my_id`***, ***`my_port`*** and ***`my_server`*** should be replaced by your userid for the database, the port of the database and the IP address or the server name of the database server respectively. You will be prompted to enter your password.

This creates table chrom in the database.

Building the GENDB module involves several steps. To simplify the process, a perl script, *comgencron_odbc.pl* groups together all of the necessary scripts or binaries for each individual step. These scripts and binaries must be present in this directory. They are:

*comgencron_odbc.pl*

*shconfig.pm*

*gen_cxx*

*pregen.pl*

*gen.pl*

*ncbi.bacteria.pl*

*genftp.pl*

*humoasn.pl*

*chrom*

*iterateparti*

*humouse_build.sh*

*mother*

*comgen*

Before building the GENDB module, the `[crons]` section in configuration file *.intrezrc* should be set up properly. It should look like the following. Text in ***`italics`*** must be changed. Variable `mail` should have the e-mail address where you want the message to be sent to. Variable `defaultrelease` should have the release number of the GenBank files you use to build the core tables of SeqHound database (see Step 15):

```
[crons]
;customizable variables in cron jobs
;NOTE: all paths must end in '/'
pathupdates=./
pathinputfiles=./
pathinputfilescomgen=./genfiles/
mail=your_email_addr
defaultrelease=141
pathflags=./flag/
```

Make a subdirectory *flag* where the flag file *comgen_complete.flg* will be saved.

**`mkdir flag`**

Run the script to build the GENDB module:

**`./comgencron_odbc.pl`**

*comgencron_odbc.pl* generates flat file *genff*, log files *bacteria.log*, *chromlog, comgenlog, gen.log, iteratapartilog*, a subdirectory *genfiles* and a lot of logs file with postfix *run* which will be moved to a subdirectory *logs*. It also downloads many *.asn* files which will be moved to subdirectory *genfiles*. During the process, temporary file *comff* and directory *asn* are created. They are deleted before the end of the build process. If the build process fails in the middle, they should be removed along with file *genff* manually.

There are several lines printed on the screen during the build like:

```
mail = your_email_addr
pathupdates = ./
pathinputfilescomgen = ./genfiles/
defaultrelease = 141
pathflags = ./flag/
No source or subsource Plasmpdium falciparum NC_03043.
Update 1 chromosome type by hand.
```

It is OK to see above line.

An e-mail will be sent to the address you provide to inform if the process succeeds or fails. If everything went ok, you will see the last line in file *comgenlog* as:

```
NOTE: [000.000] {comgen.c, line 504} Main: Done.
```

The last line in file *iteratepartilog* as:

```
NOTE: [000.000] {iterateparti.c, line 170} Done.
```

The last line in file *chromlog* as:

```
NOTE: [000.000] {chrom.c, line 173} Done.
```

The last two lines in file *bacteria.log* as:

```
deleteing asn
See bacteria.results for changes to ./genff
```

The last two lines in file *gen.log* as:

```
Removing asn
Deleting comff
```

*The following is a detailed explanation of the script comgencron_odbc.pl. You may skip it.*

21. Generate flat file *genff*.

genff is a tab-delimited text file where each line in this file represents one "DNA unit" (chromosome, plasmid, extrachromosomal element etc.) belonging to a complete genome.

```
Column  Description
1       Taxonomy identifier for the genome
2       Unique integer identifier for a given chromosome
3       Type of molecule (1 or chromosome, 8 for plasmid, …)
4       FTP file name for the genome without the .asn
        extension)
5       Full name of the organism
```

Here is an example of several rows from genff:

```
305          286     8     NC_003296     Ralstonia solanacearum plasmid pGMI1000MP
258594       287     1     NC_005296     Rhodopseudomonas palustris CGA009 chromosome
781          288     1     NC_003103     Rickettsia conorii chromosome
782          289     1     NC_000963     Rickettsia prowazekii chromosome
90370        290     1     NC_003198     Salmonella typhi chromosome
90370        291     8     NC_003384     Salmonella typhi plasmid pHCM1
90370        292     8     NC_003385     Salmonella typhi plasmid pHCM2
209261       293     1     NC_004631     Salmonella typhi Ty2 chromosome
```

The genff flat file is generated in two steps.

a) *gen.pl* which will CREATE *genff* using the eukaryotic complete genomes.

b) *ncbi.bacteria.pl* which will UPDATE *genff* with bacteria complete genomes.

* both *gen.pl* and *ncbi.bacteria.pl* are dependent on *pregen.pl* so this must be in the same directory as *gen.pl* and *ncbi.bacteria.pl* when you run it.

*gen.pl* will backup the current (if it exists) *genff* as *genff.backup* and then create a new *genff* file. *gen.pl* will download asn files from NCBI's ftp site and then extract the relevant fields (as described above) and store them as records in *genff*.

The data of bacteria complete genome is written to genff by running *ncbi.bacteria.pl*.

This perl utility will compare the data in *genff* to the contents of the */genomes/bacteria* directory in NCBI's ftp site and then automatically update *genff*. *ncbi.bacteria.pl* will save the names of the bacteria that have been newly added to *genff* in a separate file called *bacteria.results*. You can use this file to quickly verify the results.

A sample output of *bacteria.results.pl*

```
***********PERFECT MATCH***********
Aeropyrum pernix


***********SEMI MATCHED NCBI BACTERIA*************
NCBI BACTERIA               CHROMFF
---------------------------------------
Buchnera aphidicola         Buchnera sp
Buchnera aphidicola Sg      Buchnera sp


***********UNMATCHED NCBI BACTERIA*************
Agrobacterium tumefaciens C58 Cereon
Agrobacterium tumefaciens C58 UWash
```

Perfectly matched bacteria are already present in *genff*. Semi matched bacteria means that there is an organism that is closely related to a new organism. For the above example, *Buchnera aphidocola Sg* and *Buchnera aphidocola* were newly released and closely related to the *Buchnera sp*. The newly released data will have been added to *genff.* Unmatched bacteria are completely new organism and will be added to *genff.*

Both *gen.pl* and *ncbi.bacteria.pl* will create an intermediate file called *comff*, and a temporary directory *asn*. These are temporary and are critical to the functionality of the perl scripts. Both *gen.pl* and *ncbi.bacteria.pl* will delete *comff* and *asn* after execution.

While running *gen.pl* and *ncbi.bacteria.pl* you may see the following on the screen.

```
No source or subsource Plasmodium falciparum NC_03043.
Update 1 chromosome type by hand.
```

It means that for the specified organism, the asn file is missing the chromosome type. In such a scenario, the chromosome type will default to 1 (chromosome

Once you have generated file *genff*, you will likely need to run it again periodically, in case some of the data in *genff* has changed, for example if an organism taxid changes, in which case it is crucial to rerun *gen.pl*.

Script genftp.pl downloads complete genome files from *ftp://ftp.ncbi.nih.gov/genomes/**.

A script called *humoasn.pl* must be in the same directory as *genftp.pl* since *genftp.pl* calls the script.

---

*humoasn.pl* is a misnomer because the script actually processes files for human, mouse AND rat genomes.

---

Each of these genomes has two files called *rna.asn* and *protein.asn* (these files are called the same thing regardless of the organism that they refer to: the only way you can tell which organism the file refers to is by looking at the directory name that it came from or by looking at the contents. *genftp.pl* renames *rna.asn* and *protein.asn* files to more specific names so they can be processed with the *humoasn.pl* script.

*rna.asn* and *protein.asn* files mostly contain XM's and XP's sequences: see for example *genomes/H_sapiens/protein*. The sequences in these files are "loose" bioseqs that have to be "stitched" together into bioseq sets by *humoasn.pl*. This allows these sequences to be processed by the mother parser in the next step.

Many new **.asn* files will appear in the *comgenomes* directory after this is run. There is no log file for this script.

a) Populate table chrom

Binary chrom is used to populate table chrom from the list of complete genomes found in genff. Chrom generates the log file "*chromlog*". This log will look something like:

```
============[ Sep 5, 2003  2:30 PM ]===================
NOTE: [000.000] {chrom.c, line 130} Assigned TaxId 56636.
NOTE: [000.000] {chrom.c, line 137} Assigned Kloodge 1.
NOTE: [000.000] {chrom.c, line 144} Assigned Chromfl 1.
NOTE: [000.000] {chrom.c, line 149} Assigned Access NC_000854
NOTE: [000.000] {chrom.c, line 152} Assigned Name Aeropyrum pernix.
…
NOTE: [000.000] {chrom.c, line 167} Done.
```

b) Delete all records from division `gbchm` from the tables of the core module.

This step is carried out for data integrity purpose. All the records that are inserted into the core module tables are labeled as from division `gbchm`. Before they are inserted, it needs to ensure no such record exists in the database. This is accomplished using binary iterateparti. iterateparti takes the division name as one parameter and deletes all GI's that are part of that division from all of the tables in the core module.

c) Set kloodge to 0 in table taxgi

This step is also carried out for data integrity purpose. The field "kloodge" in table taxgi for all records should be set to 0 before they are updated in a later step by binary comgen.

d) Move all *Apis mellifera* related files to a subdirectory.

The chromosome, rna and protein files of *Apis mellifera* are not processed at the time of writing. They are moved to a subdirectory.

e) Add records to the core module tables.

Since the human, mouse and rat sequences from this source (the "Complete Genomes" directory) are not a part of the GenBank release, the records are added to the core module tables by script *humouse_build.sh*. **141**

This script feeds all chromosome, rna and protein files downloaded by *genftp.pl* to the mother parser. The mother parser makes a new division called "gbchm" (GenBank Chromosome Human and Mouse) and touches all core module tables.

Log files will be created by mother for every chromosome file processed (called **run*).

f) Update field kloodge in table taxgi and field name in table accdb

Parser comgen is used to label sequences as belonging to a complete genome.

This program uses the files downloaded by *genftp.pl* and marks the complete genomes in table taxgi. This program also adds loci names into table accdb (if they are not present). comgen is dependent on the chrom table and writes to accdb and taxgi. The comgen program has to be executed after all databases are built.

Comgen writes to the log file *comgenlog* in the same directory where it is run.

22. Build the Strucdb module

Change to the *mmdbdata* directory.

**cd $SEQH/7.mmdb.files**

Create tables of the Strucdb module in the database.

Make sure file *strucdb. sql* has line use seqhound close to the beginning of the file.

**mysql –u *my_id* –p –P my_port –h my_server < gendb.sql**

Where ***my_id***, ***my_port*** and ***my_server*** should be replaced by your userid for the database, the port of the database and the IP address or the server name of the database server repectively. You will be prompted to enter your password.

This creates tables mmdb, mmgi and domdb in the database.

Make certain that the configuration files have been properly set up. These include: *.mmdbrc*, *.ncbirc* and *.intrezrc*.

In file *.mmdbrc*, variable "Gunzip" should have a value which is the path of gunzip on the machine (change text in ***italics***). File *.mmdbrc* looks like:

```
[MMDB]
;Database and Index required when local MMDB database is used
Database = ./
Index = mmdb.idx
Gunzip = /bin/gunzip

; [VAST]
;Database required for local VAST fetches.
; Database = .
```

In file *.ncbirc*, variable DATA should have a value which is the path of directory *ncbi/data* on your machine. File *.ncbirc* looks like (change text in ***italics***):

```
[NCBI]
ROOT=/
DATA=/my_home/compile/ncbi/data/
```

Copy file *bstdt.val* from the *ncbi/data* directory:

**cp ~/compile/ncbi/data/bstdt.val ./**

Run the *mmdbftp.pl* script to download the mmdb (Molecular Model Database) ASN.1 files from *ftp://ftp.ncbi.nih.gov/mmdb/mmdbdata*. This will take approximately 10 hours..

**./mmdbftp.pl**

This script writes to the *mmdb.log* file and records the files downloaded. Approximately 20000 **.val.gz* files will appear in the *mmdbdata* directory after running this. Look at the first line in the *mmdb.idx* index file and this states the number of files that should have been downloaded.

Run the cbmmdb parser to make the MMDB and MMGI datafiles. Use:

**./cbmmdb –n F -m F**

This program takes about 12 hours to run and writes errors to the *cbmmdblog* file. After a typical run this file will contain:

```
============[ Nov 3, 2003  1:21 AM ]=====================
ERROR: [004.001] {cbmmdb.c, line 125} Error opening MMDB id 22339
```

```
WARNING: [011.001] {cbmmdb.c, line 240} Total elapsed time: 41857 seconds
NOTE: [000.000] {cbmmdb.c, line 245} Main: Done!
```

And records are inserted into tables mmdb and mmgi.

Run the vastblst parser to make the DOMDB datafile.

**`./vastblst –n F`**

This program writes errors to the *vastblstlog* file. After a typical run this file will contain no messages and records are inserted into table domdb

In addition, vastblst makes a FASTA datafile of domains called *mmdbdom.fas* in the directory where it is run.

Get the most recent *nrpdb.** file from the NCBI ftp site in hand (*ftp://ftp.ncbi.nih.gov/mmdb/nrtable/nrpdb*

Run the pdbrep parser to label representatives of nr chain sets in the domdb datatable. This parser writes to the domdb table. Use:

**`uncompress nrpdb*.Z`**
**`pdbrep –i nrpdb.*`**

Where *nrpdb.** is the name of the input file set. pdbrep will write errors to the *pdbreplog* file in the same directory where it is run.

23. Build the Neighdb module

The sequence neighbours tables can be downloaded from *ftp://ftp.blueprint.org/pub/SeqHound/NBLAST/* as MySql database table files, as well as mysqldump output, which should be adaptable to most SQL database systems. See the readme on the ftp site for information on these files. To incorporate the mysql database table files into your instance of seqhound, simply copy the files extracted from the nblastdb and blastdb archives, downloaded from the ftp site, into your seqhound database directory in your mysql instance. To incorporate the mysql dumps of these tables into your seqhound instance, you need only pipe the contents of the dump(which are SQL statements) to your database server. In the case of mysql, simply execute:

```
gunzip -c  seqhound.blastdb.SQLdump.YYYYMMDD.gz | mysql seqhound
gunzip -c  seqhound.nblastdb.SQLdump.YYYYMMDD.gz | mysql seqhound
```

Be sure to fill in any required mysql options, such as `username`, `hostname` and `port number`.

24. Build the Rpsdb and Domname modules

The pre-computed rps-blast table and the domname table can be downloaded from *ftp://ftp.blueprint.org/pub/SeqHound/RPS/* as MySQL database table files, as well as mysqldump output, which should be adaptable to most SQL database systems. To incorporate the mysql database table files into your instance of seqhound, simply copy the files extracted from the rpsdb and domname archive, downloaded from the ftp site, into your seqhound database directory in your mysql instance. To incorporate the mysql dumps of these tables into your seqhound instance, you need only pipe the contents of the dump(which are SQL statements) to your database server. In the case of mysql, simply execute:

```
gunzip -c  seqhound.rpsdb.SQLdump.YYYYMMDD.gz | mysql seqhound
gunzip -c  seqhound.domname.SQLdump.YYYYMMDD.gz | mysql seqhound
```

Be sure to fill in any required mysql options, such as username, hostname and port number.

25. Build the histdb table.

```
cd $SEQH/8.hist.files
./histparser –n F
```

This parser populates table histdb. An entry will be generated for each of the sequences that have valid accessions in table accdb that indicates that the sequence was added on this day (when you ran histparser). This parser writes to the *histparserlog*. This parser requires the accdb table and will take about 15 hours to run.

26. You are done with the initial build of SeqHound.

---

If you did not build any of the optional modules, you will have to remember this when setting up the *.intrezrc* configuration file for any SeqHound application.

---

Set module values to zero if you did not build them. See the following section of the *.intrezrc* configuration file.

```
example:
[sections]
;indicate what modules are available in SeqHound
;1 for available, 0 for not available
;gene ontology hierarchy (did you run goparser?)
godb = 1
;locus link functional annotations (did you run llparser and addgoid?)
lldb = 1
;taxonomy hierarchy (did you run importtaxdb?)
taxdb = 1
;protein sequence neighbours (did you download neighbours tables?)
neigdb = 1
;structural databases (did you run cbmmdb, vastblst and pdbrep?)
strucdb = 1
;complete genomes tracking (did you run chrom and comgen?)
gendb = 1
;redundant protein sequences (did you run redund?)
redundb = 1
;open reading frame database (currently not exported at all)
cddb = 0
;RPS-BLAST tables (did you download RPS-BLAST tables?)
rpsdb = 1
```

**Catch up on SeqHound daily updates**

27. Download all daily update files for genbank

---

Warning: There might have been a new GenBank release while you were building SeqHound, in this case you cannot get updates from *ftp://ftp.ncbi.nih.gov/ncbi-asn1/daily-nc/* any more. You have to rebuild SeqHound with a fresh GenBank release. You should check the file *ftp://ftp.ncbi.nih.gov/ncbi-asn1/daily/Last.Release* to make certain that it contains the same release number that was present when you started step 15.

---

```
cd $SEQH/
mkdir seqsync
```

```
cd seqsync
ftp ftp.ncbi.nih.gov
```

When prompted for a name enter **anonymous**

When prompted for a password type ***myemail@home.com*** **cd ncbi-asn1**

```
cd daily-nc
bin
prompt
mget nc*.aso.gz
bye
```

Do not download the *con_nc*.aso.gz* files from this directory. SeqHound does not use them.

28. Download all daily update files for refseq.

    From *ftp://ftp.ncbi.nih.gov/refseq/daily/* download all files past the date stamp on *gbrscu.aso.gz*. *gbrscu.aso.gz* is the latest cumulative RefSeq division which was downloaded by *asnftp.pl* and is located (in this example) in *seqhound/build/asofiles*.

    ```
    cd $SEQH/seqsync
    ftp ftp.ncbi.nih.gov
    ```

    enter **anonymous** and your email address when prompted

    ```
    cd refseq
    cd daily
    bin
    get rsnc.****.2003.bna.Z
    ```

    (where ******** are files with timestamps greater than *gbrscu.aso.gz*)

    ```
    bye
    ```

    You must uncompress all of these files and rezip them so they can be processed by the mother parser.

    ```
    compress –d *.Z
    gzip *.bna
    ```

29. Run update and mother on all downloaded files (excluding today's one; crons will do it in the evening).

    You can use the scripts *all_update.sh* and *all_update_rs.sh*. You will also need mother, update and a properly configured *.intrezrc* file in the same directory as all of the daily update files.

    ```
    cd $SEQH/seqsync
    cp $COMPILE/slri/seqhound/scripts/all_update.sh .
    cp $COMPILE/slri/seqhound/scripts/all_update_rs.sh .
    cp $SEQH/1.core.files/.intrezrc .
    cp $SEQH/1.core.files/mother .
    cp $SEQH/1.core.files/update .
    ```

    Run *all_update.sh* first

**`./all_update.sh 141`**

where **`141`** is the release number.

Run *all_update_rs.sh second*.

**`./all_update_rs.sh 141`**

These scripts will run update and mother executables (consecutively) on all downloaded files present in the current directory.

All daily updates in SeqHound are stored in one division called `gbupd` regardless how long SeqHound runs without a core rebuild.

mother will make a log file called "**run*" for every file that it processes

update will make two log files called "**gis*" and "**log*" for every file that it processes

You can check that the two parsers have completed successfully. Each of the following queries should return the same number (the number of starting input files):

```
ls *aso.gz | wc –l
ls *gis | wc –l
ls nc*log | wc –l
ls nc*run | wc –l
grep Done nc*run |wc -l
```

**Setting up daily sequence updates**

30. Make a new directory from where you will run daily sequence updates.

    Populate this with the necessary scripts and programs.

```
cd $SEQH
mkdir updates
cd updates
cp $SLRI/seqhound/scripts/*cron_odbc.pl .
cp $SLRI/seqhound/scripts/shconfig.pm .
cp $SLRI/seqhound/build/odbc/redund .
cp $SLRI/seqhound/build/odbc/mother .
cp $SLRI/seqhound/build/odbc/update .
cp $SLRI/seqhound/build/odbc/precompute .
cp $SLRI/seqhound/build/odbc/isshoundon .
cp $SLRI/seqhound/build/odbc/importaxdb .
cp $SLRI/seqhound/build/odbc/goparser .
cp $SLRI/seqhound/build/odbc/llparser .
cp $SLRI/seqhound/build/odbc/addgoid .
cp $SLRI/seqhound/build/odbc/comgen .
```

```
cp $SLRI/seqhound/build/odbc/chrom .
cp $SLRI/seqhound/scripts/genftp.pl .
cp $SLRI/seqhound/scripts/humoasn.pl .
cp $SLRI/seqhound/scripts/humouse_build.sh .
cp $SLRI/seqhound/genomes/gen_cxx .
cp $SLRI/seqhound/genomes/pregen.pl .
cp $SLRI/seqhound/genomes/gen.pl .
cp $SLRI/seqhound/genomes/ncbi.bacteria.pl .
mkdir logs
mkdir asofiles
mkdir inputfiles
mkdir genfiles
mkdir flags
```

31. Copy the *.intrezrc* config file to the updates directory and edit it.

```
cd $SEQH/updates
cp $SLRI/seqhound/config/.intrezrc .
cp $SEQH/1.core.files/.intrezrc .
```

Text in ***italics*** must be changed. in `[crons]` section, variable `pathupdates` points to the path where the update jobs will be set up; variable `pathinputfiles` points to the path that saves the input files (other than **.aso.gz* and **.bna.gz* files from the core module and **.asn* files from the gendb module); variable `pathinputfilescomgen` points to the path that saves the input files **.asn* for the gendb module; variable `mail` indicates your e-mail address; variable `defaultrelease` is the GenBank release you build SeqHound database with; variable `pathflags` points to the path that save the flag files generated by each updating job.

```
[crons]
;customizable variables in cron jobs
;NOTE: all paths must end in '/'
pathupdates=./
pathinputfiles=./inputfiles/
pathinputfilescomgen=./genfiles/
mail=my_email
defaultrelease=141
pathflags=./flags/
```

The cron daemon may consider your home directory to be the “current directory”. For this reason, the *.intrezrc* file should be copied to your home directory too.

```
cd $SEQH/updates
cp .intrezrc  ~/.
```

32. Set up the *dupdcron_odbc.pl* cron job.

*dupdcron_odbc.pl* (daily update cron) is a PERL script that retrieves the latest GenBank and RefSeq update files from the NCBI ftp site and then passes them to

"update" and "mother" where they are used to update the SeqHound data tables. Specifically, it

a) downloads update files with today's date (from *ftp://ftp.ncbi.nih.gov/ncbi-asn1/daily-nc/ nc*.aso.gz* and *ftp://ftp.ncbi.nih.gov/refseq/daily/ rsnc*.bna.Z*

b) runs update

(`update -i nc*.aso.gz`)

and then

c) runs mother

(`mother -i nc*.aso.gz -r version# -n F -m F -u T`).

---

You need to know this because if you miss a few updates before setting up the cron job (and after completing the seqsync steps above) you have to run update and mother in hand using the above commands.

---

All scripts (like *dupdcron_odbc.pl*) report success or failure via email. The mailto address is set in the *shconfig.pm* script which you have just edited.

*dupdcron_odbc.pl* is the first cron job that has to be set up. Make a new text file called *list_crontab* where you will list the cron jobs.

```
cd $SEQH/updates
pico list_crontabs
```

This file should have the single line

```
30 22 * * * cd /seqhound/update; LD_LIBRARY_PATH=libpath ./dupdcron_odbc.pl
```

where ***libpath*** should be replaced by the correct path you set up in Step 11 for environment variable `LD_LIBRARY_PATH`. You can find it out by:

```
echo $LD_LIBRARY_PATH
```

This line specifies the time to run a job on a recurring basis. It consists of 6 fields separated by spaces. The fields and allowable values are of the form:

| | |
|---|---|
| `minute` | `(0-59)` in this case 30 |
| `hour` | `(0-23)` in this case 22 |
| `day of the month` | `(1-31)` in this case * |
| `month` | `(1-12)` in this case * |
| `day-of-week` | `(0-6 where 0 is Sunday)` in this case * |
| `command to run` | |

The above line indicates that *dupdcron_odbc.pl* is to be run at 10:30 PM every day of the month, every month, regardless of the day of the week. The ***** character is a wild-card. The actual command consists of changing to the directory where *dupdcron_odbc.pl* exists (this path will have to be modified depending on your set up)

```
cd /seqhound/update;
```

and then executing the perl script

```
./dupdcron_odbc.pl
```

After adding the above line and editing it to match your setup, close the file.

To activate this crontab file, type

**crontab list_crontabs**

If for some reason, you want to deactivate the cron job, type:

**crontab –r list_crontabs**

To find out what cron jobs you have activated, type

**crontab -l**

For more information on setting up cron jobs on UNIX type:

**man crontab**

33. Set up *redundcron_odbc.pl* to run daily.

**cd $SEQH/updates**
**pico list_crontabs**

Add the following line:

```
30 23 * * * cd /seqhound/update; LD_LIBRARY_PATH=libpath ./redundcron_odbc.pl
```

See Step 32 for the explanation of `libpath`.

After adding the above line, edit it to match your setup and close the file.

To activate this crontab file, type

**crontab list_crontabs**

This script basically does three things:

a) checks if file "*nr*" is updated on the ftp site *ftp://ftp.ncbi.nlm.nih.gov/blast/db*. If it is, retrieves it

b) drops table redund from the database and recreate it.

c) rebuilds table redund using the downloaded *nr* file and the redund parser.

34. Run precompute for the first time.

First set up the configuration file

**cd $SEQH/updates**
**pico .intrezrc**

Edit the section under [precompute] to make it look like:

```
[precompute]
;precomputed taxonomy queries
MaxQueries = 0
MaxQueryTime = 10
QueryCount = 0
#path to precomputed searches has to have "/" at the end !!
path = /seqhound/precompute/
indexfile = /seqhound/precompute/index
```

Make sure the value of `path` is the absolute path of directory `precompute` you make in Step 14 and the value of `indexfile` is the value of `path` plus `index`. Variable `path` is the directory that holds results of the precompute executable. `indexfile` is a path to the index that will be created by precompute.

Finally, run the precompute executable:

```
cd $SEQH/updates
./precompute –a redo
```

Where `–a redo` specifies that the program is being run for the first time.

This program basically precomputes the number of proteins and nucleic acids (and their GI values) for each taxon in the taxgi table. The results of this query are stored and indexed in text files (in the directory specified by `path`) if this query takes longer than `x` seconds (where `x` is defined by `MaxQueryTime` in the above *.intrezrc* file). These text files are used by SeqHound API calls such as `SHoundProteinsFromTaxIDIII(taxid)`

35. Set up *precomcron_odbc.pl* to run daily.

```
cd $SEQH/updates
pico list_crontabs
```

Add the following line:

```
30 1 * * * cd /seqhound/update; LD_LIBRARY_PATH=libpath ./precomcron_odbc.pl
```

See Step 32 for the explanation of `libpath`.

After adding the above line and editing it to match your setup, close the file.

To activate this crontab file, type

```
crontab list_crontabs
```

This script basically runs the command

```
precompute  -a update
```

and updates the precomputed search results.

36. Set up *isshoundoncron_odbc.pl* to run daily.

```
cd $SEQH/updates
pico list_crontabs
```

Add the following line:

```
30 7 * * * cd /seqhound/update; LD_LIBRARY_PATH=libpath ./isshoundoncron_odbc.pl
```

See Step 32 for the explanation of "`libpath`".

After adding the above line and editing it to match your setup, close the file.

To activate this crontab file, type

```
crontab list_crontabs
```

This script basically does two things:

a) runs the executable called `isshoundon`. This program makes a single call to the local SeqHound API to ensure that it is working.

b) moves all log, run and gis log files into a directory called *logs*

37. Set up *llcron_odbc.pl* to run daily.

```
cd $SEQH/updates
pico list_crontabs
```

Add the following line:

```
30 21 * * * cd /seqhound/update; LD_LIBRARY_PATH=libpath ./llcron_odbc.pl
```

See Step 32 for the explanation of `libpath`.

After adding the above line and editing it to match your setup, close the file.

To activate this crontab file, type

```
crontab list_crontabs
```

This script basically repeats the actions listed in step 14 above and re-creates the locus link tables in SeqHound. This includes:

a) getting the latest *LL_tmpl.gz* file from the NCBI ftp site.

b) removing the locus link tables from SeqHound

c) running llparser

d) getting 2 GO annotation files from GO ftp site

e) running the addgoid parser on these two files

38. Set up *comgencron_odbc.pl* to run daily.

```
cd $SEQH/updates
pico list_crontabs
```

Add the following line:

```
30 21 * * * cd /seqhound/update; LD_LIBRARY_PATH=libpath ./comgencron_odbc.pl
```

See Step 32 for the explanation of `libpath`.

After adding the above line and editing it to match your setup, close the file.

To activate this crontab file, type

```
crontab list_crontabs
```

This script basically repeats the actions listed in step 15 above and re-creates the chrom table in SeqHound and updates the complete genome information in the core tables. This includes:

a) generating a list of "DNA units" that belongs to a complete genome,

b) downloading complete genome files from NCBI ftp site,

c) rebuilding table chrom

d) removing all records in the core tables that belongs to division "gbchm",

e) running script *humous_build.sh* to insert records into core tables

f) resetting the kloodge field in table taxgi for all records to 0

g) updating kloodge by running parser comgen

**Setting up SeqHound servers. Overview**

39. Setting up SeqHound servers. Overview.

There are two web server applications that make up the SeqHound system:

a) wwwseekgi produces html pages for the SeqHound web interface and

b) seqrem processes requests to the SeqHound remote API.

Step 40 shows you how to find the two directories where you will set up these two applications (assuming that you are using a default installation of Apache). The two directories are called:

*cgi-bin*

*htdocs*

Step 40 may be skipped if you already know or have already been told where these two directories are.
Steps 41 - describe the files that must be placed into these two sub-directories in order to start the wwwseekgi and seqrem servers.

40. Examining the *httpd.conf* file for Apache.

These instructions assume that you already have an Apache server running. In order to proceed further you must locate the directory where executables will be run from (called "*cgi-bin*" in a default set-up of Apache) and a directory that contains html documents (called "*htdocs*" in a default set-up of Apache). You can find (and reset) the location of these two directories in an Apache configuration file called "*httpd.conf*". In a default set-up of Apache, the *httpd.conf* file can be accessed by changing to the directory:

```
cd /etc/apache
```

and then opening the *httpd.conf* file found in this directory using a text editor such as pico:

```
pico httpd.conf
```

To find the *cgi-bin* directory location, look for the line beginning with "`ScriptAlias`". In the default set-up, this line looks like this:

```
ScriptAlias /cgi-bin/ "/var/apache/cgi-bin/"
```

In this example, the path to the *cgi-bin* directory is `/var/apache/cgi-bin/`. Write this path down, whatever it is.

To find the *htdocs* directory, look for the line beginning with "`DocumentRoot`". In the default set-up, this line looks like this:`

```
DocumentRoot "/var/apache/htdocs/"
```

In this example, the path to the *cgi-bin* directory is `/var/apache/htdocs/`. Write this path down, whatever it is.

Also make a note of the line beginning with "`User`" and "`Group`" (who has ownership to the server). In a default Apache set-up, these lines are likely

```
User nobody
Group nobody
```

Make a note of this, whatever it is.

Exit from the *httpd.conf* file and save your changes. If you made changes to the file, you must restart the Apache server using the command:

```
/usr/apache/bin/apachectl restart
```

See the *Trouble Shooting* section at the end for more information on this.

In the steps below you will set up the SeqHound server by adding to these two directories

| **Contents of the *cgi-bin* and *htdocs* directories** | |
|---|---|
| **directory** | **contents** |
| *cgi-bin* | the SeqHound wwwseekgi and seqrem server applications will placed here |
| *htdocs* | all of the static html pages used by the SeqHound interface will be placed here |

41. Set up the *cgi-bin* directory.

    Move to the *cgi-bin* directory you found in the step above. For the default set-up:

    ```
    cd /var/apache/cgi-bin/
    ```

    make a new subdirectory here called SeqHound

    ```
    mkdir seqhound
    cd seqhound
    ```

    copy the SeqHound server applications here:

    ```
    cp $COMPILE/slri/seqhound/build/odbc/seqrem .
    cp $COMPILE/slri/seqhound/build/odbc/wwwseekgi .
    ```

    also copy the following files to this directory:

    ```
    cp $COMPILE/slri/seqhound/html/seekhead.txt .
    cp $COMPILE/slri/seqhound/html/seektail.txt .
    cp $COMPILE/slri/seqhound/html/seekhead.txt pics/.
    cp $COMPILE/slri/seqhound/config/.intrezrc .
    cp $COMPILE/slri/seqhound/config/.ncbirc .
    ```

42. Edit the *.ncbirc* configuration file.

    Open the file with a text editor such as pico.

    The setting for `Data` should contain a path to the *ncbi/data* directory. This directory was downloaded as part of the ncbi toolkit in step 2.

    ```
    --------------------example .ncbirc file begins----------------------
    [NCBI]
    Data=/home/ncbi/data
    --------------------example .ncbirc file ends-----------------------
    ```

43. Edit the *.intrezrc* configuration file.

    Refer to step 14 in the current section for setting up of the *.intrezrc* file. The settings for `username`, `password`, `dsn` and `database` in section `[datab]` should be valid for the SeqHound database you have just built, and the setting for `path` and

`indexfile` in section `[precompute]` should point to the valid path as in step 34 in the current section. Set up the *index.html* file for the web interface.

Move to the *htdocs* directory for your web-server. In the default case:

**`cd /var/apache/htdocs/`**

Make a SeqHound directory here:

**`mkdir seqhound`**

**`cd seqhound`**

Copy the *index.html* page to this directory:

**`cp $COMPILE/slri/seqhound/html/index.html .`**

Open the file in a text editor like pico and edit it so that its action points to the wwwseekgi server.

**`pico index.html`**

then edit the line

`<FORM ACTION="/cgi-bin/seqhound/wwwseekgi" METHOD="GET">`

where `"/cgi-bin/seqhound/wwwseekgi"` should specify the path to the wwwseekgi executable.

44. Set up ODBC configuration file *.odbc.ini*:.

    Move to the home directory of the owner of the binary seqrem in directory */var/apache/cgi-bin/*. Text in ***`italics`*** should be changed (see Step 10):

    **`cd /homedir`**

    Set up file *.odbc.ini* as the following (text in ***`italics`*** should be changed):

```
[mysqlsh]
Description  = MySQL ODBC 3.51 Driver DSN
Trace        = On
TraceFile    = stderr
Driver       = /software/64/unixodbc/odbc/lib/libmyodbc3.so
DSN          = mysqlsh
SERVER       = my_server
PORT         = my_port
USER         = user_id
PASSWORD     = my_pwd
DATABASE     = seqhound
```

45. Set permissions on the *cgi-bin* directory.

    Move to the *cgi-bin* directory.

    **`cd /var/apache/cgi-bin/`**

    Change the user and group ownership to nobody (or whatever the values of "`User`" and "`Group`" were set to in step 40).

    **`chown –R nobody:nobody seqhound`**

46. Set permissions on the *htdocs* directory.

    Move to the *htdocs* directory.

    **`cd /var/apache/htdocs/`**

Change the user and group ownership to `nobody` (or whatever the values of "`User`" and "`Group`" were set to in step 40).

**`chown -R nobody:nobody seqhound`**

47. Test the SeqHound web interface.

    Open an internet browser and, in this example, go to the url

    **`http://`*`yourmachinename`*`/cgi-bin/seqhound/`**

    You should see the front page of the SeqHound wwwseekgi interface.

**Trouble-shooting notes**

**Error logs**

Error logs for each of the SeqHound parsers are described in the steps above where the parser is used to initially build a given SeqHound module.
Error logs for the SeqHound wwwseekgi server software is located in the same directory as the executable; see *wwwseekgilog*.
Error logs for the seqrem server are located in the same directory as the executable; see *seqremlogs*.
Error logs for the Apache server software are located (in a default set-up) in */var/apache/logs*.

**Recompiling SeqHound**

If you make changes to and recompile SeqHound, you should first do a clean of the existing object files and executables. If you are still in a super-user shell, you may wish to exit this shell and return to the shell where you had set all of your environment variables. These variables are required by the clean and make scripts.

| | |
|---|---|
| COMPILE | compile directory |
| SLRI | slri directory |
| NCBI | ncbi directory |
| CC | gcc |
| PATH | /usr/local/bin:/usr/ccs/bin:${PATH} |
| EXTRAOPT | -D_FILE_OFFSET_BITS=64 |
| ODBC | (path to unixodbc) |
| LD_LIBRARY_PATH | (path to mysql and odbc libraries) |

The first three variables refer to directories that are created during the above instructions. To clean, run any make file with the 'clean' target. For example, to clean the cgi executables, type:

```
cd $COMPILE/slri/seqhound/cgi
make –f make.seqrem clean
make –f make.wwwseekgi clean
```

**Restarting the Apache server**

If changes are made to the *httpd.conf* file, the Apache server must be restarted for the changes to take effect. Use the apachectl script to do this
For a default install of Apache this script is in the directory
*cd /usr/apache/bin*
and to start the server, type

```
./apachectl restart
```

or to get a list of apachectl script commands type

```
./apachectl
```

**Other useful links**

| | |
|---|---|
| SLRI on Sourceforge | *http://sourceforge.net/projects/slritools/* |
| NCBI Info Engineering branch: | *http://www.ncbi.nlm.nih.gov/IEB/* |
| Concurrent Versioning System (CVS) | *http://www.cvshome.org/* |
| MySQL | *http://www.mysql.com/* |

**Parser schedule**

Parsers are run on a periodic basis as "cron" jobs on Unix platforms and as "Schedules tasks" on Windows platforms.
The cron job schedule is set up in the file "*seqhound/update/list_crontabs*" on UNIX platforms
The setup for the current production version of SeqHound described in these instructions is shown below:

```
0 19 * * * /arena/seqhound/update/llcron_odbc.pl
0 21 * * * /arena/seqhound/update/redundcron_odbc.pl
30 22 * * * /arena/seqhound/update/dupdcron_odbc.pl
30 24 * * * /arena/seqhound/update/precomcron_odbc.pl
0 7 * * * /arena/seqhound/update/isshoundoncron_odbc.pl
```

**MySQL errors**

`ERROR 1153 at line X: Got a packet bigger than 'max_allowed_packet'`

When MySQL receives a packet bigger than `max_allowed_packet` bytes, it issues a Packet too large error and closes the connection. For example, when a single SQL statement from a mysqldump being imported exceeds the value for "`max_allowed_packet`" configured on the MySQL server. Increasing this value to 64MB from the default 16MB should resolve the error. This value may be changed in the global config or setting this on the running server via:

**`set global max_allowed_packet=67108864;`**

Please see *http://dev.mysql.com/doc/mysql/en/Packet_too_large.html* for more information

# 5. Description of the SeqHound parsers and data tables by module

## What are modules?

The SeqHound system is divided into one required "core" module and several optionally configured modules. Modules are groups of tables and API calls that are filled using a common data resource, for example the 3D structures. The purpose of this division is to give the user an option to control hardware resources and complexity of system administration when parts of the SeqHound system are not required. The list of SeqHound modules and their data resources is contained in the table below.
After a system build, the module information is recorded in the configuration file which is then utilized by the API to determine if certain operations can be achieved with the current setup. The configuration file is called *.intrezrc* (Unix platforms) The relevant section of this file is under the heading "[sections]". Consult *Section 4* under "*Building the SeqHound system*" for more information on specifying the available modules in this file.

## How to use this section.

This section describes the SeqHound system in detail module by module.
Parser and data tables associated with a given module are described under the section for that module.
A brief description of all of the parsers can be found below and in the Table 2 of the *SeqHound paper*. The table is repeated below and will be updated here.

Note: It is assumed that you have read the material in *section 3* and *section 4* before delving into this material. These two sections include everything you need to know to start using the SeqHound remote API or to install you own local version of SeqHound. This section is intended for users who may want more details about how SeqHound is constructed and exactly what it is doing behind the scenes. This section is also meant as background material for developers who want to further develop the SeqHound system

## Parser descriptions

Parser descriptions contain the following headings and information:

| | |
|---|---|
| **purpose:** | a brief description of what the parser is for |
| **logic:** | more details on the parser – see update parser for example |
| **module:** | what module the parser belongs to |
| **input files:** | input files required by the parser (also available in Table 2) |
| **tables altered:** | tables in SeqHound that are modified or created by the parser (also available in Table 2) |
| **source code location:** | location of the parser source code in the slri development tree |
| **config file dependencies:** | what configuration file parameters must be set for the parser to work |
| **command line parameters:** | used by the parser |
| **example use:** | of the parser from the command line |
| **associated scripts:** | that are used to run the parser |
| **error and run-time logs:** | where they are located and what is in them |
| **troubleshooting:** | problems that may occur with this parser |
| **additional info:** | where to find it |

## Table descriptions

Each table that is relevant to a module is described under that module.
Here is an example with comments in brackets. A data table description consists of the following sections and content:

| | |
|---|---|
| **Database:** | that the table belongs to (almost always SeqHound) |
| **Table:** | name of the table like “accdb” |
| **Definition:** | a brief description of the table's purpose (for example, “This table |

correlates gi's to accession identifiers).

**Observation:** notes about the table

**Source db:** where does this table's information come from

**Source file:** the source file (used by the parser to fill this table) location is listed here

**Parser:** the name of parser if a single parser is responsible for filling this entire table.

This is followed by a summary of the table's definition (for example):

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto number row identifier |
| gi | int(11) | No | 0 | GenInfo Identifier |
| asn1 | longblob | Yes | NULL | BioSeqs: Sequences |

and indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | gi |
| iasndb_rowid | INDEX | rowid |
| iasndb_gi | INDEX | gi |

(each field is then described...only one field description is shown for this example)

*****gi*****

**description:** definition of the column (for example, GenInfo sequence record identifier")

**example:** of a column entry (for example, "1232452")

**default value:** if the value has a default value, it is listed here

**ASN.1 structure:** If the value in this column is derived from an NCBI data structure, this gives you a quick idea of where to locate it--you can find more info by searching for this data structure at:
*http://www.ncbi.nlm.nih.gov/IEB/ToolBox/SB/hbr.html*.

| | |
|---|---|
| | for example, “Bioseq->Seq-id (choice 12)<br>Alternatively, the column may store a binary object that is an NCBI or SLRI ASN.1 object. Descriptions of SLRI ASN.1 objects may be found at *http://cvs.sourceforge.net/cgi-bin/viewcvs.cgi/slritools/slri/seqhound/asn*. |
| **source:** | If the value in this column is derived from a text file, this describes how to find the information present in this column in the source file (for example in the fourth column) |
| **parser:** | this is the parser(s) that retrieves the value from some other db (for example, mother) |
| **function:** | this is the parser function that retrieves the value |
| **API:** | if a SHound API function retrieves this value from this table it is listed here (for example, `ShoundFindAcc`) |
| **more info:** | (other notes) |

## An overview of the SeqHound data table structure

An overview of the SeqHound data table structure is available as a separate document in pdf format. See *http://www.blueprint.org/seqhound/api_help/docs/SeqHound_Schema_Prod.pdf*.

## Parsers and resource files needed to build and update modules of SeqHound.

This table will be updated shortly

| Input File | Resource | Parser | Tables Modified | Module |
|---|---|---|---|---|
| ASN.1 sequences | *ftp://ftp.ncbi.nih.gov/ncbi-asn1/*.aso*<br>*ftp://ftp.ncbi.nih.gov/refseq/cumulative/*.bna* | mother | asndb, parti, nucprot, accdb, pubseq, taxgi, sendb, sengi | core |
| ASN.1 sequences | *ftp://ftp.ncbi.nih.gov/ncbi-asn1/daily-nc/*.aso*<br>*ftp://ftp.ncbi.nih.gov/refseq/daily/*bna* | update | asndb, parti, nucprot, accdb, pubseq, taxgi, sendb, sengi | core |
| FASTA nr database | *ftp://ftp.ncbi.nih.gov/blast/db/nr* | redund | redund | redundb |
| List of complete genomes (flat file) | *http://cvs.sourceforge.net/cgi-bin/viewcvs.cgi/slritools/slri/seqhound/genomes/chromff* | chrom | chrom | gendb |
| ASN.1 for complete genomes | *ftp://ftp.ncbi.nih.gov/genomes/*/*.asn* | comgen | taxgi, accdb | gendb |
| Taxonomy release (flat file) | *ftp://ftp.ncbi.nih.gov/pub/taxonomy/taxdump.tar* | importtaxdb | TAX, GCODE, DIV, del, merge | taxdb |
| ASN.1 MMDB release | *ftp://ftp.ncbi.nih.gov/mmdb/mmdbdata/*.val* | cbmmdb | mmdb, mmgi | strucdb |
| MMDB (database table) | mmdb table | vastblst | domdb | strucdb |

| | | | | |
|---|---|---|---|---|
| 3-D chain BLAST sets (flat file) | *ftp://ftp.ncbi.nih.gov/mmdb/nrtable/nrpdb.** | pdbrep | domdb | strucdb |
| FASTA nr database | *ftp://ftp.ncbi.nih.gov/blast/db/nr* | nblast | nrB | neigdb |
| BLAST ASN.1 results | nrB table available nrB and nrN tables available at *ftp://ftp.blueprint.org/pub/SeqHound/NBLAST/* | nbraccess | nrN | neigdb |
| LL_tmpl (flat file) | *ftp://ftp.ncbi.nih.gov/refseq/LocusLink/LL_tmpl* | llparser | ll_omim, ll_go, ll_llink, ll_cdd | lldb |
| gene_associaton.com | | | | |
| pugen.GenBank/Swissprot (flat files) | *http://www.geneontology.org* | addgoid | ll_go | lldb |
| function.ontology<br>process.ontology<br>component.ontology (flat files) | *http://www.geneontology.org* | goparser | go_parent, go_name, go_reference, go_synonym | godb |
| CDD database | *ftp://ftp.ncbi.nih.gov/pub/mmdb/cdd/* | domname | domname | rpsdb |
| FASTA nr database and CDD database | *ftp://ftp.ncbi.nih.gov/blast/db/nr*; *ftp://ftp.ncbi.nih.gov/pub/mmdb/cdd/* DOMNAME and RPSDB tables available at *ftp://ftp.blueprint.org/pub/SeqHound/RPS/* | rpsdb | rpsdb | rpsdb |

**core module**

Last updated April 11, 2005. This section is maintained bt Elizabeth Burgess.

**mother parser**

Last updated April 11, 2005

**purpose:**

The mother parser is the first parser that is used to initially build the SeqHound "core" set of data tables. The input files consist of the latest release of GenBank and RefSeq in binary ASN.1 format available on the NCBI ftp site. The resulting SeqHound data tables hold DNA, RNA and protein sequence record information.
As of release 4.0, the mother parser is also used with the GenBank and RefSeq daily updates to update SeqHound so that that sequence information is synchronized with that of NCBI. Previously, updates were handled by a separate parser called "update".

**logic:**

The mother parser is run on a daily basis in update mode (-u T) to update with two input files. One input file is the daily update from GenBank and the other is the daily update from the RefSeq database.

For each bioseq in the input file, mother retrieves the GI and accession number.
Mother then looks for this pair of GI and accession identifiers in the SeqHound accdb table.

If neither the accession (nor the GI) is found, then the record in the daily update represents a GI that is to be ADDED to SeqHound.

If the accession in the update file is found in SeqHound and is associated with the same GI (as listed in the update file) then the record in the daily update represents a GI that has been CHANGED. This means that the sequence record was resubmitted to GenBank with the same GI; the sequence remains the same but the associated annotation has changed.

If the accession in the update file is found in SeqHound but the GI associated with this accession differs between the update file and SeqHound, then the GI that is newly associated with the accession represents a change in the sequence. The accession and updated GI

pair point to a sequence record that will be ADDED to SeqHound. The accession and old GI (currently in SeqHound) point to a record in SeqHound that will be KILLED (deleted).

Mother then records in the SeqHound history table whether the GI and accession in the update file represent an ADDED or CHANGED record. The previous gi associated with the accession is also recorded, if there is one. Mother also records in the history table those sequence records currently in SeqHound that will be KILLED (see above).

This process is completed for every bioseq in the update file.
A list of ADDED, CHANGED and KILLED GI's is written to the file *rsncmmddgis* where *rsncmmdd* refers to the update file that was being processed.

Mother then deletes from the following tables: parti, accdb, sendb,sengi, taxgi, pubseq, nucprot asndb. If the record is a complete genome record, then the gi will be deleted from gichromid, contigchromid, gichromosome and contigchromosome. The strategy for complete genome deletions is as follows:

Complete genome information in NCBI may be stored in several different places in the record.

1. Records from organisms other than those for certain higher eukaryotes ( e.g. human, mouse, rat, chicken and bee). These records contain the flag NCBI_GENOMES and list the RNA and protein gis in the annotation. The RNA and protein gis will be written to gichromid. The gi of the contig that contains the annotation is also written to this record if it is known.
2. Records from human, mouse, rat etc. The top level contig contains the NCBI_GENOMES flag, but no annotation. Instead, it lists the gis for contigs that make up this chromosome. The annotation of these contig records contains the gis and proteins that belong to this chromosome. The lower level contig gis are written to contigchromid so that the protein and RNA gis can be parsed later from the contig bioseqs by the postcomgen parser. The gi of the top level contig is also written to this record.
3. Some records exist that only contain a chromosome number in the description of the bioseq. These records can be a contig record or a record for an individual protein or RNA. These records are first written to gichromosome or contigchromosome and later moved to gichromid and contigchromid by postcomgen.

For updating, we check to see if the accession for that gi is in the chrom table. The only records that are written to this table are the top level gis that contain the NCBI_GENOMES flag. If the gi belongs to a top level contig, then all gis in contigchromid that belong to that contig are retrieved and all gis in gichromid that belong to each low level contig gi are deleted. The low level contig gis are then deleted from contigchromid.

If the record is present in contigchromid, then all gis in gichromid from that contig are deleted before the record is deleted from contigchromid.
If the gi is present in only gichromid and contains a contig gi, then the appropriate record in contigchromid is marked as changed. That way, after mother finishes, postcomgen will only process those contigs that have changed.
Mother writes errors and messages to a log file called *rsncmmddrun* where *rsncmmdd* refers to the update file that was being processed.

**module:** core

**input files:**

latest GenBank release (*ftp://ftp.ncbi.nih.gov/ncbi-asn1/*.aso*)

latest RefSeq release (*ftp://ftp.ncbi.nih.gov/refseq/cumulative/*.bna*)

daily GenBank release (*ftp://ftp.ncbi.nih.gov/ncbi-asn1/daily-nc/*.aso*)

daily RefSeq release (*ftp://ftp.ncbi.nih.gov/refseq/daily/*.bna*)

**tables altered:**

asndb, parti, nucprot, accdb, pubseq, taxgi, sendb, sengi, bioentity, bioname, chrom, gichromid, contigchromid, gichromosome, contigchromosome

**source code location:**

*slri/seqhound/parsers/mother.c*

**config file dependencies:**

The relevant configuration file is:

*slri/seqhound/config/.intrezrc*
The relevant section of the configuration file is:

```
[datab]
;seqhound database that you are connecting
username=your_user_name
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=
```

Text in ***italics*** must be changed for the *.intrezrc* file to function correctly with your SeqHound set-up. Variables `username`, `password`, `dsn`, `database` in section `[datab]` should have the same values as `USER`, `PASSWORD`, `DSN` and `DATABASE` respectively in your *.odbc.ini* (see section 4).

**command line parameters:**

Typing "**`./mother -`**" at the command line while in the directory where mother resides will return a list of command line parameters and default settings.

---

Note that `-n` and `-m` are listed for historical Codebase purposes. These values are always `F` for ODBC.

---

For example:

```
> ./mother -
mother   arguments:
  -i  Filename for asn.1 input [File In]
  -r  Release [String]
  -n  Initialize the ASNDB database file [T/F]  Optional
    default = F
  -m  Initialize the remaing database files [T/F]  Optional
    default = F
  -u  Is this an update [T/F]  Optional
    default = F
  -c  Is this a file for human/mouse complete genome [T/F]  Optional
    default = F
  -t  Read input file in text mode [T/F]  Optional
    default = F
```

**example use:**

```
mother –i nc1227.aso -r 135 -n F -m F
mother –I nc1227.aso –r 135
```

Note that mother is normally run under the control of a script (see below).

**associated scripts:**

The initial build of SeqHound is executed using the script called "*seqhound_build.sh*"
See "*slri/seqhound/scripts/seqhound_build.sh*"
This script cycles through all the GenBank and RefSeq release files downloaded by *asn_ftp.pl* unzips them, processes them with mother and then zips them up again.
The script must be run in the directory containing the GenBank and RefSeq release files and a copy of the mother parser The script takes one argument (a release number).

```
./seqhound_build.sh 135
```

mother is also called by the scripts that generate the daily updates (see "associated scripts" under update parser).

**error and run-time logs:**

mother writes to a log file called "*rsncmmddrun*" where *rsncmmdd* refers to the GenBank release or update file that was being processed. When run in update mode, it also writes the gis to a file called *"rsncmmddgis"*. The log files are created in the directory *logs*.

**troubleshooting:**

**additional info:**

See readme files that accompany the input files on the GenBank ftp site.
See data table descriptions for each of the tables that are listed under "tables altered".

**update parser**

Last updated April 11, 2005

**note:**

As of Release 4.0, update functionality has been moved to the mother parser and associated scripts. See above.

**postcomgen parser**

Last updated April 11, 2005

**purpose:**

The postcomgen parser is used in conjunction with the mother parser. It is used to update the taxgi table with complete genome information using the chrom, contigchromid, gichromid, gichromosome and contigchromosome tables. It is run after the initial build and after any updates.

**logic:**

Complete genome information in NCBI may be stored in several different places in different records.

1.Records from organisms other than those for certain higher eukaryotes ( e.g. human, mouse, rat, chicken and bee) contain the flag NCBI_GENOMES and list the RNA and protein gis in the annotation.

2.Records from certain higher eukaryotes (human, mouse, rat etc) are different. The top level contig contains the NCBI_GENOMES flag, but no annotation. Instead, it lists gis for the contigs that make up this chromosome. The annotation of these records contains the gis and proteins that belong to this chromosome.

3. Some records exist that only contain a chromosome number in the description of the bioseq. These records can be contig records or records for an individual protein or RNA.

At the time that mother is run, gis in the annotation may not yet have been entered into accdb and taxgi. For this reason, mother writes these gis out to the table gichromid. When mother encounters a record that contains only contig gis, these gis are written out to contigchromid. The records that contain only a chromosome number are written to gichromosome or contigchromosome.

After mother is finished, postcomgen is run to process the data in these tables and write the kloodge to the taxgi table for each gi:

1. Postcomgen first writes every gi in gichromosome to gichromid with the appropriate chromid. After this is done, all records are deleted from gichromosome.

2. Next, all contigchromosome gis are written to contigchromid with the appropriate chromid and all records are deleted from contigchromosome.
3. For each gi in contigchromid, the bioseq is obtained from asndb and any protein or RNA gis in the annotation are written to gichromid. In addition to the chromid, the contiggi is stored so that the appropriate contigchromid record can be reread on update if necessary.
4. Each record in contigchromid is marked as read, so that upon update only records that have been modified need be read.
5. Finally, taxgi is updated for each gi in gichromid with the appropriate kloodge.

**module:** core

**input files:**

There are no input files. The parser uses the tables gichromid, contigchromid, gichromosome and contigchromosome, which are filled by mother, to update the taxgi table.

**tables altered:**

taxgi, gichromid, contigchromid, gichromosome, contigchromosome

**source code location:**

*slri/seqhound/genomes/postcomgen.c*

**config file dependencies:**

The relevant configuration file is:
*slri/seqhound/config/.intrezrc*

The relevant section of the configuration file is:

```
[datab]
;seqhound database that you are connecting
username=your_user_name
```

```
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=
```

Text in *italics* must be changed for the .intrezrc file to function correctly with your SeqHound set-up. Variables username, password, dsn, database in section [datab] should have the same values as USER, PASSWORD, DSN and DATABASE respectively in your .odbc.ini (see 4).

**command line parameters:**

None.

**example use:**

```
postcomgen
```

**associated scripts:**

**error and run-time logs:**

Postcomgen writes to a log file called "*postcomgen.log*".

**troubleshooting:**

**additional info:**

See data table descriptions for each of the tables that are listed under "tables altered".

**asndb table**

Last updated April 11, 2005

**Database:** SeqHound

**Module:** core

**Table:** asndb

**Definition:** Central table that stores sequence records in binary ASN.1 format and indexed by gi.

asndb table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| rowid | int(11) | No | NULL | Mysql autoincrement column | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | timestamp | 2005-03-23 12:32:16 | | |
| gi | int(11) | No | 0 | GenInfo primary sequence record identifier | 4001923 | FillASNDB calls GetGi. See Bioseq->seqid->gi | |
| asn1 | longblob | Yes | NULL | bioseq in binary ASN.1 | An example of a bioseq is included in the Appendix (Example of GenBank record). | `ToBioseqSEQENTRY` See Bioseq->seqid->gi | `SHoundGetBioseq` `SHoundSequenceLength` |
| division | varchar(25) | No | | NCBI division | PRI | GetDivisionFromGBBlock. See Bioseq->descr->source ->org->orgname->div | |
| release | varchar(10) | No | | The name of the release given as a command line input to the mother parser | 135 | | |
| type | varchar(15) | No | | The type of molecule that this record refers to. | protein | FillASNDB calls GetType. See Bioseq-> mol | SHoundMoleculeType |

asndb indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | gi |
| iasndb_rowid | INDEX | rowid |
| iasndb_ts | INDEX | ts |
| iasndb_gi | INDEX | gi |

**parti table**

Last updated April 11, 2005

Note: This table is documented for historical purposes and may be deprecated in a future release. PARTI was required by codebase as an index to the ASNDB table.

**Database:** seqhound

**Table:** parti

**Module:** core

**Definition:** This table maps the gi to the NCBI division.

parti table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| rowid | int(11) | No | | MySQL autoincrement column. | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 12:32:16 | | |
| gi | int(11) | No | 0 | GenInfo Identifier | 21676275 | `FillASNDB` calls `AppendRecordPARTI`. See Bioseq->Seqid->gi (choice 12) | |
| division | char(15) | Yes | NULL | NCBI Division | PRI | GetDivisionFromGBBlock. See Bioseq->descr->source ->org->orgname->div | |

parti indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | gi |
| iparti_rowid | INDEX | rowid |
| iparti_ts | INDEX | ts |
| iparti_gi | INDEX | gi |
| iparti_div | INDEX | division |

**nucprot table**

Last updated April 11, 2005

**Database:** seqhound

**Table:** nucprot

**Module:** core

**Definition:** This table maps the gi of a protein to the gi of its encoding DNA.

**Observation:** A DNA may map to more than one protein. A protein can only map to one DNA. Not every DNA may map to a protein, eg synthetic DNA fragments typically do not have a protein. In a bioseqset structure of type nucprot, the first bioseq record is a nucleic acid, subsequent bioseq records correspond to proteins. In such a case, the entries added to the nucprot database would be:

record 1) gi_1 gi_2

record 2) gi_1 gi_3

record 3) gi_1 gi_4

Each record would be a mapping of the nucleic acid (gi_1) to each protein (gi_2 ... gi_N)

nucprot table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| rowid | int(11) | No | | MySQL autoincrement column. | | | |
| gin | int(11) | No | 0 | DNA GenInfo Identifier | 27464927 | FillNUCPROT. See Bioseq->Seqid->gi (choice 12) | `SHoundDNAFromProtein` |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 12:32:16 | | |
| gia | int(11) | No | 0 | Protein GenInfo Identifier | 27464928 | FillNUCPROT. See Bioseq->Seqid->gi (choice 12) | `SHoundProteinFromDNA` |

nucprot indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | gia |
| inucprot_rowid | INDEX | rowid |
| inucprot_ts | INDEX | ts |
| inuc_gin | INDEX | gin |
| inuc_gia | INDEX | gia |

**accdb table**

Last updated April 11, 2005

**Database:** seqhound

**Table:** accdb

**Definition:** This table maps gi's to accession numbers and other identifiers (a combination of a database name and identifier) found in GenBank sequence records.

**Observation** Note that gi is not unique in ACCDB. Also note that a gi does not always have an accession associated with it. There are 2 kinds of records in ACCDB. In one case the gi is associated with an accession and in the other case, the gi is associated with a database name and some identifier from that database (name column). Any given gi may have both record types and may be associated with more than one name.

Note that internal NCBI databases may be stored in ACCDB, for example NCBI_GENOMES. In this case the record will not have an accession, but it will have a name.

accdb table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| rowid | int(10) | No | | MySQL autoincrement column. | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 12:32:16 | | |
| gi | int(11) | No | 0 | GenInfo Identifier | 2313082 | FillACCDB calls GetGi. See Bioseq->seqid->gi | SHoundGiFromGBAcc (ShoundFindAcc) |
| db | varchar(15) | No | | The source database of the sequence record. See note 1 below. | pdb | FillACCDB. See Bioseq->Seq-Id->dbtag->db | SHoundDbNameAndIdListFromGBAcc |
| name | varchar(30) | No | | This is an accession number from a foreign database. | 1AAP | See note 2 below. | SHoundDbNameAndIdListFromGBAcc (ShoundFindName) (ShoundGetNameByGi) |
| namelow | varchar(30) | Yes | NULL | Same as name but in lower case. Present for historical reasons and may probably be removed in the future. | 1aap | See note 2 below. | |
| access | varchar(20) | No | | Genbank Accession. The primary sequence record identifier. | n/a | `WriteACCDB`. See Bioseq->Seq-id->Textseq-id->accession. This field is n/a for sequences from PDB and other databases. This field is only relevant when name field is n/a. | SHoundGBAccFromGi (ShoundAccFromGi) |
| chain | varchar(20) | Yes | NULL | This describes which one of (possibly) many chains in a structure a sequence refers to. This only refers to PDB sequences. | A | FillACCDB. See Bioseq->Seq-id->PDB-seq-id->chain. See note 5 below. | `SHoundGiFromPDBchain` |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| release | varchar(20) | Yes | NULL | release date of the record | Sep 14, 1990 | See note 3 below. | `SHoundSeqIdFromGi` |
| version | int(11) | Yes | NULL | version of the record | 0 | See note 4 below. | This value cannot be directly retrieved from the table by the API but a Seq-id can be retrieved using `ShoundSeqIdFromGi` given a gi. |
| title | text | Yes | NULL | a brief description of the sequence | Chain A, Protease Inhibitor Domain Of Alzheimer's Amyloid Beta-Protein Precursor (APPI) | FillACCDB calls CreateDefline. | |

Notes

1.

A complete list of db names that may appear in this column is listed under API supplementary material at *http://www.blueprint.org/seqhound/apisupplement.html*. Some common db name abbreviations are listed below.

gb means GenBank
embl means EMBL
pir means Protein Information Resource (PIR)
sp means Swiss-Prot
pbs means other database
ref means RefSeq
dbj means DNA Database of Japan (DDBJ)
prf means PRF
pdb means Protein Data Bank (PDB)
tpe means third party annotation from embl

tpg means third party annotation from genbank
tpd means third party annotation from ddbj
other means some other database

2.
WriteAccdb.
For all db's except PDB and 'other':
Bioseq->Seq-id->Textseq-id->name
For PDB sequences:
Bioseq->Seq-id->PDB->seq-id->PDB-mol-id (4 characters)
For other databases:
Bioseq->Seq-id->Dbtag->Object-id->string or integer

3.
`FillACCDB`, given a Bioseq pointer, retrieves a Seq-id pointer. If the Seq-id is of the type, pdb (protein data bank), then a PDB-seq-id ptr is passed to `WriteACCDB` which retrieves the value of rel. If the Seq-id is of the type, genbank, embl, pir, swissprot, other, ddbj, prf, tpg, tpd or tpe then a Textseq-id pointer is passed to `WriteACCDB` which retrieves the value of release. If the Seq-id is of the type, giimport then a Giimport-id ptr is passed to `WriteACCDB` which retrieves the value of release. In all cases, the formatting of the date is attempted with NCBI's function `DatePrint` (like this 07-OCT-2004). If the Formatting cannot be done, then the string is just copied.
Bioseq->Seq-id->Textseq-id->release (an INTEGER) for all databases besides PDB, Giimport and 'other'
Bioseq->Seq-id->PDB->seq-id->rel (a string or an NCBI data type) for PDB sequences
Bioseq->Seq-id->Giimport-id->release (a string) for Giimport
n/a for all 'other' databases.

4.
`FillACCDB`, given a Bioseq pointer, retrieves a Seq-id pointer. If the Seq-id is of the type, genbank, embl, pir, swissprot, other, ddbj, prf, tpg, tpd or tpe then a Textseq-id pointer is passed to `WriteACCDB` which retrieves the value of version. For all other databases, this value is n/a. See

5.
Sequences that are part of structures will have a PDB identifier. Since there may be more than one chain (sequence) in a structure, the PDB identifier must be accompanied by a chain identifier to uniquely identifiy a chain within the structure. A PDB identifier supplemented with a chain identifier will be associated with a single sequence record (GI). For example, see PDB id "9XIM" and chain A; this corresponds to GI sequence 443580. See example ASN.1 record for 9XIM_A in the Appendix.
Chain in the ASN.1 annotation is of type character, not of type string so it appears in its decimal form. So 65 is A and so on.

accdb indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | gi<br>db<br>access |
| iaccdb_rowid | INDEX | rowid |
| iaccdb_ts | INDEX | ts |
| iaccdb_gi | INDEX | gi |
| iaccdb_db | INDEX | db |
| iaccdb_name | INDEX | name |
| iaccdb_namelow | INDEX | namelow |
| iaccdb_acc | INDEX | access |

**histdb table**

Last updated April 11, 2005

**Database:** seqhound

**Table:** histdb

**Module:** hist

**Definition:** A history table of gis. Includes the date and any action taken on them.

**Observation:** As of release 4.0, histdb is no longer populated by the histparser and update. Instead, mother populates this table, both during the initial build and the update. During the initial build, gi-accession number pairs, the version number, filename and date are stored in histdb with an action ACTION_ADDED.

During updates, mother extracts the gi-accession number pairs from ACCDB. If neither the gi nor the accession are found, then this is a new record (ACTION_ADDED). If the accession is found in SeqHound but is associated with a different gi, then the record represents a changed record (ACTION_CHANGED), and if the gi-accession pair is present in SeqHound, then the record represents a deleted record (ACTION_KILLED). The gi, accession, action along with the version, filename and date (current date update executed) are logged in histdb. Gi's with ACTION_ADDED will get added to accdb, nucprot, taxgi, pubseq, sengi, sendb, parti by mother. Gi's with ACTION_CHANGED will be deleted and the new updated information will be added to the core databases. For gi's with ACTION_KILLED, the old record information in the core databases is now obsolete and will be deleted from the core databases and the new information will be added to the databases . For any gi that is killed, there will be another gi (with the same accession) that is added.

histdb table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| rowid | int(11) | No | | MySQL autoincrement column. | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 12:32:16 | | |
| gi | int(11) | No | 0 | GenInfo Identifier | 21676275 | GetGi is called by ToBioseqUp in the initial build and by ToBioseqUp in updates. See: Bioseq-->Seqid->id (choice 12) | |
| oldgi | int(11) | Yes | NULL | The gi previously associated with this accession. Not used during the initial build. | 10954454 | ToBioseqUp retrieves the gi from ACCDB using GetACCDBRecord. | |
| access | char(20) | No | | The genbank accession from ACCDB for the gi. If the accession is 'n/a', then the 'name' is written here. See details in accdb table description. | NC_001911 | ToBioseqUp retrieves the accession or name from ACCDB using GetACCDBRecord. | |
| version | int(11) | Yes | NULL | Version of the record. See details in accdb table description. | 1 | ToBioseq and ToBioseqUp call GetSeqIdInfoFromBioseq. See Bioseq->Seq-id->Textseq-id->version. | |
| date | date | No | 0000-00-00 | current date when histdb is updated in the form (YYYYMMDD) | 20040128 | Mother uses the current date. | |
| action | int(11) | No | 0 | the action taken on the record: ACTION_ADDED, ACTION_KILLED, ACTION_CHANGED | ACTION_CHANGED | ToBioseq and ToBioseqUp calls LogHistory. | |
| filename | Varchar(80) | No | | The name of the file that contains this gi for debugging purposes. | rsnc0311.bna | Main passes this to ToBioseq and ToBioseqUp. | |

histdb indices

| Keyname | Type | Field |
|---|---|---|
| ihistdb_rowid | INDEX | rowid |
| ihistdb_ts | INDEX | ts |
| ihistdb_gi | INDEX | gi |
| ihistdb_date | INDEX | date |
| ihistdb_action | INDEX | action |
| ihistdb_acc | INDEX | access |
| ihistdb_filename | INDEX | filename |
| ihistdb_oldgi | INDEX | oldgi |

**pubseq table**

Last updated April 11, 2005

**Database:** seqhound

**Table:** pubseq

**Definition:** This database maps a geninfo identifier to the medline/pubmed article(s) found in the sequence record indicating who first published the sequence.

pubseq table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| rowid | int(11) | No | | MySQL autoincrement column. | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 12:32:16 | | ts |
| gi | int(11) | No | 0 | GenInfo Identifier | 25992759 | ToBioseq calls GetGi. See Bioseq-->Seqid (choice 12) | SHoundGiFromReferenceID<br>SHoundGiFromReferenceList |
| muid | int(11) | No | 0 | Medline identifier found in this record (points to same article as pmid (if listed)). | 99091706 | FillPUBSEQ calls GetMuid. See Seq-entry->Bioseq->Seqdescr->Pubdesc->Pub-equiv->Pub->muid (choice 4) | SHoundGetReferenceIDFromGi<br>SHoundGetReferenceIDFromGiList<br>SHoundMuidFrom3D<br>SHoundMuidFrom3Dlist<br>(ShoundMuidFromGi)<br>(ShoundMuidFromGiList) |
| pmid | int(11) | No | 0 | Pubmed identifier found in this record (points to same article as muid (if listed)) | 9873079 | FillPUBSEQ calls GetMuid. See Seq-entry->Bioseq->Seqdescr->Pubdesc->Pub-equiv->Pub->pmid (choice 13) | |

pubseq indices

| **Keyname** | **Type** | **Field** |
|---|---|---|
| PRIMARY | PRIMARY | gi<br>pmid |
| ipubseq_rowid | INDEX | rowid |
| ipubseq_ts | INDEX | ts |
| ipubseq_gi | INDEX | gi |
| ipubseq_muid | INDEX | muid |
| ipubseq_pmid | INDEX | pmid |

**taxgi table**

Last updated April 11, 2005

| | |
|---|---|
| **Database:** | seqhound |
| **Table:** | taxgi |
| **Module:** | core |
| **Definition:** | This table associates a gi with a taxon identifier. |
| **Observation.:** | Gis are stored in taxgi even if they are not associated with any taxonomy id. This occurs, for example, for some patent gis. |

taxgi table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| rowid | int(11) | No | | MySQL autoincrement colulmn. | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 16:50:42 | | |
| gi | int(11) | No | 0 | GenInfo Identifier | 42565179 | WriteTAXGI calls GetGi.<br>See Bioseq-->Seq-id (choice 12) | SHoundDNAFromTaxID()<br>SHoundDNAFromTaxIDList()<br>SHoundProteinsFromTaxID()<br>SHoundProteinsFromTaxIDList()<br>SHoundProteinsFromChromosome()<br>SHoundProteinsFromChromosomeList()<br>SHoundDNAFromChromosome()<br>SHoundDNAFromChromosomeList() |
| taxid | int(11) | No | 0 | Taxonomy Identifier from NCBI's taxonomy database. | 3702 | See note 1 below. | SHoundTaxIDFromGi()<br>SHoundTaxIDFromGiList() |
| kloodge | int(11) | Yes | NULL | Blueprint chromosome id from the chrom table. | 392 | See note 2 below. | |
| type | varchar(50) | Yes | NULL | Type of macromolecule DNA, RNA, protein, NA, other, "not specified". | protein | WriteTaxgi calls GetType. See Bioseq->mol (see note 3 below). | SHoundDNAFromChromosome()<br>SHoundDNAFromChromosomeList()<br>SHoundProteinsFromChromosome()<br>ShoundProteinsFromChromosomeList() |

Notes:

1.

FillTAXGI calls GetTaxId. See Bioseq-->Seq-desc->BioSource->Org-ref->Dbtag.db == "taxon"
Bioseq-->Seq-desc->BioSource->Org-ref->Dbtag.tag

2.

Mother: ToBioseq calls SearchCHROMByChromNum.
Postcomgen: GetAllRecordsFromGICHROMID and UpdateTaxgiWithKloodge

3.
DNA = 1
RNA = 2
Protein = 3
NA = 4
Other = 255

taxgi indices

| **Keyname** | **Type** | **Field** |
|---|---|---|
| PRIMARY | PRIMARY | gi |
| itaxgi_rowid | INDEX | rowid |
| itaxgi_ts | INDEX | timestamp |
| itaxgi_gi | INDEX | gi |
| itaxgi_taxid | INDEX | taxid |
| itaxgi_kl | INDEX | kloodge |
| itaxgi_type | INDEX | type |

**sengi table**

Last updated April 11, 2005

**Database:** seqhound

**Table:** sengi

**Module:** core

**Definition:** Seqentry to 'gi' conversion.

**Observation:** Seqhound keeps track of which Bioseqs come from which Bioseq-sets using the sengi table. In the sengi table, each Bioseq is represented by a GI (a unique identifier for the sequence record) and each Bioseq-set is represented by the first GI in the set of sequences, the seid.

Sengi also stores the division for historical purposes.

sengi table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| rowid | int(10) | No | | MySQL autoincrement column | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 12:32:16 | | |
| gi | int(11) | No | 0 | GenInfo Identifier | 2313082 | ToBioseqSEQENTRY calls GetGi. See Seq-entry->Bioseq-set->Bioseq-->Seqid (choice 12) | |
| seid | int(11) | No | 0 | GenInfo Identifier: the first one in the bioseq-set. seid means seqentry id. | 231308 | ToBioseq calls GetGi for the first Bioseq in a SeqEntry See Seq-entry->Bioseq-set->Bioseq-->Seqid (choice 12). | |
| division | char(15) | Yes | NULL | Genbank division. | PRI | ToBioseqSEQENTRY calls GetDivisionFromPARTI. | |

sengi indices

| **Keyname** | **Type** | **Field** |
|---|---|---|
| PRIMARY | PRIMARY | gi |
| isengi_rowid | INDEX | rowid |
| isengi_ts | INDEX | ts |
| isengi_gi | INDEX | gi |
| isengi_seid | INDEX | seid |

**sendb table**

Last updated April 11, 2005

**Database:** seqhound

**Table:** sendb

**Module:** core

**Definition:** SeqEntry Data Base

**Observation:** Sequences are distributed by GenBank in packages. Each package is referred to as a seq-entry.

A seq-entry may contain either a single sequence record (called a Bioseq) or a set of sequence records (called a Bioseq-set). If a Seq-entry contains a Bioseq-set then that Bioseq-set contains a list of Seq-entry packages (yes, this data structure is recursive). Each of these Seq-entry packages contains a single sequence record (a Bioseq). There is annotation that is associated with single sequence records (Bioseqs). An example of annotation is a list of authors who are responsible for submitting a sequence record. There is also annotation associated with sets of sequence records (Bioseq-sets). This type of annotation applies to all of the sequence records that are in the set. For example a set of authors may be responsible for all of the sequence records in the set.

Seqhound stores Bioseqs and their associated GenInfo id's in one central table (called asndb). Since each of these Bioseqs may have come from a Bioseq-set, Seqhound needs a way to store the Bioseq-set associated annotation (that applies to each of the Bioseqs in the set). To accomplish this, Seqhound takes the Bioseq-set, removes the Bioseqs that it contains, and stores the remainder of the Bioseq-set (annotation) in the sendb table. Seqhound keeps track of which Bioseqs come from which Bioseq-sets using the sengi table. In the sengi table, each Bioseq is represented by a GI (a unique identifier for the sequence record) and each Bioseq-set is represented by the first GI in the set of sequences (the seid).

sendb table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| rowid | int(10) | No | | Auto number row identifier | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 12:32:16 | | |
| seid | int(11) | No | 0 | Gene Info identifier for the first bioseq in the SeqEntry. | 2313082 | ToBioseq calls GetGi for the first Bioseq in a SeqEntry. Main calls AppendRecordSENDB. See Seq-entry->Bioseq-set->Seq-entry->Bioseq->Seqid (choice 12) | |
| asn1 | mediumblob | No | | ASN1 Binary SeqEntry. Note that the bioseqs themselves have been removed to save space. | binary data | ToBioseqSeqEntry removes the bioseqs. Main calls AppendRecordSENDB. | These functions return the Seqentry or BioseqSet stored in this field after first replacing all of the Bioseqs that belong in it.<br><br>`SHoundGetBioseqSet()`<br>`SHoundGetSeqEntry()` |

sendb indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | seid |
| isendb_rowid | INDEX | rowid |
| isendb_ts | INDEX | ts |
| isendb_seid | INDEX | seid |

**chrom table**

**Database:** seqhound

**Table:** chrom

**Module:** core

**Definition:** This table maps taxonomy ids with their complete genome information (chromid, chromflag, accession, and name)

**Observation:** This table keeps track of all completely sequenced chromosomes of a particular organism (**taxid**). We also store the NCBI chromid (**chromid**), the type of sequence (**chromflag**), the name (**name**) and accession number (**access**).

Every chromid will have a corresponding **kloodge** identifier (this is Blueprint's internal version of the NCBI chromid. In addition, every taxon will have one kloodge identifier that has no corresponding chromid. This kloodge id is assigned to any proteins or RNAs that are have no chromid; i.e. they have not been assigned to a chromosome yet. The kloodge is the value of an autoincrement column and is written to taxgi by postcomgen.

We also store the chromosome number (**chromnum**) as text. This is used so that we can assign records which have no complete genome information other than taxid and chromosome number to a chromosome identifier.

For example, let's say that chromosome 4 (circular plasmid, named chr_4, access XIV) of species "species X" (taxid 123) is completely sequenced and that NCBI has assigned this chromosome a chromid of 191. Let us say our internal kloodge id for this same chromosome is 1254. Then a record is added to the chrom table with fields:

```
kloodge: 1254
taxid: 123
chromid: 191
chromflag: plasmid
accession: XIV
name: species X chr_4
chromnum: chr 4
```

See more example entries in the notes section below.

chrom table

| Field | Type | Null | Default | Column_Definition | Example[1] | Source | API |
|---|---|---|---|---|---|---|---|
| kloodge | int(11) | No | | Blueprint chromosome id (used internally). Mysql Autoincrement column. | 568 | | |
| ts | timestamp | No | CURRENT_TIMESTAMP | | 2005-03-23 16:17:11 | | |
| taxid | int(11) | No | 0 | Taxonomy identifier | 9606 | ToBioseq calls GetTaxid See Bioseq-->Seq-desc->BioSource->Org-ref->Dbtag->tag | SHoundAllGenomes |
| chromid | int(11) | No | 0 | NCBI chromsome identifier (see note 2 below) | 1 | ToBioseq calls GetChromIdFromBioseq. See Bioseq->SeqId->Dbtag->tag | |
| chromflag | int(11) | No | 0 | the type of chromosome (chromosome, plasmid, mitochrondria etc) defined as byte macros in intrez.h. (see note 3 below) | 1 | ToBioseq calls GetGenomeInfo, See Bioseq->descr->source->subtype->subtype | SHoundChromosomeFromGenome |
| access | varchar(20) | No | NULL | Accession for the sequence (see note 2 below). | NC_000001 | GetGenomeInfo calls Misc_GetAccession. See Bioseq->Seq-id->Textseq-id->accession | |
| name | text | No | | The scientific name of the organism with the chromosome name. | Homo sapiens Chromosome 1 | GetGenomeFromBiosource constructs this from various places in the Biosource. See Bioseq->descr->source | |
| chromnum | varchar(10) | Yes | NULL | Chromosome number as text. | 1 | GetGenomeFromBiosource constructs this from various places in the Biosource subtype. See Bioseq->descr->source->subtype | |

Notes.
1.
Example entries from the chrom table.

| kloodge | ts | taxid | chromid | chromflag | access | name | chromnum |
|---|---|---|---|---|---|---|---|
| 1 | '2005-03-23 12:33:24' | 9 | 13723 | 9 | 'NC_001911' | 'Buchnera aphidicola Plasmid pLeu-Dn' | 'pLeu-Dn' |
| 2 | '2005-03-23 12:33:24' | 9 | 17119 | 9 | 'NC_004843' | 'Buchnera aphidicola Plasmid pBPS1' | 'pBPS1' |
| 567 | '2005-03-23 16:06:41' | 9606 | -9606 | 1 | | 'Homo sapiens Chromosome Un' | 'Un' |
| 568 | '2005-03-23 16:17:11' | 9606 | 1 | 1 | 'NC_000001' | 'Homo sapiens Chromosome 1' | '1' |
| 569 | '2005-03-23 16:17:12' | 9606 | 2 | 1 | 'NC_000002' | 'Homo sapiens Chromosome 2' | '2' |
| 570 | '2005-03-23 16:17:12' | 9606 | 3 | 1 | 'NC_000003' | 'Homo sapiens Chromosome 3' | '3' |
| 592 | '2005-03-23 16:35:05' | 9606 | 2000021 | 5 | 'AC_000021' | 'Homo sapiens Mitochondria' | |
| 4289 | '2005-04-05 09:29:55' | 287944 | 18301 | 5 | 'NC_006916' | 'Harpiosquilla harpax Mitochondria' | |
| 4290 | '2005-04-05 09:29:55' | 302098 | 18316 | 5 | 'NC_006931' | 'Eubalaena japonica Mitochondria' | |

Note that the third entry down represents an entry corresponding to an “unknown” chromosome. Proteins or RNAs that have not been mapped to a chromosome will be assigned this kloodge identifier (567) in the accdb and table.

2.
Kloodge identifiers representing unknown chromosmomes will not have a corresponding chromid from NCBI. The negative value of the taxid is used instead. See third entry in example table above. These entries will also have no accession associated with them.

notes continued…

3.
CHROM_PHAGE (phage sequence)
CHROM_NR
CHROM_ECE
CHROM_PLMD (plasmid sequence)
CHROM_CHLO (chloroplast sequence)
CHROM_MITO (mitochrondrial sequence)
CHROM_CHROM (chromosome sequence)
CHROM_ALL

chrom indices

| **Keyname** | **Type** | **Field** |
|---|---|---|
| PRIMARY | PRIMARY | kloodge |
| ichrom_chromid | INDEX | chromid |
| ichrom_taxid | INDEX | taxid , chromnum |
| ichrom_kl | INDEX | kloodge |
| ichrom_acc | INDEX | access |
| Ichrom_chromnum | INDEX | chromnum |

**gichromid table**

Last updated April 11, 2005

**Database:** SeqHound

**Table:** gichromid

**Module:** core

**Definition:** Stores RNA and protein gis that are part of a complete genome. Used to update taxgi with the kloodge.

**Observation:** This table is used internally to store RNA and Protein gis parsed from contigs that are part of a complete genome. After a complete build is done, the gis and chromids from this table are used by postcomgen to update taxgi with the kloodge.

gichromid table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Primary key. Mysql auto-increment column. | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 12:32:16 | | |
| gi | int(11) | No | 0 | Gene Info identifier | 231308 | ToBioseq calls FillGiChromid. See Bioseq-->Seqid (choice 12) | |
| chromid | int(11) | No | 0 | NCBI chromosome id | 3144 | NCBI chromid | |
| contiggi | int(11) | Yes | NULL | Gi of the contig that contains this gi. | 231308 | ToBioseq calls GetChromidFromBioseq. See Bioseq->Seqid(choice 11)->tag->id | |

gichromid indices

| Keyname | Type | Field |
|---|---|---|

| | | |
|---|---|---|
| id | PRIMARY | gi |
| gi | INDEX | gi |
| igits | INDEX | ts |
| igichromid | INDEX | chromid |
| igicontiggi | INDEX | contiggi |

**contigchromid table**

Last updated April 11, 2005

**Database:** SeqHound

**Table:** contigchromid

**Module:** core

**Definition:** Stores contig gis that are part of a complete genome. Used to update taxgi with the kloodge.

**Observation:** This table is used internally to store lists of GI's that make up a contig sequence for a complete genome. After a complete build is done, the gis and chromids from these contigs are used by postcomgen to update taxgi with the kloodge.

contigchromid table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Mysql auto-increment column. | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 12:32:16 | | |
| contiggi | int(11) | No | 0 | Gene Info identifier for this sequence record that is part of a contig. | 50754263 | ToBioseq calls GetGi. See Bioseq-->Seqid (choice 12) | |
| topgi | int(11) | Yes | NULL | Genbank gi of the contig that contains multiple sequences (i.e. multiple contiggi's). | 51039201 | ToBioseq calls GetGi. See Bioseq-->Seqid (choice 12) | |
| chromid | int(11) | No | 0 | NCBI chromosome id. | 461 | ToBioseq calls GetChromidFromBioseq. See Bioseq->Seqid(choice 11)->tag->id | |
| changed | Int(11) | Yes | NULL | Indicates whether the record needs to be processed by postcomgen. Used by mother in update mode. | 1 = process<br>2 = do not process | ToBioseq calls FillContigChromid. See Bioseq->Seqid(choice 11)->tag->id | |

contigchromid indices

| Keyname | Type | Field |
|---|---|---|
| contiggi | PRIMARY | id |
| icontigts | INDEX | ts |
| contigi | UNIQUE | contiggi |
| iccontigi | INDEX | contiggi |
| ictopgi | INDEX | topgi |

**gichromosome table**

Last updated April 11, 2005

**Database:** SeqHound

**Table:** gichromosome

**Module:** core

**Definition:** Stores RNA and protein gis that have a chromosome name, but no other complete genome info.

**Observation:** This table is used internally to store RNA and protein gis that have a chromosome name, but no other complete genome info. After a complete build is done, postcomgen will write these gis to gichromid with the appropriate chromid.

gichromosome table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Primary key Mysql auto-increment column. | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 12:32:16 | | |
| gi | int(11) | No | 0 | GenInfo Identifier | 231308 | ToBioseq calls GetGi. See Bioseq-->Seqid (choice 12) | |
| chromnum | varchar(10) | No | | Chromosome number | 1 | ToBioseq calls GetGenomeInfo. See Bioseq->descr->source->subtype->name | |

gichromosome indices

| Keyname | Type | Field |
|---|---|---|
| id | PRIMARY | id |
| igichrom_ts | INDEX | ts |
| gi | UNIQUE | gi |
| igichrom_gi | INDEX | gi |
| igichrom_num | INDEX | chromnum |

**contigchromosome table**

Last updated April 11, 2005

**Database:** SeqHound

**Table:** gichromosome

**Module:** core

**Definition:** Stores contig gis that have a chromosome name, but no other complete genome info.

**Observation:** This table is used internally to store contig gis that have a chromosome name, but no other complete genome info. After a complete build is done, postcomgen will writethese gis to contigchromid with the appropriate chromid.

contigchromosome table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Primary key Mysql auto-increment column. | | | |
| ts | timestamp | Yes | CURRENT_TIMESTAMP | MySQL timestamp column | 2005-03-23 12:32:16 | | |
| contiggi | int(11) | No | | GenInfo gi | 231308 | ToBioseq calls GetGi. See Bioseq-->Seqid (choice 12) | |
| chromnum | Varchar(10) | No | | Chromosome number | 1 | ToBioseq calls GetGenomeInfo. See Bioseq-->Seqid (choice 12) | |

contigchromosome indices

| **Keyname** | **Type** | **Field** |
|---|---|---|
| id | PRIMARY | id |
| igichrom_ts | INDEX | ts |
| contiggi | UNIQUE | contiggi |
| icontigchrom_gi | INDEX | contiggi |
| icontigchrom_num | INDEX | chromnum |

**Redundant protein sequences (redundb) module**

Last updated: August 4, 2004

**redund parser**

**purpose:**

The redund parser builds the redundb module, which consists of the redund table. The input file consists of information pertaining to redundant GIs, accession numbers and the sequence information which the GIs refer to. The resulting data table contain information on the GIs, redundant GI groups and the ranking of each GI within their redundant group.

**module:**

redundb

**input files:**

*nr.gz* from *ftp://ftp.ncbi.nih.gov/blast/db/FASTA/*

**table created:**

redund

**source code location:**

*slri/seqhound/parsers/redund.c*

**config file dependencies:**

*slri/seqhound/config/.intrezrc* (UNIX platform)

The relevant section of the configuration file is:

```
[datab]
;seqhound database that you are connecting
username=your_user_name
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=

 [sections]
```

```
;this should be set to 1 to allow usuage of the redundb

;redundant protein sequences
redundb = 1
```

Text in ***italics*** must be changed for the *.intrezrc* file to function correctly with your SeqHound set-up. Variables `username`, `password`, `dsn`, `database` in section `[datab]` should have the same values as `USER`, `PASSWORD`, `DSN` and `DATABASE` respectively in your *.odbc.ini* (see Step 10 in section 4.4.) In section `[sections]` redundb should be `1`.

**commandline parameters**

Typing **`./redund`** at the command line will return a list of command line parameters and default settings. For example:

```
>./redund
redund   arguments:
  -i  Input non-redundant database fasta file [File In]
  -n  Initialize database file [T/F]  Optional
    default = F
```

example use:

```
./redund -i nr -n T
```

**associated scripts:**

*nrftp.pl*: retrieves the relevant data file from NCBI's ftp site

**error & run-time logs:**

redund writes to a log file called *redundlog*

**additional information:**

*ftp://ftp.ncbi.nih.gov/blast/db/FASTA/*

See data table descriptions for each of the tables that are listed under “tables altered”

**redund table**

Last updated: August 4, 2004

**Database:** seqhound
**Table:** redund
**Module:** redundb
**Definition:** Partitions GIs into groups based on sequence redundancy, and ranks each GI within their group.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto number row identifier |
| gi | int(11) | No | 0 | GenInfo Identifier |
| rordinal | int(11) | No | 0 | Position in redundant group |
| rgroup | int(11) | Yes | NULL | ID of redundant group(not static) |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | gi |
| iredund_rowid | INDEX | rowid |
| iredund_gi | INDEX | gi |
| iredund_ordinal | INDEX | rordinal |
| iredund_rgroup | INDEX | rgroup |

**Observation:** redund is a database table that places GIs with equivalent sequences into redundant groups. The same sequence may be worked on by independent researchers. Each discovery is submitted and assigned a different gi. When the discoveries concern a common sequence, the GIs point to sequence records that describe redundant sequences, i.e. a single sequence has multiple GIs. These GIs then belong to a common group (rgroup). In such cases, it is common for one particular GI to be used more than the others because it is better annotated. The ordinal (rordinal) is a ranking of the GIs, 1 for the best annotated GI, 2 for the second, 3 for the third etc. This ordering is determined by the ordering of the sequence headers in the nr source file. These 3 pieces of information form the redund database table.
**Source org:** NCBI
**Source file:** *nr.gz* from *ftp://ftp.ncbi.nih.gov/blast/db/FASTA/nr.gz*
**parser:** redund

*****gi*****
**description:** GenInfo Identifier for a sequence record.
**example:** 7228451
**default value:** 0
**source:** parsed from nr (line 1 of record) as token(|) delimited fields
**parser:** redund
**function:** `LabelGI`, `AssignRedund` (*redund.c*)

**API:** `SHoundRedundantGroup` (returns all GIs in the same group as the input GI)
`SHoundRedundantGroupFromID` (returns GIs from the group with input group ID)
`SHoundFirstOfRedundantGroupFromID` (GI of rank 1, given a group)
`SHoundIsNRFirst` (true/false, is this GI is ranked 1 in it's group)

*****rordinal*****
**description:** rank position in redundant set
**example:** 1
**default value:** n/a
**source:** based on the position of the gi within the record, the first gi has rordinal 1, the 2nd has ordinal 2
**parser:** redund
**function:** `LabelGI`, `AssignRedund` (*redund.c*)
**API:** `SHoundIsNRFirst` (tells if a gi has rordinal = 1)

*****rgroup*****
**description:** redundant group the gi is a member of
**example:** 1
**default value:** n/a
**source:** rgroup IDs are assigned to GIs as the input file is parsed. Each GI encountered is assigned the rgroup ID of those GIs already encountered which have an identical sequence. If no such GIs have been encountered, the GI is assigned a new rgroup ID one number higher than the largest current rgroup ID in the database. The first GI encountered is given an rgroup ID of 1.
**parser:** redund

**function:** `LabelGI, AssignRedund` (*redund.c*)
**API:** `SHoundRedundantGroupIDFromGI`[List] (returns the ID of the rgroup that the input GI is a part of)

**Complete genomes tracking (gendb) module**

As of release 4.0 of SeqHound, the complete genomes module has been moved into the core module. The initial build and updates to these tables are handled by the mother and postcomgen parsers. See the description of the core module above for more details.

**Taxonomy hierarchy (taxdb) module**

Last **updated** August 18, 2004

**importtaxdb parser**

**purpose:**

The importtaxdb parser builds the taxonomy module, which consist of the taxdb, gcodedb, divdb, del and merge table. The input file consists of taxonomic information such as the taxonomy nodes, names, division, genetic codes, deleted nodes and merged nodes. Table taxdb holds taxonomy ids and a binary file associated with each id. Table gcodedb holds genetic code ids and a binary file associated with each id. Table divdb holds division ids and a binary file associated with each id. Table del holds the taxonomy id of the deleted nodes. Table merge holds the taxonomy ids of nodes which has been merged and which is result of merging.

**module:**

taxdb

**input files:**

*taxdump.tar.gz* from *ftp://ftp.ncbi.nih.gov/pub/taxonomy/*

**tables created:**

taxdb

gcodedb

divdb

del

merge

**source code location:**

*slri/seqhound/taxon/importtaxdb.c*

**config file dependencies:**

*slri/seqhound/config/.intrezrc* (UNIX platform)

The relevant section of the configuration file is:

```
[datab]
;seqhound database that you are connecting
username=your_user_name
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=


 [sections]
;taxonomy hierarchy
taxdb = 1
```

Text in ***italics*** must be changed for the *.intrezrc* file to function correctly with your SeqHound set-up. Variables `username`, `password`, `dsn`, `database` in section `[datab]` should have the same values as `USER`, `PASSWORD`, `DSN` and `DATABASE` respectively in your *.odbc.ini* (see Step 10 in section 4.4.) In section `[sections]` `taxdb` should be `1`.

**commandline parameters**

There are no command line parameters. Typing **`./importtaxdb`** will run the program:

example use:

```
./importtaxdb
```

**associated scripts:**

*taxftp.pl*: retrieves the relevant data file from NCBI's ftp site

**error & run-time logs:**

importtaxdb writes to a log file called *importtaxdb_log.txt*

**additional information:**

readme files at *ftp://ftp.ncbi.nih.gov/pub/taxnomy/*

See data table descriptions for each of the tables that are listed under “tables altered”

**taxdb table**

**Database:** seqhound

**Table:** taxdb

**Module:** taxdb

**Definition:** Maps a taxid to information about the taxid. The information about the taxid is stored as an ASN blob.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto number row identifier |
| tid | int(11) | No | 0 | Taxonomy identifier |
| asn | mediumblob | Yes | NULL | Information about tid |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | tid |
| itax_rowid | INDEX | rowid |
| itax_tid | INDEX | tid |

**Observation:** The entire taxonomy can be viewed as a hierarchical taxonomy tree. The tree expresses the relationships between the nodes within the tree. At the root of the tree is a generic node that provides no information. Descendents of the root node include superkingdoms such as Archea, Eubacteria, Eukaryota, Viroids, Viruses. etc. Each of these superkingdoms have corresponding taxonomy children. Also included in the taxonomy tree are artificial sequences and unclassified taxonomies such as the prions, unidentified agents, etc. taxdb maps the taxonomy identifiers to the relevant information describing the taxonomies. Organizing the taxonomy as a tree allows users to request

complete lineages, ancestors, children and permits the user to browse the tree exploiting its tree structure.
taxdb contains information from both *nodes.dmp* and *names.dmp*

**Source org:** NCBI

**Source files:** *nodes.dmp* from *ftp://ftp.ncbi.nih.gov/pub/taxonomy/taxdump.tar.gz*
*names.dmp* from *ftp://ftp.ncbi.nih.gov/pub/taxonomy/taxdump.tar.gz*

**parser:** importtaxdb

*****tid*****

**description:** the unique taxonomy identifier.

**example:** 9606 (Human)

**default value:** n/a

**source:** *nodes.dmp*: column 1

**parser:** importtaxdb

**function:** `Parser_TaxDBNodeRecord`

**API:**
```
SHoundGetTaxChildNodes
SHoundGetTaxChildNodesList
SHoundGetAllTaxProgeny
SHoundGetTaxParent
ShoundGetAllTaxAncestors
```

Note that although relationships (parent, child) are not stored in the database, it is a part of the asn field, and as such it makes it possible to retrieve parent, children, ancestors and lineages (see asn blob).

*****asn*****

**description:** ASN blob containing information about the taxonomy.
Fields in the ASN blob include:
1) parent taxonomy of node
2) rank of node
3) embl code for node
4) division of node (see divdb)
5) inherited div flag (1 if this node inherits its division from its parent)
6) genetic code (see gcodedb)
7) inherited genetic code (1 if this nodes inherits its genetic code from parent)
8) mitochondrial genetic code
9) inherited mit. genetic code (1 if nodes inherits mitochondrial gencode from parent)
10) genbank hidden flag (1 if name is suppressed in GenBank entry lineage)
11) subtree root flag (1 if this subtree has no sequence data yet)
12) comments
13) name of taxid (from *names.dmp*)
Possible rankings of node (there may be more):
superkingdom, kingdom
genus, subgenus
subspecies, species
subfamily, family, superfamily
phylum, subphylum,
subtribe, tribe
varietas

infraorder, order, suborder
infraclass, class, subclass
no rank

**example:** A textual representation of the blob for taxid 9606:

```
SLRI-taxon ::= {
   taxId 9606 ,
   parent-taxId 9605 ,
   children-taxId {
     63221 } ,
   names {
     {
       name "Homo sapiens" ,
       name-class scientific-name } ,
     {
       name "human" ,
       name-class other ,
       other-class "genbank common name" } ,
     {
       name "man" ,
       name-class common-name } } ,
     rank {
     rank species ,
     premod none ,
     postmod none } ,
   embl-code "HS" ,
   division 5 ,
   inherited-div TRUE ,
   gencode 1 ,
   inherited-gencode TRUE ,
   mito-gencode 2 ,
   inherited-mito-gencode TRUE ,
   genbank-hidden FALSE ,
   hidden-subtree-root FALSE }
```

**default value:** n/a

**source:** *nodes.dmp*: column 2 - 13 and *names.dmp*: column 2, 3

**parser:** importtaxdb

**function:** `Parser_TaxDBNodeRecord`

**API:** The ASN object is not directly accessible through the API. Instead,

fields in the ASN object may be retrieved and be accessible from the API. eg.

`SHoundGetTaxNameFromTaxIDByClass`
`SHoundGetTaxNameFromTaxID`
`SHoundGetTaxLineageFromTaxID`

You can also directly retrieve the ASN SLRITaxon by:

```
#include <taxdb_db.h>
AsnIoPtr aip  = NULL;
SLRITaxonPtr ptax = NULL;
SHoundInit(FALSE, "name");
ptax = DB_GetTaxRec(9606);
aip = AsnIoNex(ASNIO_TEXT_OUT, stdout, NULL, NULL, NULL);
SLRITaxonAsnWrite(ptax, aip, NULL);
AsnIoClose(aip);
```

This will produce the text in the example above.

**gcodedb table**

**database:** seqhound

**table:** gcodedb

**Module:** taxdb

**definition:** Maps a genetic code identifier to the corresponding ASN taxonomy genecode record.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto number row identifier |
| gcid | int(11) | No | 0 | genetic code |
| asn | mediumblob | Yes | NULL | ASN taxon-gencode record |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | gcid |
| igcode_rowid | INDEX | rowid |
| igcode_gcid | INDEX | gcid |

**Observation:** gcodedb is part of a group of databases (taxdb, gcodedb, divdb) that can be used to form a taxonomy hierarchy tree. In the case of gcode, the records map a genetic code identifier to an ASN object that holds information about that genetic code. taxdb (see taxdb later) will specify the type of genetic material each taxonomy uses, eg if the taxonomy has a plasmid as a genetic code, mitochrondria DNA, or standard chromosomal DNA etc. gcodedb houses information concerning each of the genetic code. Relevant information include the translation table (the mapping of nucleic acid codons to amino acids), & the start codon. Further information at: *http://www.ncbi.nlm.nih.gov/Taxonomy*

**Source org:** NCBI

**Source file:** *gencode.dmp* from *ftp://ftp.ncbi.nih.gov/pub/taxonomy/taxdump.tar.gz*

**Parser:** importtaxdb

*****gcid*****

**description:** The genetic code identifier. The identifiers may not be consecutive because historically codes may have merged or new ones were created. The code and their corresponding names:

0 Unspecified

1 Standard

2 Vertebrate Mitochondrial

3 Yeast Mitochondrial

4 Mold Mitochondrial; Protozoan Mitochondrial; Coelenterate Mitochondrial; Mycoplasma; Spiroplasma

5 Invertebrate Mitochondrial

6 Ciliate Nuclear; Dasycladacean Nuclear; Hexamita Nuclear

9 Echinoderm Mitochondrial; Flatworm Mitochondrial

10 Euplotid Nuclear

11 Bacterial and Plant Plastid

12 Alternative Yeast Nuclear

13 Ascidian Mitochondrial

14 Alternative Flatworm Mitochondrial

15 Blepharisma Macronuclear

16 Chlorophycean Mitochondrial

21 Trematode Mitochondrial

22 Scenedesmus obliquus mitochondrial

23 Thraustochytrium mitochondrial code

**example:** Because many of the taxonomy groups are bacterial, 11 is a common genetic code.

**default value:** n/a

**source:** *gencode.dmp*: column 1

**parser:** importtaxdb

**function:** `Parse_TaxDBGenCodeRecord`

**API:** n/a

*****asn*****

**description:** An ASN blob for the genetic code information corresponding to the genetic code identifiers. The individual fields in the blob are:

1) an optional abbreviation

2) name of genetic code (see gcid for names)

3) translation table

4) start codon

The translation table maps the nucleic acid codon to amino acids:

In the source file, the map is represented as:

```
FFLLSSSSYY**CC*WLLLLPPPPHHQQRRRRIIIMTTTTNNKKSSRRVVVVAAAADDEEGGGG
```

There are 64 characters in this map. Each position in the map corresponds to a codon (see below) and the letter at that position corresponds to the resulting amino acid that will be translated from that codon. The same can map be better expressed as a direct mapping from codon to amino acid where

1) first 3 letters represent a nucleic acid sequence (codon),

2) an amino acid letter identifier

3) an amino acid abbreviation

```
TTT  F Phe      TCT  S Ser      TAT  Y Tyr      TGT  C Cys
TTC  F Phe      TCC  S Ser      TAC  Y Tyr      TGC  C Cys
TTA  L Leu      TCA  S Ser      TAA  * Ter      TGA  * Ter
TTG  L Leu      TCG  S Ser      TAG  * Ter      TGG  W Trp

CTT  L Leu      CCT  P Pro      CAT  H His      CGT  R Arg
CTC  L Leu      CCC  P Pro      CAC  H His      CGC  R Arg
CTA  L Leu      CCA  P Pro      CAA  Q Gln      CGA  R Arg
CTG  L Leu      CCG  P Pro      CAG  Q Gln      CGG  R Arg

ATT  I Ile      ACT  T Thr      AAT  N Asn      AGT  S Ser
ATC  I Ile      ACC  T Thr      AAC  N Asn      AGC  S Ser
ATA  I Ile      ACA  T Thr      AAA  K Lys      AGA  R Arg
ATG  M Met      ACG  T Thr      AAG  K Lys      AGG  R Arg

GTT  V Val      GCT  A Ala      GAT  D Asp      GGT  G Gly
GTC  V Val      GCC  A Ala      GAC  D Asp      GGC  G Gly
GTA  V Val      GCA  A Ala      GAA  E Glu      GGA  G Gly
GTG  V Val      GCG  A Ala      GAG  E Glu      GGG  G Gly
```

The start codon is the particular codon that signals the start of protein translation for that particular genetic molecular (i.e. a standard chromosome starts translation at a different codon than a protozoan mitochrondrial DNA).

The start codon is shown in the same manner as the translation table:

```
----------------------------------MM----------------------------
```

This indicates that M (methionine) is the start codon.

Further information can be found at:
*htpp://www.ncbi.nlm.nih.gov/Taxonomy* in Genetic codes link.

**example:** A textually representation of a blob for genetic code 11:

```
SLRI-taxon-gencode ::= {
   gencode-id 11 ,
   name "Bacterial and Plant Plastid" ,
   trans-table
"FFLLSSSSYY**CC*WLLLLPPPPHHQQRRRRIIIMTTTTNNKKSSRRVVVVAAAADDEEGGG
G " ,
start-codons "---M---------------M------------MMMM--------------
```

```
-M------------ " }
```

**default value:** n/a

**source:** *gencode.dmp*: column 2, 3, 4, 5 are stored in the database as an ASN SLRITaxonGencode structure.

**parser** importtaxdb

**function:** `Parse_TaxDBGenCodeRecord`

**API:** not directly accessible from the API, but you can retrieve the SLRITaxonGencode object using:

```
#include <taxdb_db.h>


AsnIoPtr aip  = NULL;
SLRITaxGencodePtr ptax = NULL;
SHoundInit(FALSE, "name");
ptax = DB_GetTaxGencodeRec(11);
aip = AsnIoNex(ASNIO_TEXT_OUT, stdout, NULL, NULL, NULL);
SLRITaxGencodeAsnWrite(ptax, aip, NULL);
AsnIoClose(aip);
```

This will produce the text in the example above.

**divdb table**

**Database:** seqhound

**Table:** divdb

**Module:** taxdb

**Definition:** Maps taxonomy division ID to an ASN SLRI-taxon-div object

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto number row identifier |
| did | int(11) | No | 0 | Taxonomy Division ID |
| asn | mediumblob | Yes | NULL | ASN taxonomy division record |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | did |
| idiv_rowid | INDEX | rowid |
| idiv_did | INDEX | did |

**Observation:** divdb is part of a group of databases (taxdb, gcodedb, divdb) that can be used to form a taxonomy hierarchy tree. In the case of divdb, the records map a division identifier to an ASN object that holds information about that division. This information include a 3-character GenBank division code, a division name and an optional comment. There are 10 divisions (see below).

**Source org:** NCBI

**Source file:** *division.dmp* from *ftp://ftp.ncbi.nih.gov/pub/taxonomy/taxdump.tar.gz*

**Parser:** importtaxdb

*****did*****

**description:** The division identifier (0-11, see asn for the names of division).

**example:** 0

**source:** *division.dmp*: column 1

**parser:** importtaxdb

**function:** `Parse_TaxDBDivRecord`

**API:** n/a

*****asn*****

**description:** The ASN blob for the taxonomy division. The individual fields in the ASN blob are:
1) a 3 character division code (see below)
2) a division name (see below)
3) an optional comment
Possible division codes and corresponding division names are:
BCT Bacteria
INV Invertebrates
MAM Mammals
PHG Phages
PLN Plants
PRI Primates
ROD Rodents
SYN Synthetic
UNA Unassigned

VRL Viruses
VRT Vertebrates

**example:** the entire field is one ASN blob. A possible blob could be represented textually as:

```
SLRI-taxon-div ::= {
   div-id 1 ,
   div-code "INV" ,
   div-name "Invertebrates" }
```

**source:** Column 2, 3, and 4 of *division.dmp* are stored as one ASN blob (SLRITaxonDiv) created in-house.

**parser:** importtaxdb

**function:** `Parse_TaxDBDivRecord` (importtaxdb)

**API:** there is no API function that allows you to retrieve the entire ASN blob. The information is used to construct information about a taxid, (see taxdb). You can retrieve a TaxonDivRec using:

```
#include <taxdb_db.h>

AsnIoPtr aip  = NULL;
SLRITaxonDivPtr ptax = NULL;
SHoundInit(FALSE, "name");
ptax = DB_GetTaxDivRec(1);
aip = AsnIoNex(ASNIO_TEXT_OUT, stdout, NULL, NULL, NULL);
SLRITaxonDivAsnWrite(ptax, aip, NULL);
AsnIoClose(aip);
```

This will produce the text in the example above.

**del table**

**Database:** seqhound

**Table:** del

**Module:** taxdb

**Definition:** Contains all the deleted taxonomy identifiers.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto number row identifier |
| tid | int(11) | No | 0 | Taxonomy ID |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | tid |
| idel_rowid | INDEX | rowid |
| idel_tid | INDEX | tid |

**Observation:**

**Source org:** NCBI

**Source files:** *delnodes.dmp* from *ftp://ftp.ncbi.nih.gov/pub/taxonomy/taxdump.tar.gz*

**parser:** importtaxdb

***tid***

**description:** The taxonomy identifier

**example:** 15

**default value:** n/a
**source:** column 1 of *delnodes.dmp*
**parser:** importtaxdb
**function:** `main` of importtaxdb
**API:** `SHoundIsTaxDeleted` (true if taxid parameter is deleted)

**merge table**

**Database:** seqhound

**Table:** merge

**Module:** taxdb

**Definition:** Contains all tax nodes that have merged. Maps an old taxid before merging with its new taxid after the merge. A taxonomy may be deleted because initially it was considered species X, but when its DNA is analyzed, it is deemed to be insignificantly different from species Y, in which case one of the species gets merged.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto number row identifier |
| otid | int(11) | No | 0 | old taxonomy id |
| ntid | int(11) | No | 0 | new taxonomy id |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | otid |
| imerge_rowid | INDEX | rowid |
| imerge_ntid | INDEX | ntid |
| imerge_otid | INDEX | otid |

**Observation:**

**Source org:** NCBI

**Source files:** *merged.dmp* from *ftp://ftp.ncbi.nih.gov/pub/taxonomy/taxdump.tar.gz*

**parser:** importtaxdb

*****otid*****

**description:** the old taxid
**example:** 12
**default value:** n/a
**source:** *merged.dmp*: column 1
**parser:** importtaxdb
**function:** `main` of importtaxdb
**API:** `SHoundIsTaxMerged` (takes an old taxid and checks if it has been merged into a new taxid)

*****ntid*****

**description:** the new taxid
**example:** 74109
**default value:** n/a
**source:** *merged.dmp*: column 2
**parser:** importtaxdb
**function:** `main` of importtaxdb
**API:** `SHoundIsTaxMerged` (takes an old taxid and checks if it's been merged into a new taxid)

**Structural databases (strucdb) module**

Last updated October 6, 2004

**cbmmdb parser**

**purpose:**

The cbmmdb parser builds the strucdb module databases. The input files to cbmmdb contain data for experimentally determined macromolecular 3D structures. The data files are in ASN.1 format available from the NCBI ftp site.

**Module:**

Build the Strucdb module

Change to the mmdbdata directory.

```
cd $SEQH/7.mmdb.files
```

Create tables of the Strucdb module in the database.

Make sure file *strucdb.sql* has line `use seqhound` close to the beginning of the file.

```
mysql -u my_id -p -P my_port -h my_server < strucdb.sql
```

Where ***my_id***, ***my_port*** and ***my_server*** should be replaced by your userid for the database, the port of the database and the IP address or the server name of the database server repectively. You will be prompted to enter your password.

This creates tables mmdb, mmgi and domdb in the database.

strucdb

input files:

**.val.gz* (*ftp://ftp.ncbi.nih.gov/mmdb/mmdbdata*)

**tables altered:**

mmdb, mmgi

**source code location:**

*slri/seqhound/parsers/cbmmdb.c*

**config file & other dependencies:**

The relevant configuration files are:

*slri/seqhound/config/.intrezrc* (UNIX platform)

*slri/seqhound/config/.mmdbrc* (UNIX platform

*ncbi/config/.ncbirc* (UNIX platform)

*ncbi/data/bstdt.val* (optional)

* The requirement that *bstdt.val* be in the same directory as the parser is not strictly enforced. As long as *.ncbirc* (see below) is properly configured, *bstdt.val* will be located. However, if *bstdt.val* is not in the same directory as parser, a warning will be issued in cbmmdb's log file. Despite the warning, the parser should work properly, granted the configurations files are all set properly.

The *.mmdbrc* file should have at least 1 section [MMDB] with 3 fields:

1) Database: the path where the data source files (**.val.gz*) are located

2) Index: the index file for the data source files (*mmdb.idx*: this is also downloaded by *mmdbftp.pl*)

3) `Gunzip`: path to gunzip

sample *.mmdbrc* file:

```
[MMDB]
;Where the data source files are located
Database = ./
;Index of all data source files
Index = mmdb.idx
;Path to gunzip
Gunzip = /bin/gunzip
```

The *.ncbirc* file should have 1 section `[NCBI]` with 1 field:

1) Data: the path to *bstdt.val*

sample *.ncbirc* file:
In file *.ncbirc*, variable `DATA` should have a value which is the path of directory *ncbi/data* on your machine. File *.ncbirc* looks like (change text in italics):

```
[NCBI]
ROOT=/
DATA=/my_home/compile/ncbi/data/

[NCBI]
;where bstdt.val is located
Data=/ncbi/data
```

The *.intrezrc* file should have the `pathmm` set to where you want the databases to be stored.

sample *.intrezrc* file:

```
[datab]
;seqhound database that you are connecting
username=your_user_name
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=

 [sections]
;structural databases
strucdb = 1
```

Text in ***italics*** must be changed for the *.intrezrc* file to function correctly with your SeqHound set-up. Variables `username`, `password`, `dsn`, `database` in section `[datab]` should have the same values as `USER`, `PASSWORD`, `DSN` and `DATABASE` respectively in your *.odbc.ini* (see Step 10 in section 4.4.) In section `[sections]` `strucdb` should be `1`.
*mmdb.idx* should be stored in the same directory as the data sources *(*.val.gz* files). It is an index, containing a list of MMDB ID and PDB code pairs. The first line is the number of Biostrucs in MMDB in the current release. The * in *.*val.gz* is the MMDB ID. The cbmmdb parser will initially parse the content of *mmdb.idx* to ensure its integrity.

**command line parameters:**

Typing "**./cbmmdb**" at the command line will return a list of parameters

and default settings. For example:

```
> ./cbmmdb
cbmmdb   arguments:

  -n  Initialize Database File for Biostrucs [T/F]
  -m  Initialize Database File for MMDB Id and GI pairs [T/F]
```

example use:

```
    ./cbmmdb -i T -m T
```

associated scripts:

*mmdbftp.pl* retrieves all the data files for input to cbmmdb.

error and run-time logs:

cbmmdb writes to *cbmmdblog*

**additional info:**

See additional readme files on the NCBI ftp site (*ftp://ftp.ncbi.nih.gov/mmdb*)

See data table descriptions for each of the tables that are listed under “tables altered”

**vastblst parser**

**purpose:**

The vastblst parser constructs the 3D domain information that is extracted from the MMDB 3D structures. vastblst builds the domdb table to store this information.

**module:**

strucdb

**input files:**

mmdb table

**tables altered:**

domdb

**source code location:**

*slri/seqhound/domains/vastblst.c*

**config file dependencies:**

*slri/seqhound/config/.intrezrc* (UNIX platform)

The relevant section in the configuration file is:

```
[datab]
;seqhound database that you are connecting
username=your_user_name
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=

 [sections]
;structural databases
strucdb = 1
```

Text in ***italics*** must be changed for the *.intrezrc* file to function correctly with your SeqHound set-up. Variables `username`, `password`, `dsn`, `database` in section `[datab]` should have the same values as `USER`, `PASSWORD`, `DSN` and `DATABASE` respectively in your *.odbc.ini* (see Step 10 in section 4.4.) In section `[sections]` `strucdb` should be `1`.

**command line parameters:**

Typing **`./vastblst`** at the command line will return a list of the command line parameters and default setting. For example:

```
> ./vastblst
vastblst   arguments:
  -n  Initialize Database File for Domains [T/F]
```

**example use**

```
  ./vastblst -n T
```

**associated scripts:**

n/a

**additional information:**

See data table description for each table listed under “tables altered”

**pdbrep parser**

**purpose:**

The pdbrep parser fills in the 'rep' field in the domdb table. 'rep' is the best representative domain for that blast set. The input files consist of non-redundant PDB chain set, BLAST rankings for the set and the representative for that chain set. pdbrep stores the representative into the domdb table.

**module:**

strucdb

**input files:**

*nrpdb.** from *ftp://ftp.ncbi.nih.gov/mmdb/nrtable*

**tables altered:**

domdb

**source code location:**

*slri/seqhound/domains/pdbrep.c*

**config file dependencies:**

The relevant configuration file is:

*slri/seqhound/config/.intrezrc* (UNIX platform)

The relevant sections are:

```
[datab]
;seqhound database that you are connecting
username=your_user_name
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=

 [sections]
;structural databases
```

```
strucdb = 1
```

Text in ***italics*** must be changed for the *.intrezrc* file to function correctly with your SeqHound set-up. Variables `username`, `password`, `dsn`, `database` in section `[datab]` should have the same values as `USER`, `PASSWORD`, `DSN` and `DATABASE` respectively in your *.odbc.ini* (see Step 10 in section 4.4.) In section `[sections]` `strucdb` should be `1`.

**command line parameters:**

Typing **`./pdbrep`** at the commandline will generate a listing of commandline

parameters. For example:

```
>./pdbrep
pdbrep   arguments:

  -i  Input nrpdb table [File In]
```

**example use:**

```
./pdbrep -i nrpdb.010400
```

associated scripts:

n/a

**error & run-time log:**

pdbrep writes to *pdbreplog*

**additional information:**

README's at *ftp://ftp.ncbi.nih.gov/mmdb/nrtable*

see data table descriptions for each of the tables that are listed under "tables altered"

**mmdb table**

**Database:** seqhound

**Table:** mmdb

**Module:** strucdb

**Definition:** Is a database of experimentally determined macromolecular 3D structures (Molecular Modeling DB).

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto number row identifier |
| mmdbid | int(11) | No | 0 | Molecular modeling database identifier |
| asn1 | mediumblob | No | | Biostruc blob |
| pdbid | varchar(20) | No | | PDB id |
| bwhat | int(11) | Yes | NULL | types of molecules in the biostruc |
| models | int(11) | Yes | NULL | number of models in record |
| molecules | int(11) | Yes | NULL | number of molecules in record |
| size | int(11) | Yes | NULL | size of uncompressed biostruc |
| bzsize | int(11) | Yes | NULL | size of compressed biostruc |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | mmdbid |
| immdb_rowid | INDEX | rowid |
| immdb_mmdbid | INDEX | mmdbid |
| immdb_pdbid | INDEX | pdbid |

**Observation:** Most 3D structures are obtained through X-ray crystallography and NMR-spectroscopy. MMDB is a subset of Protein Data Bank (PDB), excluding theoretical models. 3D structures can provide information pertaining to the biological function, mechanism of function, evolutionary history and relationships of a biomolecule.

**Source org:** NCBI

**Source file:** **.val.gz* from *ftp://ftp.ncbi.nih.gov/mmdb/mmdbdata*

**FTP script:** *slri/seqhound/scripts/mmdbftp.pl*

**parser:** cbmmdb

***mmdbid***

**description:** a unique, stable numerical identifier. MMDB ID are assigned when a new structure enters MMDB. If an entry is deleted from PDB, then its MMDB entry is obsolete. Obsolete structures get archived.

**example:** 10

**default value:** n/a

**ASN.1 struct:** Biostruc->Biostruc-id (choice 1)

**parser:** cbmmdb

**function:** `Biostruc2Modelstruc` (*ncbi/biostruc/mmdbapi1.c*)

**API:** `SHound3DExists`

***asn1***

**description:** the Biostruct blob (see ASN structure below). Contains information about the 3D structure of a molecule including information about the researchers,

molecule bond information, etc.

**example:** see below

**default value:** n/a

**source:** **.val.gz*

**parser:** cbmmdb

**function:** `MMDBBiostrucGet`

**API:** `SHoundGet3DfromPdbId`
`SHoundGetPDB3D`
`SHoundGet3D`

**pdbid
***

**description:** a 4 character identifier from the Protein Data Bank.

**example:** 100D

**default:** n/a

**ASN.1 struct:** Biostruc->Biostruc-id(choice 2)

**parser:** cbmmdb

**function:** `Biostruc2Modelstruc` (*ncbi/biostruc/mmdbapi1.c*)

**API:** no functions return the pdbid from mmdb, it is used as a key to retrieve a 3D structure, see asn1 API.

***bwhat
***

**description:** an integer that represents the type of molecule.
The possible flags are (defined in *ncbi/biostruc/mmdbapi1.h*) and their corresponding byte values are:
1) AM_ION 0x80

2) AM_RNA 0x40
3) AM_WAT 0x20
4) AM_SOL 0x10
5) AM_HET 0x08
6) AM_DNA 0x04
7) AM_PROT 0x0
8) AM_POLY 0x01
9) AM_UNK 0x00

**example:** AM_ION
**default:** AM_UNK
**ASN.1 stuct:** Biostruc->Biostruc-graph->Molecule-graph->Bio-mol-descr->molecule-type
**parser:** cbmmdb
**function:** `Biostruc2Modelstruc` (*ncbi/biostruc/mmdbapi1.c*)
**API:** `SHound3DbWhat`

***models***
**description:** an enumeration of the different models for this structure
**example:** 3
**default:** n/a
**source:** this is enumerated by NCBI code, increment for EACH Biostruc->Biostruc-model in the ASN structure
**parser:** cbmmdb
**function:** `Biostruc2Modelstruc` (*ncbi/biostruc/mmdbapi1.c*)
**API:** n/a, no public interface provided to this field

***molecules***

**description:** an enumeration of the number of molecules in the structure

**example:** 3

**default:** n/a

**source:** this is enumerated by NCBI code, increment for EACH Biostruc->Biostruc-graph->Molecule-graph in the ASN structure

**parser:** cbmmdb

**function:** `Biostruc2Modelstruc` (*ncbi/biostruc/mmdbapi1.c*)

**API:** n/a, no public interface provided to this field

***size***

**description:** the size of the uncompressed biostruc

**example:** 7691

**default:** n/a

**source:** the size of the uncompressed biostruc is determined just before it is compressed and appended

**parser:** cbmmdb

**function:** `AssignASNMemBZMemo` (*intrez_cb.c*)

**API:** n/a, no public interface provided to this field

***bzsize***

**description:** the size of the compressed biostruc

**example:** 31

**default:** n/a

**source:** the compressed size is determined after it is compressed

**parser:** cbmmdb
**function:** `AssignASNMemBZMemo` (*intrez_cb.c*)
**API:** n/a, no public interface provided to this field

**mmgi table**

**Database:** seqhound

**Table:** mmgi

**Module:** strucdb

**Definition:** A mapping of mmdbid to gi.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto number row identifier |
| mmdbid | int(11) | No | 0 | mmdb identifier |
| gi | int(11) | No | 0 | GenInfo Identifier |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | mmdbid<br>gi |
| immgi_rowid | INDEX | rowid |
| immgi_mmdbid | INDEX | mmdbid |
| immgi_gi | INDEX | gi |

**Observation:**

**Source org:** NCBI

**Source file:** **.val.gz* from *ftp://ftp.ncbi.nih.gov/mmdb/mmdbdata*

**FTP script:** *slri/seqhound/scripts/mmdbftp.pl*

**parser:** cbmmdb (see mmdb for initialization info)

***mmdbid***

**description:** 3D molecular model unique identifier
**example:** 1
**ASN.1 struct:** Biostruc->Biostruc-id (choice 1)
**parser:** cbmmdb
**function:** `Main`
**API:**
`SHound3DExists`
`SHound3DFromGi`
`SHound3DFromGiList`

***gi***

**description:** GenInfo Identifier
**example:** 1420979
**ASN.1 struct:** Biostruc->Biostruc-id
**parser:** cbmmdb
**function:** `Main`
**API:**
`SHoundGiFrom3D`
`SHoundGiFrom3DList`

**domdb table**

**Database:** seqhound

**Table:** domdb

**Module:** strucdb

**Definition:** Stores the information of structural domains.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto number row identifier |
| mmdbid | int(11) | No | 0 | mmdb identifier |
| asn1 | mediumblob | No | | asn blob |
| pdbid | varchar(20) | No | | pdb identifier |
| pdbchain | varchar(10) | Yes | NULL | pdb chain |
| gi | int(11) | No | 0 | geninfo identifier |
| domno | int(11) | Yes | NULL | domain number |
| domall | int(11) | No | 0 | number of domains in the whole structure |
| domid | int(11) | No | 0 | vast domain id |
| rep | int(11) | Yes | NULL | representative of blast set |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | domid |
| idomdb_rowid | INDEX | rowid |
| idomdb_mmdbid | INDEX | mmdbid |
| idomdb_pdbid | INDEX | pdbid |
| idomdb_gi | INDEX | gi |

| | | |
|---|---|---|
| idomdb_domall | INDEX | domall |
| idomdb_domid | INDEX | domid |

**Observation:** VAST (vector alignment search tool) is an NCBI-developed algorithm used to identify similar 3-D structures that may not possess sequence similarities. Structural information is taken from the mmdb database. 3D structures are converted into vectors (which corresponding to structurally significant regions of the protein). Adjacent vectors are grouped into domains. Domain information is used to determine distant homologs and provide structural information. The domains of proteins can be compared with other protein domains. Those with similar domain overlaps are likely to be distant homologs. The domdb database stores the domain information.

**Source org:** NCBI

**Source file:** MMDB database & *nrpdb.* from ftp://ftp.ncbi.nih.gov/mmdb/nrtable*

**Parser:** vastblst & pdbrep

**Note:** vastblst parser uses SHoundGet3D to retrieve the MMDB information..

***mmdbid***

**description:** the 3D structure id from which the domain was computed.

**example:** 3446

**default value:** n/a

**source:** retrieved from mmdbid by calling `SHoundAllMMDBID`.

**parser:** vastblst

**function:** `Main` calls `SHoundAllMMDBID` and `MakeAModelstruc`

**API:** not used by the API, there are other tables with more complete mmdbid's.

***asn1***

**description:** the asn structure of the domain. The structure gives the gi of the domain and the starting and ending point of the domain.

**example:** a text output of the SLRIValNode:

```
SLRIValNode ::= {
    domain {
    gi 443581 ,
    from 2 ,
    to 393 } }
```

**default value:** n/a

**source:** extracted from the biostruc reconstructed from what is stored in mmdb.

**parser:** vastblst

**function:** `WriteFASTAByDomain` calls `MakeDomain`

**API:** `SHoundGetDomain` to actually print out the ASN structure, after calling `SHoundGetDomain`, the return value (a SLRIValNodePtr object) must be opened and streamed into an asn IO stream. eg.

```
{ // start of program
  SLRIValNodePtr pdom = NULL;
  AsnIoPtr aip = NULL;

  pdom = SHoundGetDomain(443581, 0);
  aip = AsnIoNew(ASNIO_TEXT_OUT, stdout, NULL, NULL, NULL);
  SLRIValNodeAsnWrite(pdom, aip, NULL);
  AsnIoClose(aip);
} // end of program, text output as in example
```

`SHoundGetFastaDomain` (to retrieve the text, follow code above, replace `SLRIValNode` with `SLRIFasta`

***pdbid***

**description:** the PDB id of the 3D structure from which the domain was computed
**example:** 9XIM
**default value:** n/a
**ASN.1 struct:** n/a
**parser:** vastblst
**function:** `WriteFASTAByDomain`
**API:** `SHoundGetDomain`

***gi***

**description:** the gi of the chain from which the domain was computed
**example:** 443581
**default value:** n/a
**source:** extracted from the biostruc object reconstructed from data in mmdb.
Biostruc->Biostruc-id (choice 1)
**parser:** vastblst
**function:** `WriteFASTAByDomain`
**API:** `SHoundGiFromPDBchain`
This field can also be parsed from the `SLRIValNode` and `SLRIFasta` ASN structures (above).

***domno***

**description:** a protein chain may have several domains, each domain is enumerated, eg if a protein X has 10 domains, the first domain has domno 0, the

second domain has domno 1, ...etc

**example:** 0

**default value:** n/a

**source:** this is enumerated by NCBI code

**parser:** vastblast

**function:** `WriteFASTAByDomain`

**API:** n/a, by itself, the domno provides little information, so it is not provided in the API

***domall***

**description:** The total number of domains in the 3D structure. In the above example protein X, domall is 10

**example:** 1

**default value:** n/a

**source:** this is enumerated by NCBI code

**parser:** vastblast

**function:** `WriteFASTAByDomain`

**API:** n/a

***domid***

**description:** the id for the domain. domid is computed by hashing various id's, including (but not limited to) mmdbid, domno, etc.

**example:** 34460200

**default value:** n/a

**source:** hashed in `WriteFASTAByDomain`

**parser:** vastblast
**function:** `WriteFASTAByDomain`
**API:** n/a

***rep***
**description:** domains get grouped based on properties. The domains are then compared to the other domains in their group and then the best over domain representative of that group is chosen. This field reflects that representative.
**example:** 1
**default:** 0
**source:** *nrpdb.** from *ftp://ftp.ncbi.nih.gov/mmdb/nrtable* columns 6, 9 & A
**parser:** pdbrep
**function:** `Main`
**API:** n/a

**Protein sequence neighbours (neighdb) module**

Last updated: August 18, 2004

Note: The neighbours tables are precalculated on a cluster and the resulting tables are distributed in MySQL format on our ftp site. Therefore, this section is provided for informational purposes only, or for those who would like to build neighbours tables from there own sequence data; it is not necessary if one wishes simply to include the neighbours module into their own seqhound instance, in which case they should simply download the precomputed tables.

Note: the nblast development tree is in the slri directory on the same level as SeqHound (i.e.; *slri/nblast*).

This documentation includes a description of the nblast program.
The *NBLAST paper* is freely available from BioMed Central and is provided in the supplementary documents directory distributed with this manual. See:
Dumontier M, Hogue CW. *NBLAST: a cluster variant of BLAST for NxN comparisons.*
**BMC Bioinformatics.** 2002 May 8;3(1):13. Epub 2002 May 08.
PMID: 12019022

**Purpose:** This section describes how to build and use nblast, a program for generating a database of sequence neighbours.
**Installing nblast:**

There are two ways to install nblast:

* Download nblast binaries for your platform from the sourceforge website:

  *http://sourceforge.net/project/showfiles.php?group_id=17918*

or

* Compile **nblast** on your system: In order to compile nblast, two pieces of third party software are prerequisite: NCBI's C toolkit and Sequiter software's CodeBase database library. Nblast currently only supports CodeBase as its database backend, but it may be ported to other databases in the future. If your system meets these requirements, download the platform independent source code for nblast from the link above and proceed.

  The NCBI C toolkit can be downloaded from NCBI's website at

  *ftp://ftp.ncbi.nih.gov/toolbox/ncbi_tools/ncbi.tar.gz*

  CodeBase is a commercial database software library available from Sequiter software.

A description of how to compile and set up the nblast software follows. If you installed the binaries, or already have compiled the software, skip to the Configuration section. The installation procedure for CodeBase and the NCBI C toolkit are not detailed here, but are assumed to have been successful.
Once you have unpacked the source code tree, change directories into the topmost nblast directory and then exercise one of the following sets of instructions, depending on whether you are using a Unix or Windows system.
Unix:

- Modify the *nblast.mk* file for different source and library paths.
- Modify the *make.nblast* file or project settings to create an executable that incorporates NBLAST (`-D NBLAST_API`), logging (`-D NBLAST_LOG`), and/or MoBiDiCK(`-D MOBIDICK_API`) (The MoBiDick library is currently not publicly available).
- From the *src* directory type **`'make -f make.nblast'`**, if the nblast binary is built then build nblastcleanup with **`'make -f make.nblastcleanup'`** The binaries will be placed in the *build/* subdirectory of the source tree.

Windows:

- Open the *nblast.dsw* workspace in MSVC.

Build NBLAST and NBLASTCLEANUP
The two nblast executables, nblast and nblastcleanup, should now be present in the *slri/nblast/build/* directory. Set your `PATH` environment variable appropriately so that you can execute them. Before you can use nblast, you'll have to do some more configuration, described in the next section.
**Configuration of nblast environment:**

At least one configuration file is required to use nblast and it's associated applications, more if you wish to have some of the relevant files outside of the current directory. At the very least, you must have an nblast configuration file, called *.nblastrc* on Unix, and *nblast.ini* on Windows. This file must be present either in your current directory or your home directory[may not apply on windows] and has the following formats:
*.nblastrc* on Unix:

```
; NBLAST configuration file
[NBLAST]
writepath = /home/nblast/build/
```

*nblast.ini* on Windows:

```
[NBLAST]
writepath = g:\code\slri\nblast\build
```

where the directory path named after "`writepath =` " specifies where the files generated by nblast will be written to. A trailing slash(unix) or backslash(windows) is necessary for the directory path to work.
If you want to place the scoring matrix (used by the blast algorithm) and/or the formatted fasta database in any directory but the current working one, you must also have an ncbi configuration file:
*.ncbirc* on Unix:

```
[NCBI]
DATA = g:\code\ncbi\data

[BLAST]
BLASTDB = g:\blastdb\
```

*ncbi.ini* on Windows:

```
[NCBI]
DATA = /code/ncbi/data

[BLAST]
BLASTDB = /blastdb/
```

Where the path following "`DATA =`" specifies the path to find the scoring matrix file, and the path following "`BLASTDB`" specifies the path to find the formatted fasta database.
The BLAST algorithm uses the BLOSUM62 scoring matrix. The file containing this matrix is required for nblast to function. The file is named *BLOSUM62*, and comes with the NCBI C toolkit. It should also come with the binary distribution of nblast.
Once the configuration files have been properly set, you are ready to run nblast, detailed in the next section.

**Running NBLAST**

* Format the fasta database using formatdb: Before Nblast can process the protein sequences, they must be properly formatted. This is done using the formatdb program, available from NCBI, which takes a fasta formatted database of protein sequences and processes them into a form which can be BLASTed. Once you have downloaded formatdb, format your fasta database using the following command:

  **`formatdb -oT -i <`*`dbname`*`>`**

  Where **`<`*`dbname`*`>`** is the file name of your fasta formatted protein sequence database. Generally this is `nr`, the non-redundant protein sequence database, which can be downloaded from *ftp://ftp.ncbi.nlm.nih.gov/blast/db/nr.tar.gz* file (at the time of this writing, that file is ~500 MB compressed). **`<`*`dbname`*`>`** will be used throughout the rest of this document to mean the filename of your original fasta formatted sequence database.

* *Use NBLAST to build the skeleton database:* Before nblast can compare sequences, it needs to build a skeleton of the nblastdb table with information on how the sequences will be ordered and indexed. This is done by running nblast with the `-N1` command line argument as follows:

**nblast -i<*dbname*> -d<*dbname*> -N1**

* *Use Nblast to do the blast comparisons.* Before the neighbour tables can be built, nblast must do the pairwise blast comparisons. In addition to the nblast specific command line options mentioned here, you may also apply options related to NCBI's blastall to augment the BLAST results. For small databases, it is feasible to do this step on a single computer. Single computer execution:

**nblast -i<*dbname*> -d<*dbname*> -e<*eval_cutoff*> -N2**

Where **<*eval_cutoff*>** is the maximum evalue allowed for BLAST comparisons between sequences. BLAST comparisons which result in evalues higher than this are not saved.

Parallel Computer Execution: Since these comparisons are computationally intensive for large databases (like nr), nblast is capable of splitting up the task across multiple compute nodes. This is done by distributing the **<*dbname*>***N.**** files generated by the last step, and the **<*dbname*>***.p**** files generated by formatdb, to the compute nodes, and then running nblast on each compute node with node specific options:

**nblast -i<*dbname*> -d<*dbname*> -e<*eval_cutoff*> -N2 -C<*node_#*> -D<*total_#of_nodes*>**

Where **<*total_#of_nodes*>** is the total number of compute nodes in your parallel computing system, and **<*node_#*>** is the index (ranging from 1 to **<*total_#of_nodes*>**) of the current compute node with respect to the set of nodes which the nblast task is divided across. **<*eval_cutoff*>** has the same meaning as in single computer usage.

Both single and parallel computer execution of the N2 mode of nblast results in creation of files entitled **<*dbname*>***B*<*node_#*>.*** (for single computers, **<*node_#*>** defaults to 1). These contain the set of blast results which that particular compute node generated.

* *Build the nblastdb table of sequence neighbours:* Now the blastdb table of pairwise blast results can be used to build/fill the nblastdb table of neighbouring sequences. The pairwise BLAST results generated during the last step are processed and consolidated to generate the records for the neighbouring sequences table, nblastdb. Single Computer Execution:

**nblast -i<*dbname*> -d<*dbname*> -e<*eval_cutoff*> -N4**

Parallel Computer Execution: You must first collect the database files generated on the compute nodes during the last step onto the head node before running this step. Then run the following on the head node:

**nblast -i<*dbname*> -d<*dbname*> -e<*eval_cutoff*> -N4 -C<*node_#*> -D**<total_#of_nodes>

* *Cleanup the database and generate number of neighbours fields:* The neighbours table, nblastdb, is nearly complete. All that needs to be done is to fill in the #Neighbours fields of the nblastdb table. This is done using the program nblastcleanup with the following arguments:

**nblastcleanup -bT -pT -aT -qT -d<*dbname*> -n <*num_blastdbs*>**

Where **<*num_blastdbs*>** is the number of blastdb's to check/build from, generally equal to the number of compute nodes you used (1 in the single computer case).

Your Neighbours database should now be completely built.

NBLAST Update Procedure

Nblast was designed to process NCBI's non-redundant sequence database, named nr. This database contains a non-redundant list of protein sequences and their associated GenInfo identifier numbers (GIs). The NCBI's nr database is updated on a regular basis, with some GI's being removed, and others being added. It is desirable to keep the NeighDB module's nblastdb and blastdb tables updated with the nr database, without having to recompute all the neighbours. This is the purpose of nblast's update procedure, which removes GI's which have been "killed" from any entries in the nblast tables which contain them, and BLASTs and inserts "new" GI's where they are appropriate. This process involves multiple steps, which are outlined and explained here.

* Format new version of the fasta database using formatdb: Use formatdb to format your new version of the fasta database in the same way you did before. Note that your new fasta database should have the same name as the one you initially used to build the nblast tables.

**formatdb -oT -i <*dbname*>**

* *Run Nblast in Update mode* N5*:* This step compares the GIs in the out of date nblastdb with those in the updated FASTA database. It removes entries of the killed Gis from the neighbour lists of all gi's, deletes records which only exist because of the killed GI, and inserts empty records for the newly added GIs in the nblastdb. It also creates an update file called *NBLAST_UPDATE.val* which lists which GI's have been killed and which are to be added, for the next stages to use. On the head compute node, execute:

**nblast -i<*dbname*> -N5**

* *Run Nblast in Update mode* N6*:* This step performs the pairwise BLAST comparisons between the newly added sequences and all the old sequences that haven't been killed, as well as comparing the new sequences with each other. Single Computer Execution:

**nblast -i<*dbname*> -e<*eval_cutoff*> -N6**

Parallel Computer Execution:

**nblast -i<*dbname*> -e<*eval_cutoff*> -N6 -C<*node_#*> -D<*total_#of_nodes*>**

Where **<*eval_cutoff*>** is the maximum allowed evalue for comparison results, as described earlier.

* *Rebuild the Neighbouring Sequences Table:* Now rebuild the nblast database using the same command you used to build it previously. Single Computer Execution:

  **nblast -i<*dbname*> -d<*dbname*> -e<*eval_cutoff*> -N4**

  Parallel Computer Execution: First collect all the **<*dbname*>***B***<*node#*>**.* files from the compute nodes onto the head node. Then run the following command:

  **nblast -i<*dbname*> -d<*dbname*> -e<*eval_cutoff*> -N4 -C<*node_#*> -D<total_#of_nodes>**

* *Cleanup:* The cleanup procedure is done in the same manner as for the initial build of the neighbour tables. Single Computer Execution:

  **nblastcleanup -bT -pT -aT -qT -d<*dbname*> -n <*num_blastdbs*>**

  Where **<*num_blastdbs*>** is the number of blastdb's to check/build from, generally equal to the number of compute nodes you used (1 in the single computer case).

Your Neighbours database should now be properly updated.

**nbraccess program***

Note: Not available at time of release.

**BLASTDB table**

Last updated: August 4, 2004

**Database:** SeqHound
**Module:** (Sequence) Neighbours
**Source:** NBLAST
**Source File:** Derived from NxN comparison of sequences from the NR database from *ftp://ftp.ncbi.nih.gov/blast/db/FASTA/nr.gz*
**Parser/Application:** NBLAST *http://www.sourceforge.net/projects/slritools* (source & binaries)
**Published Documentation:** BMC Bioinformatics *http://www.biomedcentral.com/1471-2105/3/13/*
**Definition:** Pairwise sequence alignments from NBLAST computation

Note: The neighbours tables are precalculated on a cluster and the resulting tables are distributed in MySQL format on our ftp site. Therefore, this section is provided for informational purposes only, or for those who would like to build neighbours tables from there own sequence data; it is not necessary if one wishes simply to include the neighbours module into their own seqhound instance, in which case they should simply download the precomputed tables.

Codebase

| Column_Name | Index | NULL | Data_Type | Size | Column_Definition |
|---|---|---|---|---|---|
| UID | P | N | INTEGER/Hash Key | 14 | Perfect Hash for 2 Ordinal Numbers |
| EVAL | N | N | FLOAT | E-Value | 12.7 Alignment Evalue |
| ASNSA | N | N | MEMO | ASN.1 | Modified SeqAlign for pairwise sequence alignment |

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | Yes | NULL | Auto incremented id |
| uid | bigint(20) | Yes | NULL | Perfect Hash for 2 Ordinal Numbers |

| | | | | |
|---|---|---|---|---|
| eval | decimal(12,7) | Yes | NULL | 12.7 Alignment Evalue |
| asnsa | mediumblob | Yes | NULL | Modified SeqAlign for pairwise sequence alignment |

MySQL Indexes:

| **Keyname** | **Type** | **Field** |
|---|---|---|
| iblastdb_rowid | INDEX | rowid |
| iblastdb_uid | INDEX | uid |

***** uid *****

**Description:** 64 bit Perfect Hash Key generated from 2 32 bit Ordinal Numbers in nblastdb

**example:**

**default value:** none

**source:** NBLAST - a cluster computer extension of BLAST to compute NxN sequence comparisons

**functions:** `ShoundGetBlastResult`: Given two GIs, checks if alignment exists, returns NBlast-result-set else NULL

`SHoundGetBlastSeqAlign` : Given two GIs, calls `SHoundGetBlastResult` and formats the NBlast-result-set to a SeqAlign

***** eval *****

**Description:** The BLAST e-value reported for this alignment

**example:** 0.0001

**default value:** none

**function:** Used by NBLAST to create the NBLASTDB table using a user-specified minimum evalue

*****asnsa*****

**Description:** NBlast-Result-Set (ASN.1 definition is described in *slri/nblast/asn/NBlastasn.asn*)

- Stores the useful parts of a seqalign from the BLAST computation including the alignment, bitscore, evalue

**NBLASTDB table**

Last updated: August 4, 2004

**Database:** SeqHound
**Module:** (Sequence) Neighbours
**Source:** NBLAST
**Source File:** Derived from NxN comparison of the NR database from *ftp://ftp.ncbi.nih.gov/blast/db/FASTA/nr.gz*
**Parser/Application:** NBLAST *http://www.sourceforge.net/projects/slritools* (source & binaries)
**Published Documentation:** BMC Bioinformatics *http://www.biomedcentral.com/1471-2105/3/13/*
**Definition:** Sequence neighbour lists from NBLAST computation

Codebase

| Column_Name | Index | NULL | Data_Type | Size | Column_Definition |
|---|---|---|---|---|---|
| ORD | P | N | INTEGER Ordinal Number | 10 | The ordinal number of this entry (auto-increment) |
| GI | I | N | INTEGER GenInfo Id | 10 | The GenInfo Identifier for the sequence for which there are neighbours in the list |
| NUM | I | N | INTEGER# Neighbours | 10 | Number of neighbours in ASN.1 structure |
| ASNNBR | N | N | MEMO | ASN.1 | ASN.1 structure containing the list of GIs whose sequences neighbour that of this entries GI, and the corresponding evalues of the alignments. |

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto incremented id |
| ord | int(11) | No | 0 | The ordinal number of this entry |
| gi | int(11) | No | 0 | The GenInfo Identifier for the sequence for which there are neighbours in the list |
| num | int(11) | No | 0 | Number of neighbours in ASN.1 structure |
| asnnbr | mediumblob | No | | ASN.1 structure containing the list of GIs whose sequences neighbour that of this entries GI, and the corresponding evalues of the alignments. |

MySQL Indexes:

| Keyname | Type | Field |
|---|---|---|
| inblastdb_rowid | INDEX | rowid |
| inblastdb_ord | INDEX | ord |
| inblastdb_gi | INDEX | gi |
| inblastdb_num | INDEX | num |

*****ord*****

**Description:** The ordinal value of the entry in the database (starts with 1). The ordinal values from two GIs in a pairwise alignment are perfectly and reversibly hashed into/from the BLASTDB UID value. This approach saves on space required to store two 32 bit integers.

**Example:** 1

**Default Value:** NA

**Function:**

*****gi*****

**Description:** The GenInfo Identifier of the query sequence
**Example:** 2495000
**Default Value:** NA

**API Function:**

`SHoundNeighboursFromGiEx`: Given GI, an evalue cutoff and a limit of 100 returned results, returns FLinkSet containing list of neighbour GIs and their alignment e-value

Other functions that use SeqHound Functionality (Redundant Groups & Taxonomy Protein Lists)

`SHoundNeighboursFromGi`: Calls `SHoundNeighboursFromGiEx`, and if the GI is not found, searches through the list of redundant GIs for the respective sequence to find an equivalent GI for which there is neighbour information, returning the ShoundNeighboursFromGiEx results for that GI.

`SHoundNeighboursFromGiList`: Calls `SHoundNeighboursFromGi` with each GI in a valnode list

`SHoundNeighboursFromTaxID`: Calls `ShoundNeighboursFromGiList` for each GI in a given taxonomy (`SHoundProteinsFromOrganism`)

`SHoundNeighboursOfNeighbours`: Fetches the neighbours of supplied GI and each of their neighbours (limit 100)

`SHoundNeighboursOfNeighboursList`: Fetches the neighbours of supplied GI list and each of their neighbours

`SHoundGiAndNumNeighboursList`: returns a list of all the GIs with more than 0 neighbours

`SHoundNumNeighboursInDB`: Fetches the number of neighbours in the nblastdb

*****num*****

**Description:** Quick lookup value to find out how many neighbours are in the ASN.1 structure. Can also be used to sort the GIs with most/least neighbours
**Example:** range of integer values
**Default Value:** 0
**Function:**

*****asnnbr*****
**Description:** NBlast-GiAndEval-set (ASN.1 definition is described in *slri/nblast/asn/NBlastasn.asn*)
stores the GI and it's list of sequence neighbours (as GI, evalue pairs)

**Functions:** see above for GI

**Locus link functional annotations (lldb) module**

**llparser**

Last updated: August 5, 2004

**purpose:**

The llparser parses the LocusLink data files to create and update a set of tables that correlate curated sequence data and descriptive information about genetic loci. It retrieves information on official nomenclature, aliases, sequence accessions, phenotypes, EC numbers, MIM numbers, UniGene clusters, homology and map locations.

**module:** lldb

**input files:**

LL_tmpl

From *ftp://ftp.ncbi.nih.gov/refseq/LocusLink/*

**tables altered:**

ll_cdd, ll_go, ll_llink, ll_omim

**source code location:**

*slri/seqhound/locuslink/llparser.c*

**config file dependencies:**

The relevant configuration file is:

*slri/seqhound/parsers/.intrezrc* (for Unix platforms) or

The relevant section of the configuration file is:

```
[datab]
;seqhound database that you are connecting
username=your_user_name
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=

 [sections]
;locus link functional annotations
lldb = 1
```

Text in ***italics*** must be changed for the *.intrezrc* file to function correctly with your SeqHound set-up. Variables `username`, `password`, `dsn`, `database` in section `[datab]` should have the same values as `USER`, `PASSWORD`, `DSN` and `DATABASE` respectively in your *.odbc.ini* (see Step 10 in section 4.4.) In section `[sections]` `lldb` should be `1`.

**command line parameters:**

This parser does not have any command line parameter, Just type "**`./llparser`**" and it will parse the LL_tmpl file. This input file must be in the same directory as the llparser executable.

**associated scripts:**

see "*slri/seqhound/scripts/llftp.pl*"
This script retrieves the input file or this parser.

**error and run-time logs:**

llparser writes to a log file called "*llparserlog*" where it writes Time Stamp, Error #, goparser.c line # and cause of the problem.
e.g.

```
================[ May 21, 2003  3:49 PM ]=================
ERROR: [000.000] {llparser.c, line 81} Main: Cannot find LL_tmpl file.
```

**troubleshooting:**

**additional info:**

The LocusLink web page is at NCBI *http://www.ncbi.nlm.nih.gov/LocusLink/*

The LocusLink *README* file describes the input file for this parser *ftp://ftp.ncbi.nih.gov/refseq/LocusLink/*

See data table descriptions for each of the tables in the lldb module.

**addgoid parser**

Last updated: August 5, 2004

**purpose:**

**Correlates sequence record gi's with GO annotation identifiers.**

The Gene Ontology flat file parser adds information to the supplements ll_go table. This information correlates sequence records GI's with GO annotation identifiers. This information is retrieved from the *gene_association.compugen.Genbank* and *gene_association.compugen.Swissprot* files from *www.geneontology.org.*

Other GO annotation data is available at this site but it is not currently incorporated into SeqHound. This is actively being worked on at the time of writing.

Note that the input files used here do not contain PubMed Identifiers.

This parser is dependent on the following tables, asndb, parti, accdb and nucprot. This parser is also dependent on SeqHound API.

For this reason, the mother parser must be run before using the addgoid parser.

**module:** lldb

**input files:**

*gene_ association.compugen.Genbank*

*gene_association.compugen.Swissprot*

from *ftp://ftp.geneontology.org/pub/go/gene-associations/*

**tables altered:**

ll_go

**source code location:**

*slri/seqhound/locuslink/addgoid.c*

**config file dependencies:**

The relevant configuration file is:

*slri/seqhound/parsers/.intrezrc* (for Unix platforms) or

The relevant section of the configuration file is:

```
[datab]
;seqhound database that you are connecting
username=your_user_name
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=

 [sections]
;locus link functional annotations
lldb = 1
```

Text in ***italics*** must be changed for the *.intrezrc* file to function correctly with your SeqHound set-up. Variables `username`, `password`, `dsn`, `database` in section `[datab]` should have the same values as `USER`, `PASSWORD`, `DSN` and `DATABASE` respectively in your *.odbc.ini* (see Step 10 in section 4.4.) In section `[sections]` `lldb` should be `1`.

**command line parameters:**

Typing "**`./addgoid -`**" at the command line while in the directory where addgoid resides will return a list of command line parameters and default settings. For example:

```
> ./addgoid -
pdbrep arguments:
  -i  Input file [File In]
```

**associated scripts:**

see */slri/seqhound/goftp.pl*

The script retrieves the files used as input by the addgoid parser. This script also retrieves the three input files required by the goparser (see godb module).

**error and run-time logs:**

addgoid parser writes to a log file called *addgoidlog* where it writes Time Stamp, Error #, goparser.c line # and cause of the problem. For example

```
==================[ May 21, 2003  4:14 PM ]==================
NOTE: CoreLib [002.003] {ncbifile.c, line 624} FileOpen("gene_association.compugen.Swissprot","r")
failed
```

**troubleshooting:**

**additional info:**

The NCBI LocusLink web page is at

*http://www.ncbi.nlm.nih.gov/LocusLink/.*

The Gene Ontology Consortium documentation at is at *:http://www.geneontology.org/..*

See data table descriptions for each of the tables that are listed under the lldb module.

**ll_omim table**

Last updated: August 5, 2004

**Database** seqhound

**Table** ll_omim

**Module** lldb

**Definition** OMIM Online Mendelian Inheritance in Man.

Online Mendelian Inheritance in Man (OMIMTM) is a continuously updated catalog of human genes and genetic disorders. OMIM focuses primarily on inherited, or heritable, genetic diseases. It is also considered to be a phenotypic companion to the human genome project. OMIM is based upon the text Mendelian Inheritance in Man, authored and edited by Dr. Victor A. McKusick and a team of science writers and editors at Johns Hopkins University and elsewhere.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto incremented id |
| ll_id | int(11) | No | 0 | Locus Link Identifier |
| omim_id | int(11) | No | 0 | OMIM Identifier. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | ll_id<br>omim_id |
| illomim_rowid | INDEX | rowid |
| illomim_llid | INDEX | ll_id |
| illomim_omimid | INDEX | omim_id |

**Observation:**

**Organization:** NCBI

**Source db:** *ftp://ftp.ncbi.nih.gov/refseq/LocusLink/LL_tmpl.gz*

***** ll_id *****

**description:** Locus link record identifier.

**example:** 1

**default value:** 0

**source:** First field in each locus link record. Eg:

```
>>1
```

is the record with locus link id 1.

**parser:** llparser.c --> ll_parser.c

**function:** `LL_ParseFile()` --> `LL_LineParser`
db_layer: `LL_Append2OMIM_DB()`
**API:** `SHoundLLIDFromOMIM()`

***** omim_id *****
**description:** OMIM Online Mendelian
**example:** 138670
**default value:** n/a
**source:** After tag 'OMIM: '
**parser:** llparser.c --> ll_parser.c
**function:** `LL_LineParser()` --> `LL_ParseOMIM()`
db_layer: `LL_AppendRecord()` --> `LL_Append2OMIM_DB()`
**API:** `SHoundOMIMFromLLID()`
`SHoundOMIMFromGi()`
`SHoundOMIMFromGiList()`

**ll_go table**

Last updated: August 5, 2004

**Database:** seqhound

**Table:** ll_go

**Module:** lldb

**Definition:** Associates a locus link identifier with the gene ontology (GO) annotation.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto incremented id |
| ll_id | int(11) | No | 0 | Locus Link Identifier |
| go_id | int(11) | Yes | NULL | Gene Ontology ID. |
| pmid | int(11) | Yes | NULL | Pub Med ID. |
| evidence | varchar(50) | Yes | NULL | Evidence Code. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| illgo_rowid | INDEX | rowid |
| illgo_llid | INDEX | ll_id |
| illgo_goid | INDEX | go_id |
| illgo_pmid | INDEX | pmid |

**Observation.:**

**Organization:** NCBI

**Source file:** *ftp://ftp.ncbi.nih.gov/refseq/LocusLink/LL_tmpl.gz*

**Parser:** ll_parser.c

***** ll_id *****

**description:** Locus link identifier

**example:** 2

**default value:** n/a

**source:** see above

**parser:** *ll_parser.c -> ll_parser.c*

**function:** `LL_LineParser() -> LL_ParseNPUnit`

**API:** `SHoundLLIDFromGOIDAndECode ()`

***go_id***

**description:** Gene Ontology Identifier.

**example:** 5717
**default value:** n/a
**source:** after tag GO, 4th element
e.g.:
```
GO: cellular
component|extracellular|IDA|GO:0005574|GOA|na
```
**parser:** *ll_parser.c* or *ll_parser.c*
**function:** `LL_LineParser() -> LL_ParseGOUnit`
**API:**
```
SHoundGOIDFromLLID()
SHoundGOIDFromGi()
SHoundGOIDFromRedundantGi
SHoundGOIDFromGiList
SHoundGOIDFromRedundantGiList
```

***pmid***

**description:** PubMed Identification.
**example:** 3458201
**default value:** n/a
**source:** after tag GO, 6th element
e.g.:
```
GO: cellular component|extracellular|IDA|GO:0005574|GOA|345201
```
**parser:** `llparser.c -> ll_parser.c`
**function:** `LL_LineParser() -> LL_ParseGOUnit`
**API:** `SHoundGOPMIDFromGiAndGOID()`

***evidence***

**description:** Every GO annotation must indicate the type of evidence that supports it; these evidence codes correspond to broad categories of experimental or other support. *http://www.geneontology.org/GO.evidence.html*
**example:**
`IC:` Inferred by Curator.
`ND:` No biological Data available.
`TAS:` Traceable Author Statement.
`IEA:` Inferred from Electronic Annotation.
**default value:** n/a
**source:** After a 'GO:' line, it's the 3rd. field element
eg:
```
GO: cellular
component|extracellular|IDA|GO:0005574|GOA|34520
1
```
**parser:** `llparser.c -> ll_parser.c`

**function:** `LL_LineParser()-> LL_ParseGOUnit()`
**API:** `SHoundGOECodeFromGiAndGOID()`

**ll_llink table**

Last updated: August 5, 2004

**Database:** seqhound

**Table:** ll_llink

**Module:** lldb

**Definition:** Associates a locus link id with a sequence identifier

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto incremented id |
| ll_id | int(11) | No | 0 | Locus Link Identifier. |
| gi | int(11) | No | 0 | Gene Info Identifier |
| map | text | Yes | NULL | Gene location in chromosome. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | ll_id<br>gi |
| illll_rowid | INDEX | rowid |
| illll_llid | INDEX | ll_id |
| illll_gi | INDEX | gi |

**Observation.:** Maps a locus link id with a gi and its location in the chromosome. Not all locus link ids will have a gi. A gi may be specified as an NP gi or a XP gi ( experimentally determined ). If an NP gi is available, it will be used. If an NP gi is not available, then the XP gi will be used. If neither the NP nor XP gi is available, then no gi will be used.

**Organization:** NCBI

**Source file:** *ftp://ftp.ncbi.nih.gov/refseq/LocusLink/LL_tmpl.gz*

*** ll_id ***

**description:** Locus Link Identifier.

**example:** 2

**default value:** n/a

**source:** start of record
eg.
`>>2`

**parser:** llparser.c --> ll_parser.c

**function:** `LL_AppendLLID_DB()`
`LL_ParseFile()` -> `LL_LineParser()`

**API:** `SHoundLLIDFromGi()`
`SHoundLLIDFromGiList()`

***gi***

**description:** Gene Info Identifier

**example:** 21071030

**default value:** n/a

**source:** in the NP tag, 2nd element
eg
`NP: NP_570602|21071030`

**parser:** llparser.c --> ll_parser.c

**function:** `LL_ParseFile()` --> `LL_LineParser()` --> `LL_Append2LLID_DB()`

**API:** `SHoundGiFromLLID()`
`SHoundGiFromLLIDList()`

***map***

**description:** Location of the gene in the Chromosome

**example:** 19q13.4

**default value:** n/a

**source:** in the MAP tag: 1st element
`MAP: 19q13.4|RefSeq|C|`

**parser:** llparser.c --> ll_parser.c

**function:** `LL_ParseFile()` --> `LL_LineParser()`
`LL_Append2LLID_DB()`

**API:** `SHoundLocusFromGi()`

**ll_cdd table**

Last updated: August 5, 2004

**Database:** seqhound

**Table:** ll_cdd

**Module:** lldb

**Definition:** Conserved Domain Database.

Maps a locus link id to a Conserved Domain ID.

Proteins often contain several modules or domains, each with a distinct evolutionary origin and function. The CDD database may be used to identify the conserved domains present in a protein sequence.

Conserved Domains can be summarized with multiple local sequence alignments. Computational biologists have compiled collections of such alignments representing conserved domains, and LocusLink imports them from three major sources:

* Smart, the Simple Modular Architecture Research Tool
* Pfam (UK), Pfam-A seed alignments
* COG (Clusters of Orthologous Groups)

Smart and Pfam are public domain databases, which are offered in combination with HMM-based search engines and alignment visualization services.

COG is an NCBI-curated protein classification resource. Sequence alignments corresponding to COGs are created automatically from constituent sequences and have not been validated manually for import in CDD.

The default e-value cutoff of for data in this table is 0.01

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto incremented id |
| ll_id | int(11) | No | 0 | Locus Link Identifier |
| cdd_id | varchar(50) | Yes | NULL | CDD Source Database. |
| evalue | decimal(20,10) | Yes | NULL | Descriptive match. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| illcdd_rowid | INDEX | rowid |
| illcdd_llid | INDEX | ll_id |
| illcdd_cddid | INDEX | cdd_id |

**Observation.:** Domains can be thought of as distinct functional and/or structural units of a protein. These two classifications coincide rather often, as a matter of fact, and what is found as an independently folding unit of a

polypeptide chain also carries specific function. Domains are often identified as recurring (sequence or structure) units, which may exist in various contexts. e.g.: of the CDD Record.

```
CDD: pfam00207: Alpha-2-macroglobulin
family|5952|2318|na|8.970050e+02
CDDID: pfam00207
Evalue: 8.970050e+02
```

**Organization:** NCBI

**Source db:** *ftp://ftp.ncbi.nih.gov/refseq/LocusLink/LL_tmpl.gz*

*** ll_id ***

**description:** Locus link identifier

**example:** 2

**default value:** n/a

**source:** start of record

eg.

```
>>2
```

**parser:** llparser.c --> ll_parser.c

**function:** `LL_AppendLLID_DB()`
`LL_ParseFile()` -> `LL_LineParser()`

**API:** `SHoundLLIDFromCDDID()`
`SHoundLLIDFromGi()`
`SHoundLLIDFromGiList()`

***cdd_id***

**description:** Conserved Domain Database Identifier

**example:** pfam00207

**default value:** n/a

**source:** after CDD tag: 1st element

```
CDD: pfam00207: Alpha-2-macroglobulin
family|5952|2318|na|8.970050e+02
```

**parser:** llparser.c --> ll_parser.c

**function:** `LL_ParseNPUnit()`
`LL_ParseFile()` --> `LL_LineParser()`

**API:** `SHoundCDDIDFromGi()`
`SHoundCDDIDFromGiList()`
`SHoundCDDIDFromLLID()`

***evalue***

**description:** Describes match between CDD and the sequence

| | |
|---|---|
| **example:** | 8.970050e+02 |
| **default value:** | 0 |
| **source:** | after CDD tag: last element<br>`CDD: pfam00207: Alpha-2-macroglobulin family\|5952\|2318\|na\|8.970050e+02` |
| **parser:** | llparser.c --> ll_parser.c |
| **function:** | `LL_ParseNPUnit()`<br>`LL_ParseFile()` --> `LL_LineParser()` |
| **API:** | `SHoundCDDScoreFromGi()` |

**GENE module**

**parse_gene_files.pl parser**

Last updated September 27, 2004

**purpose:**

*parse_gene_files.pl* parses 4 files from the NCBI Gene database and populates gene_* tables in SeqHound.

**logic:**

*parse_gene_files.pl* first drops the gene_* tables and then recreates them. It then reads the files generated by *gene_cron.pl* to populate the new tables. In the future, the tables will not be dropped upon update.

**module: gene**

**input files:**

*ftp://ftp.ncbi.nih.gov/gene/DATA*

*gene2refseqUniq*
*gene_infoUniq*
*gene_historyUniq*
*gene2pubmedUniq*

**tables altered:** gene_dbxref, gene_genomicgi, gene_history, gene_info, gene_productgi, gene_pubmed, gene_object, gene_synonyms.

source code location:
*/seqhound/gene/parse_gene_files.pl*
*/seqhound/scripts/gene_cron.pl*

**config file dependencies:**

The relevant configuration file is:

*slri/seqhound/config/.intrezrc* (for Unix platforms)

The relevant section of the configuration file is:

```
[datab]
;seqhound database that you are connecting
username=your_user_name
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=
```

Text in ***italics*** must be changed for the .intrezrc file to function correctly with your SeqHound set-up. Variables `username`, `password`, `dsn`, `database` in section `[datab]` should have the same values as `USER`, `PASSWORD`, `DSN` and `DATABASE` respectively in your *.odbc.ini* (see Step 10 in section 4.4.) *.intrezrc* must reside in the directory where the parser is running and *.odbc.ini* should be in your home directory.

You should also have a copy of *shconfig.pm* in the directory where the parser is running to read *.intrezrc* and *.odbc.ini.*

**command line parameters:**

**example use:**

```
perl parse_gene_files.pl
```

**associated scripts:**

Four files are downloaded from *ftp://ftp.ncbi.nih.gov/gene/DATA* by *gene_cron.pl*:
*gene2refseq.gz*
*gene_info.gz*
*gene_history.gz*
*gene2pubmed.gz.*
*gene_cron.pl* unzips the files and makes sure that each file only contains unique records generating the following files:
*gene2refseqUniq*
*gene_infoUniq*
*gene_historyUniq*
*gene2pubmedUniq*

**error and run-time logs:**

*parse_gene_files.log*
troubleshooting:

**additional info:**

*http://www.ncbi.nlm.nih.gov/entrez/query/static/help/genehelp.html*

> Note that the NCBI gene database is experimental. This means that the input files and the SeqHound tables may change.

**gene_dbxref table**

Last updated September 28, 2004

**Database:** SeqHound

**Table:** gene_dbxref

**Module:** GENE

**Definition:** The table holds cross references to other databases for GeneIds and their associated gis.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| id | Int(11) | No | | Identifier for a cross reference. |
| geneinfoid | Int(11) | No | | Id of the gene_info record that this cross reference refers to. |
| dbname | Varchar(255) | No | | Database name |
| dbaccession | Varchar(30) | No | | Accession. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| igenedbxrefs_id | INDEX | id |
| igenedbxrefs_infoid | INDEX | geneinfoid |
| igenedbxrefs_db_name | INDEX | dbname |
| igenedbxrefs_db_access | INDEX | dbaccess |

**Observation:**

**Source org:** NCBI

**Source file:** *gene_info.gz*

**FTP script:** *gene_cron.pl*

**Parser:** *parse_gene_files.pl*

*****id*****

**description:** Identifier for the cross reference. Mysql auto-increment table.

**example:** `1`

**default value:**

**ASN.1 struct:**

**source:**

**parser:** *parse_gene_files.pl*

**function:**

**API:** not available yet

*****geneinfoid*****

**description:** Identifier for the geneinfo record where this cross reference was found.
**example:** `53577`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****dbname*****

**description:** Name of the database that contains the second reference.
**example:** `SGD`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****dbaccess*****

**description:** Accession for the record that contains the name.
**example:** `S0000572`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

**gene_genomicgi table**

Last updated September 29, 2004

**Database:** SeqHound

**Table:** gene_genomicgi

**Module:** GENE

**Definition:** Table that contains the gis of genomic DNAs that contain genes. The start, stop location and orientation on the genomic DNA are also included.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| id | int(11) | No | | Identifier of a product gi. Mysql auto-increment column. |
| geneobjectid | int(11) | No | | Identifier of the geneobject that this genomic gi refers to. |
| gi | int(11) | No | | The genomic gi. |
| start | int(11) | Yes | | The start location on the genomic DNA. |
| end | int(11) | Yes | | The start location on the genomic DNA. |
| orientation | char(1) | Yes | | The orientation on the genomic DNA. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| igenomic_id | | id |
| igenomic_objectid | | geneobjectid |
| igenomic_gi | | gi |
| | | |

**Observation:**

**Source org:** NCBI

**Source file:** *gene_info.gz*

**FTP script:** *gene_cron.pl*

**Parser:** *parse_gene_files.pl*

*****id*****

**description:** Identifier of a genomic gi.
**example:** 1
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****geneobjectid*****

**description:** The gene object that this gi refers to.
**example:**
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****gi*****

**description:** The genomic gi.
**example:** `10954454`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****start*****

**description:** The start position of the gene on the genomic DNA.
**example:** `348`
**default value:**
**ASN.1 struct:**

**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****end*****
**description:** The end position of the gene on the genomic DNA.
**example:** `1190`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****orientation*****
**description:** The orientation of the gene on the genomic DNA.
- `-` meaning "minus" strand or
- `+` meaning "plus" strand

**example:** `-`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

**gene_history table**

Last updated September 29,2004

**Database:** SeqHound

**Table:** gene_history

**Module:** GENE

**Definition:** This table has information about geneids that are no longer current.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| id | int(11) | No | | Identifier for a history record. Mysql auto-increment column. |
| taxid | int(11) | Yes | | NCBI taxonomy identifier. |
| currentgeneid | int(11) | Yes | | The current NCBI Gene Id for this gene. |
| oldgeneid | int(11) | Yes | | The discontinued Gene Id. |
| oldsymbol | varchar(20) | Yes | | The symbol assigned to the discontinued Gene Id, if the discontinued record was not replaced with another. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| igenehistory_id | Index | id |
| current_gene_id | Index | currentgeneid |
| discont_gene_id | Index | oldgeneid |
| discont_symbol | Index | oldsymbol |

**Observation:** Note that all fields except for id are optional.

**Source org:** NCBI

**Source file:** *gene_history.gz*

**FTP script:** *gene_cron.pl*

**Parser:** *parse_gene_files.pl*

*****id*****

**description:** Identifier for the history record. Mysql auto-increment column.
**example:** `212815`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****taxid*****

**description:** The NCBI taxonomy identifier for this gene..
**example:** `10116`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****currentgeneid*****

**description:** The current NCBI gene id.
**example:** `29666`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****oldgeneid*****

**description:** The discontinued NCBI gene id.
**example:**
**default value:**
**ASN.1 struct:**

**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****oldsymbol*****
**description:** The symbol associated with the discontinued gene id, if no new record replaced the discontinued record.
**example:** `hlyB`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

**gene_info table**

Last updated September 29, 2004

**Database:** SeqHound

**Table:** gene_info

**Module:** GENE

**Definition:** Information about a gene.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| id | int(11) | No | | Identifier for this record. |
| geneobjectid | int(11) | No | | geneobjectid association with this information. |
| symbol | varchar(255) | Yes | | The default symbol for this gene. |
| locustag | varchar(255) | Yes | | The LocusTag for this gene. |
| chromosome | varchar(32) | Yes | | The chromosome where this gene is found. |
| maplocation | varchar(255) | Yes | | The map location of this gene on the chromosome. |
| description | mediumtext | Yes | | A description of this gene. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| igeneinfo_id | Index | id |
| object_id | Index | geneobjectid |
| symbol | Index | symbol |
| locus_tag | Index | locustag |
| chr | Index | chromosome |

**Observation:**

**Source org:** NCBI

**Source file:** *gene_info.gz*

**FTP script:** *gene_cron.pl*

**Parser:** *parse_gene_files.pl*

*****id*****

**description:** Identifier for this record.
**example:** `74058`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

*****geneobjectid****

**description:** The geneobjectid for the gene that this information refers to.
**example:** `73870`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

*****symbol*****

**description:** The symbol for this gene.
**example:** `1A981`
**default value:**
**ASN.1 struct:** gene->locus (NCBI says this is where the data comes from).
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

*****locustag*****

**description:** The locus tag for this gene.
**example:** `1A981`
**default value:**
**ASN.1 struct:** gene->locus-tag (NCBI says this is where the data comes from).

**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

*****chromosome*****
**description:** The chromosome where this gene is found.
**example:** I
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

*****maplocation*****
**description:** The map location of this gene on the chromosome.
**example:** I;-19.13 cM (interpolated genetic position)
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

*****description*****
**description:** A description of this gene.
**example:** `putative protein (69.3 kD) (1A981)`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

**gene_object table**

Last updated September 29,2004

**Database:** SeqHound

**Table:** gene_object

**Module:** GENE

**Definition:** This table contains information on the status of gene records.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| id | int(11) | No | | Identifier for this gene. |
| geneid | int(11) | No | | NCBI's Gene Id. |
| status | varchar(64)) | Yes | | Status of the RefSeq for this gene. May be provisional, INFERRED, MODEL, PREDICTED, Reviewed or VALIDATED |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| igeneobject_id | Index | id |
| igeneobject_geneid | Index | geneid |
| igeneobject_status | Index | status |
| | | |

**Observation:**

**Source org:** NCBI

**Source file:** *gene2refseq.gz*

**FTP script:** *gene_cron.pl*

**Parser:** *parse_gene_files.pl*

*****id*****

**description:** Identifier for this gene.
**example:** `8`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****geneid****

**description:** NCBI's Gene Id.
**example:** `1246510`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****status*****

**description:** The status of the RefSeq record that contains this gene.

```
NULL
INFERRED
MODEL
PREDICTED
Provisional
Reviewed
VALIDATED
```

**example:** `Provisional`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

**gene_productgi table**

Last updated September 29, 2004

**Database:** SeqHound

**Table:** gene_productgi

**Module:** GENE

**Definition:** Stores the gis of the RNA and Proteins produced by a gene.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| id | int(11) | No | | Internal identifier for the product gi. Mysql auto-increment column. |
| geneobjectid | int(11) | No | | The geneobjectid for the gene that this gi belongs to. |
| gi | int(11) | No | | The gi. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| iproduct_id | Index | id |
| iproduct_objected | Index | geneobjectid |
| iproduct_gi | Index | gi |

**Observation:**

**Source org:** NCBI

**Source file:** *gene2refseq.gz*

**FTP script:** *gene_cron.pl*

**Parser:** *parse_gene_files.pl*

*****id*****

**description:** Internal identifier for this gi. Mysql auto-increment column.

**example:** 9

**default value:**

**ASN.1 struct:**

**source:**

**parser:** *parse_gene_files.pl*

**function:**

**API:** not available yet

*****geneobjectid*****

**description:** NCBI's identifier for the gene that this gi belongs to.
**example:** `10`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

*****gi*****
**description:** The gi. May be a protein or an RNA gi.
**example:** `32455275`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:** not available yet

**gene_pubmed table**

Last updated September 29, 2004

**Database:** SeqHound

**Table:** gene_pubmed

**Module:** GENE

**Definition:** This table stores publications that refer to genes.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| id | int(11) | No | | Internal identifier for this reference. |
| geneobjectid | int(11) | Yes | | The geneobjectid that this reference is about. |
| pmid | int(11) | Yes | | The pmid of the reference. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| ipubmed_id | Index | id |
| ipubmed_geneid | Index | geneobjectid |
| ipmid | Index | pmid |

**Observation:**

**Source org:** NCBI

**Source file:** *gene2pubmed.gz*

**FTP script:** *gene_cron.pl*

**Parser:** *parse_gene_files.pl*

*****id*****

**description:** Internal identifier of this reference or of this gene objectid-pmid pair

**example:** `112394`

**default value:**

**ASN.1 struct:**

**source:**

**source:**

**parser:** *parse_gene_files.pl*

**function:**

**API:** not available yet

*****geneobjectid*****

**description:** The geneobjectid of the gene.
**example:** `173392`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

*****pmid*****

**description:** The pmid of the reference.
**example:** `8889548`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

**gene_synonyms table**

Last updated September 28, 2004

**Database:** SeqHound

**Table:** gene_synonyms table

**Module:** GENE

**Definition:** Stores synonyms for genes.

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| id | int(11) | No | | Identifier of this synonym, Mysql auto-increment column |
| geneinfoid | int(11) | Yes | | The geneinfoid for this synonym. |
| synonym | text | Yes | | The synonym. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| igenesyn_id | Index | id |
| igeneinfoid | Index | geneinfoid |
| isynonym | Index | synonym |
| | | |

**Observation:**

**Source org:** NCBI

**Source file:** *gene_info.gz*

**FTP script:** *gene_cron.pl*

**Parser:** *parse_gene_files.pl*

*****id***

**description:** Internal identifier for this synonym geneinfoid pair. Basically a rowid. Mysql auto-increment column.

**example:** `11179`

**default value:**

**ASN.1 struct:**

**source:**

**parser:** *parse_gene_files.pl*

**function:**

**API:**

*****geneinfoid**

**description:** The geneinfoid for the record where this synonym was found.
**example:** `27686`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

*****synonym**

**description:** The synonym.
**example:** `T1J24.19`
**default value:**
**ASN.1 struct:**
**source:**
**parser:** *parse_gene_files.pl*
**function:**
**API:**

**Gene Ontology hierarchy (godb) module**

**goparser**

Last updated: August 5, 2004

**purpose:**

Go data files contain information from the Gene Ontology Consortium that describe controlled vocabularies for the description of the molecular function, biological process and cellular component of gene products.

The GO parser is responsible for generating the hierarchical gene ontology datafiles: *go_name*, *go_parent*, *go_synonym* and *go_reference*. This is accomplished by parsing the flat files *component.ontology*, *function.ontology* and *process.ontology*.

**module:** godb

**input files:**

*component.ontology*

*function.ontology*

*process.ontology.*

From *ftp://ftp.geneontology.org/pub/go/ontology/*

**tables altered:**

go_name, go_parent, GO_REF, GO_SYN

**source code location:**

*slri/seqhound/go/goparser.c*

**config file dependencies:**

The relevant configuration file is:

*slri/seqhound/parsers/.intrezrc* (for Unix platforms) or

The relevant section of the configuration file is:

```
[datab]
;seqhound database that you are connecting
username=your_user_name
password=your_pass_word
dsn=dsn_in_.odbc.ini_file
database=seqhound
local=

 [sections]
;gene ontology hierarchy
godb = 1
```

Text in ***italics*** must be changed for the *.intrezrc* file to function correctly with your SeqHound set-up. Variables `username`, `password`, `dsn`, `database` in section `[datab]` should have the same values as `USER`, `PASSWORD`, `DSN` and `DATABASE` respectively in your *.odbc.ini* (see Step 10 in section 4.4.) In section `[sections]` `godb` should be `1`.

**command line parameters:**

This parser does not have any command line parameters. Typing "**`./goparser`**" will process the three Gene Ontology files.
These files (*component.ontology*, *function.ontology* and *process.ontology*) must be present in the same directory as the compiled goparser executable

**associated scripts:**

see "*/slri/seqhound/goftp.pl*"

This script retrieves the three input files required by the goparser. The script also retrieves the files used as input by the addgoid parser (see lldb module).

**error and run-time logs:**

goparser writes to a log file called "*goparserlog*" where it writes Time Stamp, Error #, goparser.c line # and cause of the problem.
e.g.

```
================[ May 21, 2003  2:36 PM====================
ERROR: [000.000] {goparser.c, line 74} Main: Cannot find function.ontology file
in current directory.
```

**troubleshooting:**

**additional info:**

The Gene Ontology Consortium documentation is located at
*http://www.geneontology.org/*
See data table descriptions for each of the tables that are listed under SeqHound's Data Dictionary.

**go_parent table**

Last updated: August 5, 2004

**Database:** Seqhound

**Table:** go_parent

**Module:** Godb

**Definition:**

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto number row identifier |
| go_id | int(11) | No | 0 | GeneOntology ID |
| parent_goid | int(11) | No | 0 | Parent Go Id.. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | go_id<br>parent_goid |
| igoparent_rowid | INDEX | rowid |
| igoparent_goid | INDEX | go_id |
| igoparent_pid | INDEX | parent_goid |

**Observation.:** Function, process and component are represented as directed acyclic graphs (DAGs) or networks. The difference between a DAG and a hierarchy is that in the latter each child can only have one parent; a DAG allows a child to have more than one parent. A child term may be an "instance" of its parent term(isa relationship) or a component of its parent term (part-of relationship). A child term may have more than one parent term and may have a different class of relationship with its different parents.

**Organization:** Gene Ontology (*ftp://ftp.geneontology.org/pub/go/ontology*)

**Source db:** function.ontology (Molecular function)
process.ontology (Biological process)
component.ontology (Cellular component)

***go_id***

**description:** Gene Ontology identifier Child.

**example:** 0016172

```
%antifreeze activity ; GO:0016172 {Parent}
 %ice nucleation inhibitor activity ; GO:0016173 {Child}
```

**default value:** n/a

**source:** related to the indentation in the file.

**parser:** goparser.c -> go_parser.c

**function:** GODB_ParseFile()->GO_LineParser()->GO_AppendRecord()
db_layer: GO_AppendRecord()->GO_Append_Name()->GO_AppendParent()
GO_GetParentOf()
GO_GetChildrenOf()
GO_GetAllChildren()
GO_GetAllAncestors()

**API:** SHoundGODBGetChildrenOf()

***parent_goid***

**description:** Gene Ontology identifier Parent.

**example:**
```
0016173
 %antifreeze activity ; GO:0016172   {Parent}
  %ice nucleation inhibitor activity ; GO:0016173 {Child}
```

**default value:** n/a

**source:** Related to indentation in the file

**parser:** goparser.c -> go_parser.c

**function:** GODB_ParseFile()->GO_LineParser()->GO_AppendRecord()
db_layer: GO_AppendRecord()->GO_Append_Parent()
GO_GetParentOf()
GO_GetChildrenOf()
GO_GetAllChildren()
GO_GetAllAncestors()

**API:** SHoundGODBGetParentOf()

**go_name table**

Last updated: August 5, 2004

**Database:** seqhound

**Table:** go_name

**Module:** godb

**Definition:**

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto incremented id |
| go_id | int(11) | No | 0 | GeneOntology ID. |
| go_name | text | No | | Go_id Identifier name. |
| go_db | int(11) | No | 0 | GO Database name. |
| go_level | int(11) | No | 0 | Hierarchy level of the GO ID. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | go_id<br>go_name<br>go_db<br>go_level |
| igoname_rowid | INDEX | rowid |
| igoname_goid | INDEX | go_id |

**Observation.:** This table contains a list of 'go_id' and it's molecular function name as well the database where the go_id was parsed from and the level in the Gene Ontology hierarchy.

**Organization:** GeneOntology (*ftp://ftp.geneontology.org/pub/go/ontology*)

**Source db:** function.ontology (Molecular function)
process.ontology (Biological process)
component.ontology (Cellular component)

***go_id***

**description:** Gene Ontology identifier.

**example:** 15643

**default value:** n/a

**source:** See example Go File. The GO id follows 'GO:' tag.

**parser:** goparser.c -> go_parser.c

**function:** `GODB_ParseFile()->GO_LineParser()->GO_AppendRecord()`
db_layer: `GO_AppendRecord()->GO_Append_Name()`

| | |
|---|---|
| | `GO_GetRecordByID()` |
| **API:** | `SHoundGOIDFromRedundantGi`<br>`SHoundGOIDFromRedundantGiList`<br>`SHoundGOIDFromGi`<br>`SHoundGOIDFromGiList` |

***go_name***

| | |
|---|---|
| **description:** | Gene Ontology identifier name. |
| **example:** | anti-toxin; |
| **default value:** | n/a |
| **source:** | go_name follows, '%' and proceeds ';GO:'. |
| **parser:** | goparser.c -> go_parser.c |
| **function:** | `GODB_ParseFile()->GO_LineParser()->GO_AppendRecord()`<br>db_layer: `GO_AppendRecord()->GO_Append_Name()`<br>`GO_GetNameByID()` |
| **API:** | `SHoundGODBGetNameByID` |

***go_db***

| | |
|---|---|
| **description:** | Gene Ontology Database file. This is an integer 1, 2 or 3 |
| **example:** | 1<br>where:<br>1 GO_MOLFUNCTION<br>2 GO_BIOPROCESS<br>3 GO_CELLCOMPONEN |
| **default value:** | n/a |
| **source:** | NA |
| **parser:** | goparser.c -> go_parser.c |
| **function:** | `GODB_ParseFile()->GO_LineParser()->GO_AppendRecord()`<br>db_layer: `GO_AppendRecord()->GO_Append_Name()`<br>`GO_GetClassification()` |
| **API:** | `SHoundGODBGetClassification()` |

***go_level***

| | |
|---|---|
| **description:** | Hierarchy level of the GO ID. |

This is not used because the same GO ID can appear at different levels making the process to determine its level irrelevant. This was intended to be used to indicate the distance of a given GO node from the root node.

| | |
|---|---|
| **example:** | 3 |
| **default value:** | n/a |
| **source:** | Related to the indentation of<br>`'%{function name}'` |
| **parser:** | goparser.c -> go_parser.c |
| **function:** | `GODB_ParseFile()->GO_LineParser()->GO_AppendRecord()`<br>db_layer: `GO_AppendRecord()->GO_Append_Name()`<br>`GO_GetHierarchyLevel()` |
| **API:** | `SHoundGODBGetHierarchyLevel()` this function is deprecated. |

**go_reference table**

Last updated: August 5, 2004

**Database:** seqhound

**Table:** go_reference

**Module:** godb

**Definition:**

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto incremented id |
| go_id | int(11) | No | 0 | GeneOntology ID |
| go_ref | text | No | | GeneOntology Reference. |
| go_ref_db | varchar(50) | Yes | NULL | Reference Data Base Name |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | go_id<br>go_ref |
| igoref_rowid | INDEX | rowid |
| igoref_go_ref_db | INDEX | go_ref_db |

**Observation.:** This table stores the 'go_id' with its database cross-reference. The cross-reference can be an external database identifier that points to something that is equivalent to a given GO term.

**Organization:** GeneOntology (*ftp://ftp.geneontology.org/pub/go/ontology*)

**Source db:** function.ontology (Molecular function)
process.ontology (Biological process)
component.ontology (Cellular component)

***go_id***

**description:** Gene Ontology identifier.

**example:** 45174

**default value:** n/a

**source:** The go_id comes after '%{function name} ; GO:xxxxxx ; '

**parser:** goparser.c -> go_parser.c

**function:** `GODB_ParseFile()->GO_LineParser()->GO_AppendRecord()`
db_layer: `GO_AppendRecord()->Go_Append_Reference()`
`GO_GetRecordByReference()`

**API:** `SHoundGODBGetRecordByReference()`

***go_ref***

**description:** Gene Ontology Synonym Description.

**example:** ISBN: 0198506732

**default value:** n/a

**source:** go_ref comes after "GO:xxxxxx ; ISBN: 0198506732 ;"

**parser:** goparser.c -> go_parser.c

**function:** `GODB_ParseFile()->GO_LineParser()->GO_AppendRecord()`
db_layer: `GO_AppendRecord()->GO_Append_Reference()`
`GO_GetRecordByReference()`

**API:** NA

***go_ref_db***

**description:** Gene Ontology Reference Database.

**example:** EC
ISBN
TC

**default value:** n/a

**source:** After '%{function_name} ; GO:xxxxxxx ; {go_ref_db}
After '%{component_name} ; GO:xxxxxxx ; {go_ref_db}

**parser:** goparser.c -> go_parser.c

**function:** `GODB_ParseFile()->GO_LineParser()->GO_AppendRecord()`
db_layer: `GO_AppendRecord()->GO_Append_Reference()`
`GO_GetRecordByReference()`

**API:** NA

**go_synonym table**

Last updated: August 5, 2004

**Database:** seqhound

**Table:** go_synonym

**Module:** godb

**Definition:**

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto incremented id |
| go_id | int(11) | No | 0 | GeneOntology ID |
| go_syn | text | No | | GeneOntology Synonym. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| PRIMARY KEY | INDEX | go_id<br>go_syn(100) |
| igosynonym_rowid | INDEX | go_id |
| igosynonym_go_id | INDEX | go_syn |

**Observation.:**

**Organization:** GeneOntology (*ftp://ftp.geneontology.org/pub/go/ontology*)

**Source db:** function.ontology (Molecular function)
process.ontology (Biological process)
component.ontology (Cellular component)

**Example of source file:**
```
%glycine binding activity ; GO:0016594 ; synonym:Gly binding ;
synonym:aminoacetic acid binding ; synonym:aminoethanoic acid
binding
```

***go_id***

**description:** Gene Ontology identifier.

**example:** 45174

**default value:** n/a

**source:** The go_id follows '`%{function name}; GO:`'

**parser:** goparser.c -> go_parser.c

**function:** `GODB_ParseFile()->GO_LineParser()->GO_AppendRecord()`
db_layer: `GO_AppendRecord()->Go_Append_Synonym()`

**API:** n/a

***go_syn***

**description:** Gene Ontology Synonym Description. This can be a 'synonym' of a 'process' or 'component' name.

**example:** 'Gly binding'

**default value:** n/a

**source:** After `'%{function_name} ; GO:xxxxxxx ; synonym:{synonym name}'`

After `'%{component_name} ; GO:xxxxxxx ; synonym:{synonym name}'`

```
After '%{process_name} ; GO:xxxxxxx ; synonym:{synonym name}'
  glutathione dehydrogenase (ascorbate); glutamic acid binding
   %glycine binding activity ; GO:0016594 ;
       synonym:Gly binding ;
       synonym:aminoacetic acid binding ;
       synonym:aminoethanoic acid binding
```

**parser:** goparser.c -> go_parser.c

**function:** `GODB_ParseFile()->GO_LineParser()->GO_AppendRecord()`

db_layer: `GO_AppendRecord()->GO_Append_Synonym()`

**API:** n/a

## Gene Ontology Association (GOA) module

Last updated April 5, 2005
This section is maintained by Renan Cavero.

**purpose:**

The GOA Module provides Gene Ontology (GO) information for all possible organisms that have GO terms. GO terms are controlled vocabulary for molecular function, biological process and cellular component of gene products. GO Annotation assignments are derived from *ftp://ftp.geneontology.org/pub/go/gene-associations/* and from *ftp://ftp.ncbi.nlm.nih.gov/gene/DATA/gene2go.gz*.
The GO terms are linked to identifiers provided by the curating database (e.g. FlyBase) AND to the NCBI Gene Info identifier (GI) using the SeqHound DBXref Module.
The GOA Module contains

- GO term assignments to genes or proteins
- Literature references like PubMed IDs
- Evidence codes between the gene product and the GO term
- Object types that get annotated such as gene, transcript, protein or protein structure
- Gene symbols or other associated text
- Taxonomic identifiers
- Date on which the annotation was made.

**module:**

GOA

**input files:**

All files found under gene ontology FTP site
*ftp://ftp.geneontology.org/pub/go/gene-associations/*
NCBI EntrezGene
*ftp://ftp.ncbi.nlm.nih.gov/gene/DATA/gene2go.gz*

**tables altered:**

goa_association
goa_gigo
goa_reference
goa_seq_dbxref
goa_with
goa_xdb

**Table summarizing input files, parsers and command line parameters for GOA module.**

| **Input file** | **parser** | **command line parameters** |
|---|---|---|
| *All files from: ftp://ftp.geneontology.org/pub/go/gene-associations/* | goa_parser_cluster.pl<br>See note below. | **-d {Org.abbr.} (*)**<br>**-c {Cluster: T F}**<br>**-o {Offset: n}**<br>**-n {Num. Lines: n}**<br>**-f {Flag File}** |
| *ftp://ftp.ncbi.nlm.nih.gov/gene/DATA/gene2go.gz* | go_geneparser_cluster.pl<br>See note below. | **-d GO_GENE (**)**<br>**-c {Cluster: T F}**<br>**-o {Offset: n}**<br>**-n {Num. Lines: n}**<br>**-f {Flag File}** |
| *Tables: goa_gigo, dbxref, goa_seq_dbxref, goa_association, accdb, redund, taxgi.* | Seqhound_gigo_cluster.pl<br>See note below. | **-c {Cluster: T F}**<br>**-o {Offset: n}**<br>**-n {Num. Lines: n}**<br>**-f {Flag File}** |
| *Tables: goa_gigo, goa_seq_dbxref, goa_association, accdb, redund, taxgi.* | Seqhound_gigoPDB_cluster.pl<br>See note below. | **-c {Cluster: T F}**<br>**-o {Offset: n}**<br>**-n {Num. Lines: n}**<br>**-f {Flag File}** |
| *Tables: goa_gigo, dbxref, goa_seq_dbxref, goa_association.* | Seqhound_gigoCGEN_cluster.pl<br>See note below. | **-c {Cluster: T F}**<br>**-o {Offset: n}**<br>**-n {Num. Lines: n}**<br>**-f {Flag File}** |

Notes:
(*) Parser Command Line Parameters. (See dbxref.ini for details.)
**goa_parser_cluster.pl:** Parse Gene Ontology Association files and populate GOA module tables.
-d Organism Database File Abbreviation: Can be found under dbxref.ini Partition [GENE_ASSOCIATON_FILE] Ex.: GOA_DDB, GOA_CGEN.
-c Cluster Option: T: True (run in a cluster environment); F: False: (run stand alone).
The following options are optional. Needs to be set-up only if running in a Cluster environment.
-o Offset: The offset in a flat file where a cluster node will start parsing.
-n Number of lines: The number of line-records to process by a cluster node after the Offset is reached.

-f Flag File: For synchronization purpose. A file name that will be generated by a cluster node when finished parsing, telling the Cluster's head node that the parsing was completed. (Cluster Head node will track completion of all nodes before continuing with the next process in the queue.

(**)
**goa_gene_parser:** Same as above but this parser will only parse gene2go file.

**seqhound_gigo_cluster.pl:** Populates goa_gigo with GI's (GenBank assessions) extracted from dbxref table and by looking-up Xref in goa_seq_dbxref will get GO terms from goa_association. When looking up GI's in accdb, redundancy and taxonomies are considered.

**seqhound_gigoPDB_cluster.pl:** Looks up PDB records and chains from goa_seq_dbxref and by looking-up GIs in accdb populates gi-go pairs in goa_gigo. When looking up GI's in accdb, redundancy and taxonomies are considered.

**seqhound_gigoCGEN_cluster.pl:** Same as above but for GIs from Compugen records.

**source code location:**
*The parsers for this module have been updated to work in a cluster configuration. Source code is unavailable at the time of this manual release but will be released with the next code release.*
*/slri/seqhound/dbxrefgoa*

**config file dependencies:**

The relevant configuration file is:
*dbxref.ini* (for Unix platforms)
see dbxref.ini documentation.

**command line parameters:**

See summary table above.

**associated scripts:**

The following shell scripts execute the parsers:
dbxrefgoa_cron.sh: Cron job that runs dbxrefgoa_updatecron.pl
dbxrefgoa_updatecron.pl: Program that automates deployment and runs parsers in a cluster. (see dbxref.ini documentation for details)

**auxiliary scripts:**
In a cluster environment the following scripts will help dbxrefgoa_updatecron.pl in the deployment and execution:
parsers.deploy.sh: deploy files to be parsed to the cluster nodes.
generate_goa_run.pl: Generate an instruction script that distributes processes in the cluster nodes.
run{organism database_file_abbreviation}: instruction script generated by generate_goa_run.pl. Example.: runGOA_MGI.sh
clean.sh: clean (remove) files previously deployed by script deploy.sh.
wait.pl: makes the cluster's head node wait until all the nodes finish processing the parser that was deployed. When wait.pl receives a signal from all the nodes, it will continue with the next parser.
See dbxref.ini for more details.

**error and run-time logs:**

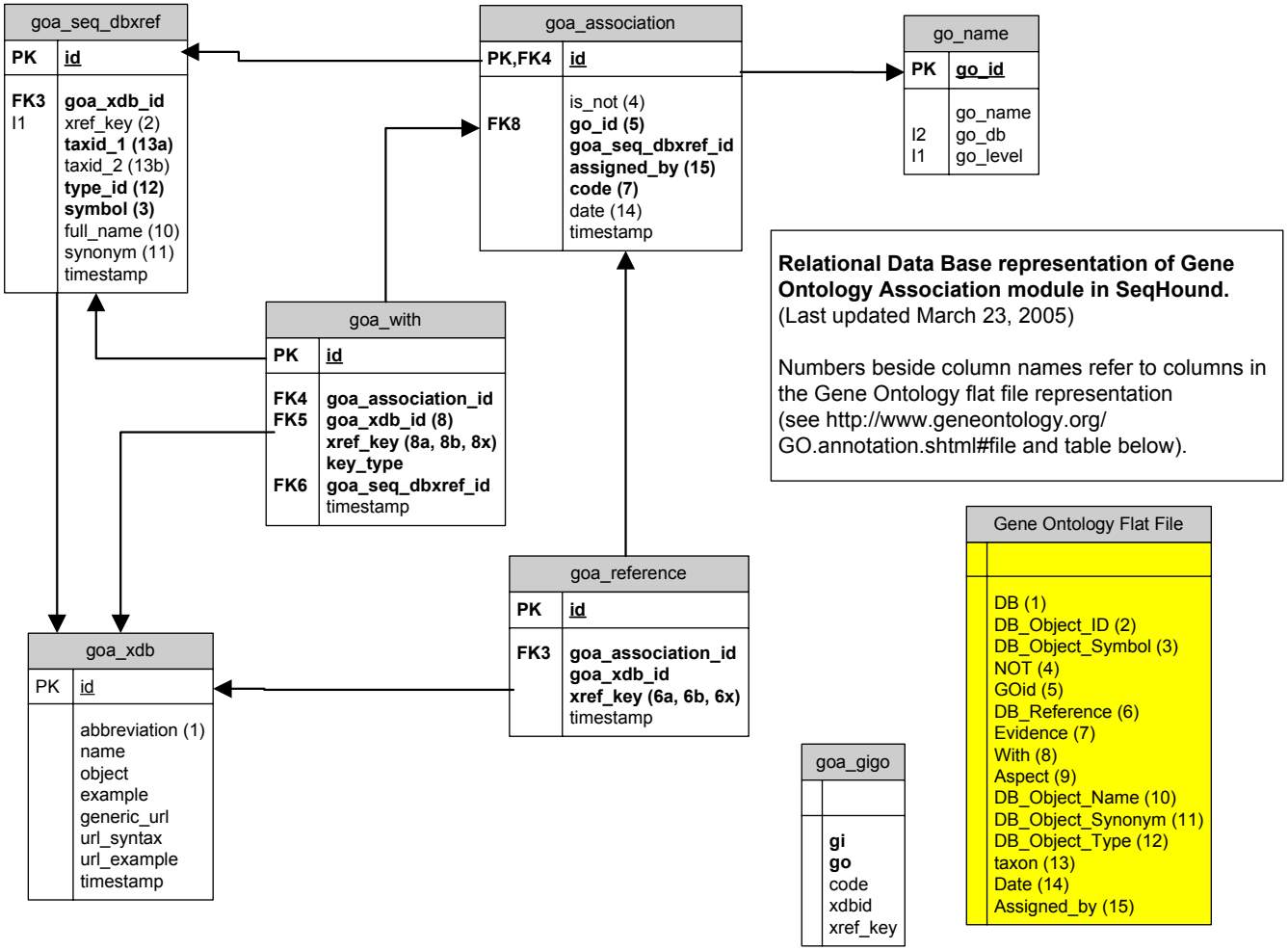
dbxrefgoa_errors.log: log that tracks run time error by the parsers.

dbxrefgoa_updatecron.log: log that indicate what parser was run, completed or failed . A copy of this log will be send by email to the SeqHound administrator.
goa_parser.log: log that summarize number of records updates by each goa parser.

**troubleshooting:**
dbxrefgoa_updatecron.pl will execute instructions from the configuration file dbxref.ini. Any error generated by this process or by the parsers will be recorded under dbxrefgoa_error.log. The final results will be summarized in dbxrefgoa_updatecron.log and goa_parser.log. By following the error messages, the SeqHound administrator will be able to adjust configuration parameters under dbxref.ini and run it again.

**additional info:**

The Gene Ontology Consortium documentation is located at
*http://www.geneontology.org/GO.contents.doc.html*
*ftp://ftp.geneontology.org/pub/go/doc/GO.xrf_abbs_spec*
**Gene Ontology Module Diagram**
The tables also appears in *http://www.blueprint.org/seqhound/api_help/docs/SeqHound_Schema_Prod.pdf*


goa_seq_dbxref
PK id
FK3 goa_xdb_id
I1 xref_key (2)
taxid_1 (13a)
taxid_2 (13b)
type_id (12)
symbol (3)
full_name (10)
synonym (11)
timestamp
goa_association
PK,FK4 id
FK8 is_not (4)
go_id (5)
goa_seq_dbxref_id
assigned_by (15)
code (7)
date (14)
timestamp
go_name
PK go_id
go_name
I2 go_db
I1 go_level
goa_with
PK id
FK4 goa_association_id
FK5 goa_xdb_id (8)
xref_key (8a, 8b, 8x)
key_type
FK6 goa_seq_dbxref_id
timestamp
goa_reference
PK id
FK3 goa_association_id
goa_xdb_id
xref_key (6a, 6b, 6x)
timestamp
goa_xdb
PK id
abbreviation (1)
name
object
example
generic_url
url_syntax
url_example
timestamp
Relational Data Base representation of Gene Ontology Association module in SeqHound.
(Last updated March 23, 2005)
Numbers beside column names refer to columns in the Gene Ontology flat file representation (see http://www.geneontology.org/GO.annotation.shtml#file and table below).
Gene Ontology Flat File
DB (1)
DB_Object_ID (2)
DB_Object_Symbol (3)
NOT (4)
GOid (5)
DB_Reference (6)
Evidence (7)
With (8)
Aspect (9)
DB_Object_Name (10)
DB_Object_Synonym (11)
DB_Object_Type (12)
taxon (13)
Date (14)
Assigned_by (15)
goa_gigo
gi
go
code
xdbid
xref_key

**goa_seq_dbxref table**

Last updated April 12, 2005

| | |
|---|---|
| **Database:** | Seqhound |
| **Table:** | goa_seq_dbxref |
| **Module:** | GOA |
| **Definition:** | The main table of the GOA Module. This table contains entries for a database record ID (e.g.: `Fly Base ID FBgn0013277`) and the information associated with the record that can be found in gene_association files from Gene Ontology. The record is the base to obtain other information like GO terms, reference and other annotation. |
| **Source org:** | Gene Ontology *ftp://ftp.geneontology.org/pub/go/gene-associations/* |
| **Source file:** | See module description above. |
| **Parser:** | See module description above. |

goa_seq_dbxref table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(10) | No | Auto incremented integer. | Internal primary record identifier. | 2099131 | Assigned by source document parser. | NA |
| goa_xdb_id | int(10) | No | 0 | Database identifier from table goa_xdb. For example, an xdb_id of 4 indicates the Candida Genome Database. | 5 | See note below. | NA |
| xref_key | varchar(30) | No | | Record ID (in the above-mentioned database) which points to the object being annotated. | PrID1098818 | See note below. | NA |
| taxid_1 | int(11) | No | 0 | Taxonomic identifier of the species encoding the gene product. | 11676 | See note below. | NA |
| taxid_2 | int(11) | Yes | 0 | Taxonomic identifier of the species where the gene product acts (in the manner described by the GO annotation). For example, if the protein is from a virus, the host organism might be listed here. | 0 | See note below. | NA |
| type_id | varchar(20) | No | | Indicates the type of object being annotated (gene, transcript, protein etc.) | protein | See note below. | NA |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| symbol | varchar(30) | No | | A unique and valid symbol to which the xref_key is matched. It can be an ORF name, gene product symbol or any other identifier. | GI424263 | See note below. | NA |
| full_name | varchar(255) | Yes | NULL | Name of gene or gene product. | cell surface glycoprotein gp138 | See note below. | NA |
| synonym | varchar(50) | Yes | NULL | Gene symbol or other text. | fusA | See note below. | NA |
| lastupdate | timestamp | No | CURRENT_TIMESTAMP | When was this entry last updated. | 2005-04-01 17:25:44 | | NA |

Note: columns in this table may be mapped to the GO Annotation flat file format described at *http://www.geneontology.org/GO.annotation.shtml#file*. Also see the Figure entitled "GOA relationships" below.

goa_seq_dbxref indices

| Keyname | Type | Cardinality | Field |
|---|---|---|---|
| id_idx | INDEX | 2138717 | id |
| goa_xdb_id_idx | PRIMARY | 91 | goa_xdb_id |
| xref_key_idx | PRIMARY | VC0002 | xref_key |
| taxid_1_idx | INDEX | 686 | taxid_1 |
| symbol_idx | INDEX | VC0002 | symbol |
| synonym_idx | INDEX | mioC | synonym |
| lastupdate_idx | INDEX | 2005-04-01 17:25:44 | lastupdate |

**goa_association table**

Last updated April 12, 2005

| | |
|---|---|
| **Database:** | Seqhound |
| **Table:** | goa_association |
| **Module:** | GOA |
| **Definition:** | This table contains GO term information associated with the Record ID (goa_seq_xref.xref_key). |
| **Source file:** | See module description above. |
| **Parser:** | See module description above. |

goa_association table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(10) | No | Auto increment integer. | Internal unique identifier for this record. | 33 | This identifier is incremented by the source file parser. | NA |
| is_not | char(1) | Yes | NULL | Flags that modify the interpretation of an annotation. A GO ID with a `Not` in this field means that a particular gene product is NOT associated with a particular GO term.<br>For more information please read "Using the Qualifier column" from *http://www.geneontology.org/GO.annotation.html*<br>"T" indicates that "NOT was found in this column.<br>"F" indicates that "NOT" was not found. | F | See note below. | NA |
| go_id | int(10) | No | 0 | Gene Ontology identifier for the term attributed to the object described by goa_seq_xref.xref_key. | 3677 | See note below. | NA |
| goa_seq_dbxref_id | int(10) | No | 0 | Foreign key pointing to goa_seq_dbxref.id | 7 | See note below. | NA |
| assigned_by | int(10) | No | 0 | database that made the annotation. | 117 | See note below. | |
| code | char(4) | No | | Evidence Code. One of IMP, IGI, IPI, ISS, IDA, IEP, IEA, TAS, NAS, ND, IC. | IEA | See note below. | NA |
| date | char(8) | Yes | NULL | Date on which the annotation was made. | 20040107 | See note below. | NA |
| lastupdate | timestamp | Yes | NULL | Date when this record was last modified. | 2005-04-01 17:25:44 | See note below. | NA |

Note: columns in this table may be mapped to the GO Annotation flat file format described at *http://www.geneontology.org/GO.annotation.shtml#file*. See the Figure entitled "GOA relationships" below.

goa_association indices

| Keyname | Type | Cardinality | Field |
|---|---|---|---|
| PRIMARY | PRIMARY | 8720064 | id |
| go_id | UNIQUE | 8720064 | go_id |
| | | | goa_seq_dbxref_id |
| | | | code |
| goa_id_idx | INDEX | 21268 | go_id |
| goa_seq_dbxref_id_idx | INDEX | 8720064 | goa_seq_dbxref_id |
| assigned_by_idx | INDEX | 19 | assigned_by |
| code_idx | INDEX | | code |
| lastupadate_idx | INDEX | 2005-04-01 17:25:44 | lastupdate |

**goa_reference table**

Last updated April 12, 2005

| | |
|---|---|
| **Database:** | Seqhound |
| **Table:** | goa_reference |
| **Module:** | GOA |
| **Definition:** | This table contains the reference identifier for the GO annotation. Reference identifiers are unique identifiers appropriate to a database authority for the attribution of the go_id to the Record ID. They may be a literature reference or a database record. |
| **Source file:** | See module description above. |
| **Parser:** | See module description above. |

goa_reference table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(10) | No | Auto increment integer. | A unique identifier for this record. | 1 | This value is autoincremented by the source file parser. | NA |
| goa_association_id | int(10) | No | 0 | Foreign key pointing to goa_association.id. | 530508 | See note below. | NA |
| goa_xdb_id | int(10) | No | 0 | Database identifier that made the reference. Foreign key pointing to goa_xdb.id.. | 49 | See note below. | NA |
| xref_key | varchar(20) | No | | Reference Identifier. For example, if the reference is a published paper that has a PubMed ID, the PubMed ID number will be in this field | MGI:1354194 | See note below. | NA |
| lastupdate | timestamp | Yes | NULL | When was this entry last updated? | 2005-04-01 17:25:44 | | NA |

Note: columns in this table may be mapped to the GO Annotation flat file format described at *http://www.geneontology.org/GO.annotation.shtml#file*. See the Figure entitled "GOA relationships" below.

goa_reference indices

| Keyname | Type | Cardinality | Field |
|---|---|---|---|
| PRIMARY | PRIMARY | 8424423 | id |
| goa_association_id_idx | INDEX | 8424423 | goa_association_id |
| goa_xdb_id_idx | INDEX | 18 | goa_xdb_id |
| xref_key_idx | INDEX | 2864 | xref_key |
| lastupdate_idx | INDEX | 17122 | lastupdate |

**goa_with table**

Last updated April 12, 2005

| | |
|---|---|
| **Database:** | Seqhound |
| **Table:** | goa_with |
| **Module:** | GOA |
| **Definition:** | This table is used to hold additional identifiers for annotations using certain evidence codes. For more information please see "With (or) From" section at *http://www.geneontology.org/GO.annotation.html* |
| **Source files:** | See module description above. |
| **Parsers:** | See module description above. |

goa_with table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(10) | No | Auto increment integer. | A unique identifier for this record. | 1 | This column is autoincremented by the source file parser. | NA |
| goa_association_id | int(10) | No | 0 | Foreign key pointing to goa_association.id | 530509 | See note below. | NA |
| goa_xdb_id | int(10) | No | 0 | Database Identifier that made the 'with' annotation. | 37 | See note below. | NA |
| xref_key | varchar(20) | No | | Reference identifier. | IPR001601 | See note below. | NA |
| key_type | int(10) | No | 0 | Type of the symbol annotated:<br>Type of the symbol annotated:<br>`1=gene_symbol,`<br>`2=allele_symbol,`<br>`3=gene_id,`<br>`4=sequence_id,`<br>`5=go_id.` | 0 | See note below. | NA |
| goa_seq_dbxref_id | int(10) | No | 0 | Foreign key pointing to goa_seq_dbxref.id for quick look-up from a 'with' annotation back to the record id. | 0 | See note below.<br>This field is not currently implemented. | NA |
| lastupdate | timestamp | No | NULL | When was this entry last updated? | 2005-04-01 17:25:44 | | NA |

Note: columns in this table may be mapped to the GO Annotation flat file format described at *http://www.geneontology.org/GO.annotation.shtml#file*. See the Figure entitled "GOA relationships" below.

goa_with indices

| Keyname | Type | Cardinality | Field |
|---|---|---|---|
| PRIMARY | PRIMARY | 1234449 | id |
| goa_association_id_idx | INDEX | 1234449 | goa_association_id |
| goa_xdb_id_idx | INDEX | 17 | goa_xdb_id |
| xref_key_idx | INDEX | | xref_key |
| key_type_idx | INDEX | | key_type |
| goa_seq_dbxref_id_idx | INDEX | | goa_seq_dbxref_id |
| lastupdate_idx | INDEX | | lastupdate |

**goa_xdb table**

Last updated April 12, 2005

| | |
|---|---|
| **Database:** | Seqhound |
| **Table:** | goa_xdb |
| **Module:** | GOA |
| **Definition:** | The table goa_xdb contains metadata about the organizations which contribute to the GO. There is a one to one relationship between abbreviations and URLs where data can be retrieved. A single URL which can be queried using database ids is referred to as a datasource. Each organization may have multiple datasources. Each abbreviation identifies one section of the file which provides the abbreviation and full name of that data source, the object type which is retrieved, an example database id, the generic url which identifies that data source uniquely and globally and the syntax of an actual query request with parameters filled in.<br>For more information please read:<br>*ftp://ftp.geneontology.org/pub/go/doc/GO.xrf_abbs_spec* |
| **Source files:** | See module description above. |
| **Parsers:** | See module description above. |

goa_xdb table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | Auto increment integer. | A unique identifier for this record. Note that this identifier is unstable and may change from one release to another. | 76 | This column is autoincremented by the source file parser. | NA |
| abbreviation | varchar(50) | No | | Database abbreviation. | SWISS-PROT | See note below. | NA |
| name | varchar(255) | Yes | NULL | Database name or description. | Swiss-Prot protein database. | See note below. | NA |
| object | varchar(255) | Yes | NULL | type of identifier returned from the data source:<br>Accession number<br>Locus identifier<br>call number<br>Gene symbol etc. | | See note below. | NA |
| example | varchar(50) | Yes | NULL | An example database identifier. | Swiss-Prot:P45867 | See note below. | NA |
| generic_url | varchar(255) | Yes | NULL | The root or representative URL for this data source. | `http://ca.expasy.org/sprot/` | See note below. | NA |
| url_syntax | varchar(255) | Yes | NULL | A string to which one can append a database ID and get a valid URL query for the object referenced by that id. There is no wild card to represent the database ID, it is simply appended to the end of the string. | *`http://www.expasy.ch/cgi-bin/sprot-search-ac`*? | See note below. | NA |
| url_example | varchar(255) | Yes | NULL | An example of what the url_syntax will look like | *`http://www.expasy.ch/cgi-bin/sprot-search-ac?P45867`* | See note below. | NA |
| lastupdate | timestamp | No | NULL | | 2005-04-01 17:25:44 | | NA |

Note: columns in this table may be mapped to the GO Annotation flat file format described at *http://www.geneontology.org/GO.annotation.shtml#file*. See the Figure entitled "GOA relationships" below.

goa_xdb indices

| Keyname | Type | Cardinality | Field |
|---|---|---|---|
| PRIMARY | PRIMARY | 117 | id |
| abbreviation_idx | INDEX | | abbreviation |
| name_idx | INDEX | | name |

**goa_gigo table**

Last updated April 5, 2005

| | |
|---|---|
| **Database:** | Seqhound |
| **Table:** | goa_gigo |
| **Module:** | GOA |
| **Definition:** | Pre-computed list of gi-go pairs.<br>Since SeqHound database is NCBI GI Centric and GOA is organism database ID centric; the process to get a GO term given a GI can be complicated and time consuming, for this reason a pair list of gi-go were pre-computed and stored in goa_gigo table. The SeqHound core database (mainly accdb and redund tables) is required to run these parsers. |
| **Source files:** | See module description above. |
| **Parsers:** | See module description above. |

goa_gigo table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| gi | INTEGER | No | 0 | Gene Info Identifier for an NCBI sequence record | 6552303 | The record indicated by the last two columns of this table are converted to a matching Gene Info Identifier using the DBXref module. | NA |
| go | INTEGER | No | 0 | Gene Ontology Identifier. | 6281 | From table goa_association:gi_id | NA |
| code | varchar(4) | Yes | NULL | Evidence Code. One of IMP, IGI, IPI, ISS, IDA, IEP, IEA, TAS, NAS, ND, IC. For more information please read *http://www.geneontology.org/GO.evidence.html* | TAS | From table goa_association:code | NA |
| xdb_id | INTEGER | Yes | NULL | Identifier for database. See also xref_key below. From table goa_xdb. | 103 | From table goa_xdb.id | NA |
| xref_key | varchar(30) | Yes | NULL | Identifier in database (see previous column) pointing to object that was originally annotated. | P38398 | From table goa_seq_dbxref:xref_key. | NA |
| lastupdate | timestamp | No | NULL | When was this entry last updated? | 2005-04-01 17:25:44 | | NA |

goa_gigo indices

| Keyname | Type | Cardinality | Field |
|---|---|---|---|
| PRIMARY | PRIMARY | 7936320 | gi<br>go<br>code |
| gi_idx | INDEX | 3968160 | gi |
| go_idx | INDEX | 7254 | go |
| code_idx | INDEX | | code |
| xdb_id_idx | INDEX | 22 | xdb_id |
| xref_key_idx | INDEX | 7936320 | xref_key |
| lastupdate_idx | INDEX | 22 | lastupdate |

**dbxref module**

Last updated April 12, 2005

**purpose:**

The purpose of the SeqHound dbxref module is to have a centralized data source (cross references) where related information can be found from a given ID. By using the dbxref module, it is possible to find one to "n" relationships between IDs from 3rd party databases for DNA, Protein Sequences, Domains and Interactions, GenBank Accession Numbers, Swiss-Prot, LocusLink, SGD, MGD, ZFIN, FB, PFAM, SMART, etc. See the “Explanation of the data table structure” below.

**Who Cross-references who?**

The following table indicates what database records we collect as cross-references from primary database records in the SeqHound DBXref module.
This table was last updated April 15th and may change on a regular basis.

| | **DB Cross references to:** | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Primary DBs** | GB | SPTR | CG | TAIR | UNIGENE | IPI | ENSEMBL | OMIM |
| GENE | X | X | X | | X | X | X | X |
| SPTR | X | X | X | X | X | X | X | X |
| ENSEMBL | X | X | | | | X | | |
| AFCS | X | | | | | | | |
| TIGR_ATH | X | | | | | | | |
| MGI | X | X | | | | | | |
| RGD | X | | | | | | | |
| FB | X | | | | | | | |
| WB | X | | X | | | | | |
| SGD | X | | | | | | | |
| DDB | X | | | | | | | |
| ZFIN | X | | | | | | | |
| GRAMINE | X | X | | | | | | |
| GENEDB_SPOMBE | | X | | | | | | |
| TIGR_ATH | X | | | | | | | |
| TIGR_CMR | | X | | | | | | |
| UNIGENE | | X | | | | | | |
| VIDA | | X | | | | | | |

**Explanation of the data table structure:**

The dbxref table is the core of the dbxref module. This explanation refers to that table.

Dbxref represents cross-references between 3rd party databases and GeneBank. This table is created by parsing 3rd party flat files and creating records in "dbxref" for each record parsed. dbxref is a self-referencing table.
The value in the "record_id" field may represent one of two things:

1. A source record:

   If the value of "parent_id" in the row is zero (0) it is referred to as an object id. Its "record_id" is the identifier/primary id for a record in the database ("source_db") from which cross-references have been retrieved.

For example, from the dbxref table content example listed below.

```
P38903      is a Primary ID in SwissProt Database
S00055403   is a Primary ID in SGD Database.
```

2. A database cross-reference found in a source record. The retrieved cross-references are stored as a combination of
   a) Source database ("source_db").
   b) an identifier for a record in that database ("record_id").
   c) the record that the cross-reference was found in. The field "parent_id" contains an integer. This integer refers to the row in this table (see "id") that contains the identifier of the record from which this cross reference was retrieved.
   d) cross references are retrieved from some field in a record. The name of this field is recorded in the "field" column or if there are no field names then the column number is recorded. For example : `Col1` or `Col4`.

### Example entries

| id | source_db | record_id | parent_id | link | field | cv |
|---|---|---|---|---|---|---|
| **1** | **SP** | **P38903** | **0** | **0** | **ID** | **0** |
| 2 | GB | U06630 | 1 | 0 | DR | 1 |
| 3 | GB | AAB38372 | 1 | 2 | DR | 2 |
| 4 | GB | S79635 | 1 | 0 | DR | 1 |
| 5 | GB | AAB35312 | 1 | 4 | DR | 2 |
| 6 | GB | X87331 | 1 | 0 | DR | 1 |
| 7 | GB | CAA60763 | 1 | 6 | DR | 2 |
| 8 | GB | Z74922 | 1 | 0 | DR | 1 |
| 9 | GB | CAA99203 | 1 | 8 | DR | 2 |
| 10 | InterPro | IPR001757 | 1 | 0 | DR | 3 |
| 11 | Pfam | PF00689 | 1 | 0 | DR | 3 |
| 12 | SGD | S0005540 | 1 | 0 | DR | 0 |
| **13** | **SP** | **P47096** | **0** | **0** | **ID** | **0** |
| 14 | GB | Z49525 | 13 | 0 | DR | 1 |
| 15 | GB | CAA89550 | 13 | 14 | DR | 2 |
| 16 | GB | X87297 | 13 | 0 | DR | 1 |
| 17 | IPR | IPR007113 | 13 | 0 | DR | 0 |
| **18** | **SGD** | **S00055403** | **0** | **0** | **Col4** | **0** |
| 19 | GB | 1420113 | 18 | 0 | GI | 0 |
| 20 | GermOnline | 143602 | 18 | 0 | Col1 | 0 |
| 21 | DIP | 4191 | 18 | 0 | Col1 | 4 |
| 22 | GB | 6324588 | 18 | 0 | GI | 0 |
| 23 | GB | AX596518 | 18 | 0 | Col1 | 1 |
| 24 | CandidaDB | CA1247 | 18 | 0 | Col1 | 0 |
| 25 | GB | CAA99203 | 18 | 0 | Col1 | 2 |
| 26 | InterPro | IPR002554 | 18 | 0 | Col1 | 0 |
| 27 | GB | NP_014656 | 18 | 0 | Col1 | 2 |
| 28 | SP | P38903 | 18 | 0 | Col1 | 0 |
| 29 | PIR | S54620 | 18 | 0 | Col1 | 0 |
| 30 | GB | S79635 | 18 | 0 | Col1 | 1 |
| 31 | GB | U06630 | 18 | 0 | Col1 | 1 |
| 32 | GB | X87331 | 18 | 0 | Col1 | 1 |
| 33 | MIPS | YOR014W | 18 | 0 | Col1 | 0 |
| 34 | GB | Z74922 | 18 | 0 | Col1 | 1 |

The "link", "field" and "cv" fields in the dbxref table help specify where the information is coming from. These are described below.

*link*

The link field was created to support some databases (for example Swiss-Prot) which may store more than one cross-reference in one field. For example a swiss-prot record for a protein may contain a "DR" field that lists two EMBL identifiers. ie.:

```
DR   EMBL; U06630; AAB38372.1; -.
```

The first identifier is a cross-reference for a nucleotide record in EMBL that encodes a protein (second identifier).

The link field was created to capture this relationship between the two cross-references. The integer in the link field points to a row in the dbxref table (see "id") and indicates that the current cross-reference is linked (or comes after) some other cross reference in the same source record and field.

The exact meaning of the database cross-reference can be discerned from the "cv" (Controled Vocabulary) column of this table. In this example, one cross-reference would be labeled as "`nucleotide`" and one would be labeled as "`protein`".
`2`: points to record "`id=2`" meaning that protein sequence identifier "`AAB38372`" comes after the identifier "U06630" in the DR field.
`0:` if no relationship exists or if the dbxref is the first one in a list

*field*

This describes the field in the source record where the database cross-reference was found. For example, "DR" is a field name in Swiss-Prot records indicating a Database Reference. Alternatively, a column number might be listed here is the source file was a tab-delimited text file.

*cv*

cv is a controlled vocabulary term that is used to describe the type of record that the database cross-reference is pointing to. This controlled vocabulary is simple at the moment and may be expanded in future. Briefly,

`1` indicates a DNA sequence record
`2` indicates a protein sequence record
`3` RNA
100 Swiss-Prot record
101 Trembl record
110 Swiss-Prot secondary accession
111 Trembl secondary accession

`0` means not defined.

**source code location**: /slri/seqhound/dbxref

**input Files:** *`See summary table.`*

**parsers:** *`See summary table.`*

**config file dependencies:**
dbxref.ini

**command line parameters:** *See summary table.*

**example use:** *See summary table.*

**associated scripts: (See associated scripts under GOA Module.)**

The following shell scripts execute the parsers.
*dbxrefgoa_cron_monthly.sh: Script to create all tables and sub-directories when running dbxref-goa module for the first time.*
*dbxrefgoa_updatecron.pl:* Program that automates deployment and runs parsers in a cluster. (see dbxref.ini documentation for details)

**error and run-time logs:**

*dbxrefgoa_errors.log:* log that tracks run time error by the parsers.
*dbxrefgoa_updatecron.log:* log that indicate what parser was run, completed or failed . A copy of this log will be sent by email to the SeqHound administrator.
*dbxref_parser.log:* log that summarizes number of record updates by each dbxref parser.
Error messages are sent by email when dbxrefgoa_updatecron.pl runs.

**troubleshooting:**
Check the email sent by dbxrefgoa_updatecron.pl to find out if any parsers had problems. For more details consult the log files.

**additional info:**

**How to update the DBXref and GO Annotation modules using a cluster.**

Last updated April 15th, 2005.
This section is maintained by Zhe Wang and Renan Cavero.

Note for those installing there own local instance of SeqHound. The data sets generated by this process are made available on the SeqHound ftp site at *ftp://ftp.blueprint.org/pub/SeqHound/Data/* . These instructions are supplied as a description of our internal process. The scripts described are provided as part of the SeqHound code release package for those who may wish to use them as a guide for setting up their own internal cluster build. The framework presented here might also be useful to others for setting up cluster jobs.

Dbxrefgoa_update.pl will generate scripts for distribution and execution of processes on a cluster. To accomplish this it uses clusterit tools. More information about clusterit can be found at: http://www.garbled.net/clusterit.html.

The file *dbxref.ini* has all the configurations to build and update the DBXRef/GOA modules on a computer cluster. This configuration file is read and executed by the script *dbxrefgoa_update.pl*.

**Understanding the dbxref.ini file**

Section *[DBXREFDATA]* describes the database to which the updated or new DBXRef/GOA data will be **written**. Variable "*database*" should be an existing database. The text in *italics* should be modified. The user must have write privilege to the database.

```
[DBXREFDATA]
# this should point to the server which has dbxref and goa modules
host            = staging_box
port            = 33306
user            = user
password        = passwd
database        = dbxrefgoa
table           = dbxref
tablegigo       = goa_gigo
```

Section *[SEQHOUND]* describes the SeqHound database from which information will be **read** in order to update the DBXRef/GOA modules specified in section *[DBXREFDATA]*. The user must have read privilege to the database.

```
[SEQHOUND]
# this should point to the server which has the most up-to-date tables of seqhound
hostshound     = production_box
portshound     = 3306
usersshound    = user
passwordshound = passwd
databaseshound = seqhound
working_dir    = /home/user123/dbxrefgoa/
data_dir       = /scratch/dbxrefgoa/download
myemail       = you@you.org
```

The variable "*working_dir*" specifies the directory in which to run script *dbxref_updatecron.pl*.
Directory */home/* is mapped to all cluster nodes.

Variable *"data_dir"* specifies where the input files are saved.
Directory */scratch/* is a local directory on each node.
Variable "*myemail*" should be the e-mail address of the SeqHound administrator who will be notified of the result of the DBXRef/GOA update.

Section *[LOG_FILES]* has the name for three logs files:

```
[LOG_FILES]
results_log    = dbxrefgoa_results.log
errors_log     = dbxrefgoa_errors.log
update_log     = dbxrefgoa_updatecron.log
```

Section *[DBXREF_FILES]* and *[GENE_ASSOCIATION_FILES]* specify the data files to be processed.

Each of sections *[ORGANISM_DBXREF]* and *[ORGANISM_GOA]* specifies the categories of data to be processed.

```
[ORGANISM_DBXREF]
ORGANISMS = "GENE;SP;TR"
```

The value of the variable "*ORGANISMS*" indicates that there are three groups of data that need to be processed. This particular order of GENE, SP and TR is important for internal purposes. By looking at the value of the variable "*ORGANISMS*", script *dbxrefgoa_update.pl* goes to the proper section in this configuration file, *dbxref.ini*, to find information such as where to download the data file and what commands to be executed on the data file.

For example, when *dbxrefgoa_update.pl* reads "*GENE*", it looks for section *[GENE]* in the *dbxref.ini* file. Section *[GENE]* is shown below. "*GENE_URL*" specifies the FTP path of the data file, "*GENE_CMD*" specifies the command to be run, and "*GENE_CMD2RUN*" specifies the command to be run on the cluster nodes.

```
[GENE]
GENE_URL="ftp://ftp.ncbi.nlm.nih.gov/gene/DATA/mim2gene"
GENE_CMD2RUN=perl dbxref_gene_cluster.pl
```

```
GENE_CMD="./deploy.sh GENE gene2accession"
GENE_CMD="./generate_dbxref_run.pl XREF_GENE > runXREF_GENE.sh"
GENE_CMD="./runXREF_GENE.sh"

GENE_URL="ftp://ftp.ncbi.nlm.nih.gov/gene/DATA/gene2accession.gz"
GENE_OMIM_CMD2RUN=perl dbxref_gene_extra.pl -d OMIM
GENE_CMD="./deploy.sh GENE mim2gene"
GENE_CMD="./generate_dbxref_run.pl XREF_GENE_OMIM > runXREF_GENE_OMIM.sh"
GENE_CMD="./runXREF_GENE_OMIM.sh"
GENE_CMD="./clean.sh GENE"

GENE_URL="ftp://ftp.ncbi.nlm.nih.gov/gene/DATA/gene2unigene"
GENE_UNIGENE_CMD2RUN=perl dbxref_gene_extra.pl -d UNIGENE
GENE_CMD="./deploy.sh GENE gene2unigene"
GENE_CMD="./generate_dbxref_run.pl XREF_GENE_UNIGENE > runXREF_GENE_UNIGENE.sh"
GENE_CMD="./runXREF_GENE_UNIGENE.sh"
GENE_CMD="./clean.sh GENE"
```

Script *dbxrefgoa_update.pl* first creates a sub-directory called "*GENE/wget/"* in the directory specified by the variable "*data_dir*". The newly created directory would be */scratch/dbxrefgoa/download/GENEl/wget/*. Script *dbxrefgoa_update.pl* then reads all GENE_URLs sequentially and downloads the data files if they been updated. These files are placed into the directory */scratch/dbxrefgoa/download/GENE/wget/*, and then subsequently copied one level up to the directory */scratch/dbxrefgoa/download/GENE/*. If no up-to-date data files are downloaded, script *dbxrefgoa_update.pl* finishes with this section and moves to the next according to the value of "*ORGANISMS*" in section `[ORGANISM_DBXREF]`. Once all the data files are downloaded, the script *dbxrefgoa_update.pl* reads the values of "*GENE_CMD*" and executes one command at a time.

The first part of section *"[GENE]*" is used to explain how this works.

```
[GENE]
#GENE_URL="ftp://ftp.ncbi.nlm.nih.gov/gene/DATA/gene2accession.gz"
GENE_CMD2RUN=perl dbxref_gene_cluster.pl

GENE_CMD="./deploy.sh GENE gene2accession"
GENE_CMD="./generate_dbxref_run.pl XREF_GENE > runXREF_GENE.sh"
GENE_CMD="./runXREF_GENE.sh"
```

The first command to be executed is *"./deploy.sh GENE gene2accession "*. Script *deploy.sh* makes directory */scratch/dbxrefgoa/download/GENE/* on each of the cluster nodes and copy the data file *gene2accession* into the newly created directory on each node.

The second command to be executed is *"./generate_dbxref_run.pl XREF_GENE > runXREF_GENE.sh"*. Script *generate_dbxref_run.pl* takes in one parameter, *XREF_GENE*, which refers to the full path of the data file specified in variable "*data_dir*" plus "*XREF_GENE*" in section *[DBXREF_FILE]* of the configuration file *dbxref.ini*. The data file has been copied to each cluster node by executing command *"./deploy.sh GENE gene2accession"*. Each of the cluster nodes will process a part of the data file. The data file will be evenly divided into multiple segments each of which is processed by one node. In this way, the jobs on the nodes can finish in approximately the same time.

The cluster nodes need to know where in the file to start and to end. Script *generate_dbxref_run.pl* reads the data file and calculates the start and end points of the file for each cluster node to process. The script also constructs the command line for each cluster node. The output of script *generate_dbxref_run.pl* is written to the file *runXREF_GENE.sh*.

An example of such a shell script is:

```
#! /usr/bin/bash
rsh an090 "cd /home/user123/dbxrefgoa; perl dbxref_gene_cluster.pl -c T -o 0 -n
269259 -f an090.dat >> /home/user123/dbxrefgoa/xref_parser.log 2>&1 &"
rsh an091 "cd /home/user123/dbxrefgoa; perl dbxref_gene_cluster.pl -c T -o 269259 -n 269259 -f an091.dat >>
/home/user123/dbxrefgoa/xref_parser.log 2>&1 &"
rsh an092 "cd /home/user123/dbxrefgoa; perl dbxref_gene_cluster.pl -c T -o 538518 -n 269259 -f an092.dat >>
/home/user123/dbxrefgoa/xref_parser.log 2>&1 &"
# Num of records: 807777
./wait.pl an090.dat an091.dat an092.dat
rm an090.dat an091.dat an092.dat
```

Where "*perl dbxref_gene_cluster.pl"* is the value of variable "*GENE_CMD2RUN*" in section *[GENE]*. In this example, the data file has 807,777 records that are evenly divided into three segments each of which is processed on one cluster node.

Script *dbxref_ll.pl* takes four parameters:

*–c* indicates whether this is a run on a cluster node *(-c F* would make the script process the entire data file regardless of the values of *–o* and *–n*),
*–o* indicates the starting point or offset in the file for this node,
–n indicates the number of records to be processed,
*–f* specifies the name of the flag file.

Since the next data file cannot be processed until the previous one is finished, it is necessary to know whether the process on every cluster node is completed. On each node, a flag file named *node.dat* (e.g. an091.dat) is generated when the process on that particular node is finished. The next data file won't be processed until script *wait.pl* finds file *node.dat* on all of the nodes. After this condition is met, *wait.pl* removes all flag files.

The last line in section *[GENE]* is:

```
GENE_CMD="./cleana.sh"
```

This command deletes all data files downloaded for this section from the cluster nodes in order to reclaim disk space.

All of the other sections in the dbxref.ini file have the same format as just described for *[GENE]*. These additional sections are:

[GENE], [SP], [TR], [FB]. [WB], [MGI], [SGD], [TIGR_ATH], [DDB], [RGD], [ZFIN], [XREFGOA], [GENEDB_SPOMBE], [TAIR], [TIGR_CMR], [UNIGENE], [VIDA], [GOA_CGEN], [GOA_DDB], [GOA_FB], [GOA_GENEDB_GMORSITANS], [GOA_GENEDB_LMAJOR], [GOA_GENEDB_PFALCIPARUM], [GOA_GENEDB_SPOMBE], [GOA_GENEDB_TBRUCEI], [GOA_GRAMENE_ORYZA], [GOA_MGI], [GOA_GOA_PDB], [GOA_RGD], [GOA_SGD], [GOA_TAIR], [GOA_TIGR_ATH1], [GOA_TIGR_CMR], [GOA_TIGR_TBRUCEI_CHR2], [GOA_TIGR_GENE_INDEX], [GOA_VIDA], [GOA_WB], [GOA_GOA_UNIPROT], [GOA_ZFIN] and [GO_GENE].

**Table summarizing input files, parsers and command line parameters for dbxref module.**

| ***Input file*** | **parser** | [1]**command line parameters** |
|---|---|---|
| *ftp://expasy.org/databases/uniprot/knowledgebase/uniprot_sprot.dat.gz* | dbxref_sptr_cluster.pl | -d XREF_SP |
| *ftp://expasy.org/databases/uniprot/knowledgebase/uniprot_trembl.dat.gz* | dbxref_sptr_cluster.pl | -d XREF_TR |
| *http://flybase.bio.indiana.edu/allied-data/extdb/external-databases.txt* | dbxref_fb_cluster.pl | none |
| *ftp://ftp.sanger.ac.uk/pub/databases/wormpep/wormpep.table* | dbxref_wb_cluster.pl | none |
| *ftp://ftp.informatics.jax.org/pub/reports/MRK_Sequence.rpt* | dbxref_mgi_cluster.pl | none |
| *ftp://ftp.informatics.jax.org/pub/reports/MRK_SwissProt_TrEMBL.rpt* | dbxref_mgi_cluster.pl | none |
| *ftp://genome-ftp.stanford.edu/pub/yeast/data_download/chromosomal_feature/dbxref.tab* | dbxref_sgd_cluster.pl | none |
| *ftp://ftp.afcs.org/pub/mpdata/afcsflat.txt* | dbxref_AFCS_cluster.pl | none |
| *ftp://ftp.tigr.org/pub/data/a_thaliana/ath1/DATA_RELEASE_SUPPLEMENT/release_5.genbank_accessions.txt.gz* | dbxref_tigr_ath_cluster.pl | -d XREF_TIGR_ATH |
| *ftp://ftp.geneontology.org/pub/go/gp2protein/gp2protein.tigr_ath* | dbxref_tigr_ath_cluster.pl | -d XREF_TIGR_ATH_GP |
| *ftp://ftp.blueprint.org/pub/SeqHound/Private/DDB/dictybaseid_gb_accession.txt.gz* | dbxref_ddb_cluster.pl | none |
| *ftp://rgd.mcw.edu/pub/data_release/genbank_to_gene_ids.txt* | dbxref_rgd_cluster.pl | none |
| *http://zfin.org/data_transfer/Downloads/genbank.txt* | dbxref_zfin_cluster.pl | none |
| *http://zfin.org/data_transfer/Downloads/refseq.txt* | dbxref_zfin_cluster.pl | none |
| *ftp://ftp.geneontology.org/pub/go/gp2protein/gp2protein.zfin* | dbxref_zfin_cluster.pl | none |
| *ftp://ftp.ebi.ac.uk/pub/databases/GO/goa/HUMAN/human.xrefs.gz* | dbxref_goa_xrefs_cluster.pl | -d XREF_XREFGOA_HUMAN |
| *ftp://ftp.ebi.ac.uk/pub/databases/GO/goa/MOUSE/mouse.xrefs.gz* | dbxref_goa_xrefs_cluster.pl | –d |

| ***Input file*** | **parser** | [1]**command line parameters** |
|---|---|---|
| | | XREF_XREFGOA_MOUSE |
| *ftp://ftp.ebi.ac.uk/pub/databases/GO/goa/RAT/rat.xrefs.gz* | dbxref_goa_xrefs_cluster.pl | -d XREF_XREFGOA_RAT |
| *ftp://ftp.sanger.ac.uk/pub/yeast/pombe/Mappings/gp2swiss.txt* | dbxref_DBs_SPTR_cluster.pl | `-d spombe` |
| *ftp://ftp.geneontology.org/pub/go/gp2protein/gp2protein.tair* | dbxref_DBs_SPTR_cluster.pl | `-d tair` |
| *ftp://ftp.geneontology.org/pub/go/gp2protein/gp2protein.tigr_cmr* | dbxref_DBs_SPTR_cluster.pl | `-d tigr_cmr` |
| *ftp://ftp.geneontology.org/pub/go/gp2protein/gp2protein.unigene* | dbxref_DBs_SPTR_cluster.pl | `-d unigene` |
| *ftp://ftp.geneontology.org/pub/go/gp2protein/gp2protein.vida* | dbxref_DBs_SPTR_cluster.pl | `-d vida` |
| *ftp://ftp.ncbi.nih.gov/gene/DATA/gene2accessions.gz* | dbxref_gene_cluster.pl | |
| *ftp://ftp.ncbi.nih.gov/gene/DATA/mim2gene.gz* | dbxref_gene_extra.pl | `-d OMIM` |
| *ftp://ftp.ncbi.nih.gov/gene/DATA/gene2unigene.gz* | dbxref_gene_extra.pl | `-d UNIGENE` |

**[1] command line parameters:**
All DBXref parsers can run in a cluster environment setting the –c argument.
-d Organism Database File Abbreviation: Can be found under dbxref.ini Partition [ORGANISM_DBXREF] Ex.: SPTR; FB.
-c Cluster Option: T: True (run in a cluster environment); F: False: (run stand alone).
The following options are optional. Needs to be set-up only if running in a Cluster environment.
-o Offset: The offset in a flat file where a cluster node will start parsing.
-n Number of lines: The number of line-records to process by a cluster node after the Offset is reached.
-f Flag File: For synchronization purposes. A file name that will be generated when a cluster node finishes parsing telling the Cluster's head node that the parsing is finished. (The Cluster Head node will track completion of all nodes before it continues with the next process in queue).

**dbxref table**

Last updated April 12, 2005

| | |
|---|---|
| **Database:** | SeqHound |
| **Table:** | dbxref |
| **Module:** | dbxref |
| **Definition:** | The dbxref table is the core of the dbxref module. It represents cross references between 3rd party databases and GeneBank. This table is created by parsing 3rd party flat files and creating records in "dbxref" for each record parsed. dbxref is a self-referencing table. See “Explanation of data table structure” above. |
| **Source org:** | multiple - *see summary table* |
| **Source file:** | multiple - *see summary table* |
| **FTP script:** | multiple - *see summary table* |
| **Parser:** | multiple - *see summary table* |

dbxref table

| Field | Type | Null | Default | Column_Definition | Example | Source[1] | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | Auto increment | Identifier for this entry. | 2 | All SQL insert statements will auto increment this field. | NA |
| source_id | int(11) | No | 0 | Foreign key pointing to an identifier for a database, in table dbxrefsourcedb. For example,<br>1 = Swiss-Prot,<br>2 = GenBank…etc. | 2 | See dbxrefsourcedb:source_id. | NA |
| record_id | char(30) | No | | Record identifier in database mentioned in previous column. The format of this identifier will be that of the source database. | AAD12597 | | NA |
| parent_id | int(11) | No | 0 | Link pointing to "id" (first column in this table) to the record that is the source id of the Cross-Reference. An entry of "0" indicates that this is a source record from which database cross-references are parsed. | 1 | See dbxref:id | NA |
| link | int(11) | Yes | NULL | The link field was created to support some databases (for example Swiss-Prot) which may store more than one cross-reference in one field. See the section above "Explanation of data table structure". | 0 | SQL insert statements for proteins that have dbXref to the nucleotide will have the "link" field pointing to the "id" record of the nucleotide.<br>If this relationship cannot be established the "link" value will be set to 0. | NA |
| field | char(20) | Yes | NULL | Describes the field in the source record where the database cross-reference was found. For example, "DR" is a field name for Database Reference found in Swiss-Prot records. | Col6 | | NA |
| cv | int(11) | Yes | NULL | Controled vocabulary. This will be used to describe the type of record that the cross-reference is pointing to. See the section above "Explanation of data table structure". | 2 | | NA |
| lastupdate | timestamp | No | NULL | When was this entry last updated | 2005-04-01 17:25:44 | | NA |

1. Multiple source files are parsed by multiple parsers. For details, *see summary table*.

dbxref indices

| Keyname | Type | Cardinality | Field |
|---|---|---|---|
| id_idx | INDEX | 16849002 | id |
| source_id_idx | PRIMARY | 18 | source_id |
| dbxref_id _idx | PRIMARY | 16849002 | record_id |
| parent_id_idx | PRIMARY | 16849002 | parent_id |
| link_idx | INDEX | 16849002 | link |
| field_idx | INDEX | | field |
| cv_idx | INDEX | 18 | cv |
| lastupdate_idx | INDEX | 51843 | lastupdate |

**dbxrefsourcedb table**

Last updated April 12, 2005

| | |
|---|---|
| **Database:** | seqhound |
| **Table:** | dbxrefsourcedb |
| **Module:** | dbxref |
| **Definition:** | This table assigns an internal identifier to all data sources where cross-references are found. These identifiers are used in the source_id column of the dbxref table. |
| **Source org:** | multiple - *see summary table* |
| **Source file:** | multiple - *see summary table* |
| **FTP script:** | multiple - *see summary table* |
| **Parser:** | multiple - *see summary table* |

dbxrefsourcedb table[1]

| Field | Type | Null | Default | Column_Definition | Example | Source[1] | API |
|---|---|---|---|---|---|---|---|
| source_id | int(11) | No | 0 | Database ID, primary key in table dbxrefsourcedb. For example,<br>1 = Swiss-Prot | 1 | | NA |
| source_db | char(50) | No | | Abbreviated name of database.<br>Abbreviations for database names are the same as those used by the Gene Ontology group see: "GO.xrf_abbs"<br>*ftp://ftp.geneontology.org/pub/go/doc/GO.xrf_abbs*<br>This value is mandatory. | SP | | NA |
| isprimary_db | tinyint(4) | No | 0 | Are cross-references retrieved from this database?<br>1 = YES<br>0 = NO | 1 | | NA |
| lastupdate | timestamp | No | | | 2005-04-01 17:25:44 | | NA |

1. The contents of this table are hand-edited as part of the dbxrefgoa.sql file. The entire contents of this table as of April 5, 2005 are listed below.

dbxrefsourcedb indices

| Keyname | Type | Cardinality | Field |
|---|---|---|---|
| PRIMARY | PRIMARY | 33 | source_id |
| source_db_idx | INDEX | 33 | source_db |
| lastupdate_idx | INDEX | | lastupdate |

**Contents of dbxrefsourcedb table**

(last updated March 22, 2005).

| source_id | source_db | isprimary_db |
|---|---|---|
| 1 | SP | 1 |
| 2 | GB | 0 |
| 3 | PFAM | 0 |
| 4 | INTERPRO | 0 |
| 5 | MGI | 1 |
| 6 | SGD | 1 |
| 7 | SMART | 0 |
| 8 | ZFIN | 1 |
| 9 | FB | 1 |
| 10 | CG | 0 |
| 11 | TR | 1 |
| 12 | SPTR | 1 |
| 13 | WB | 1 |
| 14 | LL | 0 |
| 15 | CGEN | 0 |
| 16 | TIGR_ATH | 1 |
| 17 | REFSEQ | 0 |
| 18 | GENEDB_SPOMBE | 1 |
| 19 | DDB | 1 |
| 20 | | 1 |
| 21 | TAIR | 1 |
| | TIGR_CMR | 1 |
| 23 | UNIGENE | 1 |
| 24 | VIDA | 1 |

| | | |
|---|---|---|
| 25 | RGD | 1 |
| 26 | IPI | 1 |
| 27 | ENSEMBL | 1 |
| 28 | AFCS | 1 |
| 29 | HUGO | 0 |
| 30 | OMIM | 0 |
| 31 | PIR | 0 |
| 32 | GENE | 1 |

**RPS-BLAST domains (rpsdb) module**

**domname parser**

Note: Not available at this time, as it has not been ported to an ODBC backend. Please go to our ftp site at *ftp://ftp.blueprint.org/pub/SeqHound/RPS/* to download precomputed domname tables.

**Rpsdb parser**

Last updated: August 4, 2004

Note: The rpsdb table is precalculated on a cluster and the resulting table is distributed in MySQL format on our ftp site. Therefore, this section is provided for informational purposes only, or for those who would like to build rpsdb tables from there own sequence/domain data; it is not necessary if one wishes simply to include the rpsdb module into their own seqhound instance, in which case they should simply download the precomputed tables.

**domname table**

Last updated: August 4, 2004

**Database:** SeqHound
**Table:** domname
**Definition:** Domain information parsed from CDD database.
**Parser:** The table is populated by the program "DomNameToDB" whose source file is *seqhoun/rps/domname.c*

The program traverses a directory that contains all the **.acd* files (obtained from NCBI ftp site *ftp://ftp.ncbi.nih.gov/pub/mmdb/cdd/acd.tar.gz*) which contains the CDD ASN.1 records

**Comments:** Similarly to rpsdb, this table has two API's. The CDD ASN.1 definition seems to be under constant flux and with every new release there are new and revised fields. This in turn requires that we modify the parser functions and update API functions accordingly.

Codebase (for historical purposes)

| Column_name | Indexed | NULL | Data_type | Size | Column_Definition |
|---|---|---|---|---|---|
| ACCESSION | Yes | No | String | 15 | CDD id |
| NAME | Yes | No | String | 25 | Short domain label |
| PDB-ID | Yes | Yes | String | 10 | ID of PDB structure that is used as 3D representative of the domain |
| ASN1 | | No | Binary object | | The entire CDD ASN.1 record from the source file |

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto incremented id |
| accession | varchar(15) | No | | CDD id |
| name | varchar(25) | No | | Short domain label |

| | | | | |
|---|---|---|---|---|
| pdbid | varchar(12) | No | | ID of PDB structure that is used as 3D representative of the domain |
| asn1 | mediumblob | No | | The entire CDD ASN.1 record from the source file |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| idom_rowid | INDEX | rowid |
| idom_acc | INDEX | accession |
| idom_name | INDEX | name |
| idom_pdbid | INDEX | pdbid |

*****accession*****

**Description:** This is the domain's Conserved Domain Database (CDD) unique identifier assigned by the CDD group in NCBI. It can also be SMART, Pfam, LOAD or CDD identifier.

**Default Value:** Null

**Source (ASN.1) :** CddIdPtr,

**Parser :** DomNameToDB

**Function:** `FillDomNameNode`

**More Info:** In early versions of CDD the accession was the Pfam or SMART identifier. Therefore, in some of the comments in the code this field is referred to as the Pfam or SMART identifier. Currently, most of the domains have a unique CDD id but some may not.

**More info:** The API functions return a list. The reason is that a domain label such as SH3 may have a SMART and Pfam entry each stored as a separate CDD entry. Both ID's will be returned.

**API:** `SHoundGetDomainIdFromLabel`(CharPtr label);

*****name*****
**Description:** Domain's short label.
**Default value:** Null
**source:** This information is obtained from **.csq* file that contains a FASTA description of the domain. The label is parsed from the definition line.
**Function:** `FillDomNameNode`
**More info:**
**API:** string GetDomainLabelFromDomainId(string s); CharPtr LIBCALL `SHoundGetDomainLabelFromDomainId`(CharPtr accession)

*****pdbid*****
**Description:** A 3D structure representative of the domain.
**Default value:** null
**source:** pCdd->master3d, part of Cdd record
**Function:** `FillDomNameNode`
**More info:**
**API:** `Get3DStructureFromDomainId`
`SHoundGetDomain3DStructure`

*****asn1*****
**Description:** This is the entire NCBI CDD ASN.1 structure.
**Default value:** Null
**source:** Cdd
**More info:**

---

**Important Note**: The CDD structure contains place holders for describing the domains parent, sibling and child domains. These are domains that are structurally or otherwise related to the domain on the sequence level. The program DomNameToDB collects this information. In the latest release of CDD that was parsed these fields were left empty.

NCBI plans to (or may have) include this information in future releases. This is important information pertaining to the domains that may be included in future versions of the DomName table. Currently, the table has not been expanded with additional fields to hold this information.

**rpsdb table**

Last updated: October 07, 2004

**Database:** SeqHound

**Table:** rpsdb

**Definition:** Domain annotation of proteins derived from RPS-BLAST and Conserved Domains Database (CDD).

**Comments:** The rpsdb is precalculated on a cluster and distributed in MySQL format on our ftp site.

This table contains two local API versions (C and C++) defined in *rpsdbapi.hpp* and *rpsdbapi.c*. For the most part the same information can be accessed by both API albeit in different forms. However, there may be cases where the two APIs are not identical.

The default e-value cutoff for data in rpsdb is 1

---

Note: The rpsdb table is precalculated on a cluster and the resulting table is distributed in MySQL format on our ftp site. Therefore, this section is provided for informational purposes only, or for those who would like to build rpsdb tables from there own sequence/domain data; it is not necessary if one wishes simply to include the rpsdb module into their own seqhound instance, in which case they should simply download the precomputed tables.

---

Codebase (for historical purposes)

| Column_name | Indexed | NULL | Data_type | Size | Column_Definition |
|---|---|---|---|---|---|
| GI | Yes | No | Integer | 10 | Sequence identifier |
| CDDID | Yes | No | Integer | 10 | CDD ID (domain ID from CDD) |
| DOMID | Yes | No | String | 12 | Domain ID from primary database (Pfam, SMART, COG, KOG or cd) |
| FROM | No | No | Integer | 6 | First a.a. position aligned to this domain |

| | | | | | |
|---|---|---|---|---|---|
| ALIGN_LEN | Yes | No | Integer | 6 | Length of alignment b/w protein and domain |
| SCORE | No | No | Integer | 10 | RPS-BLAST score |
| EVALUE | No | No | Double | 15,8 | Base 10 log of RPS-BLAST E- value |
| BITSCORE | No | No | Double | 15,8 | RPS-BLAST bit score |
| MISSING_N | No | No | Integer | 6 | The length of N-terminus residues on the domain that were not aligned |
| MISSING_C | No | No | Integer | 6 | The length of C-terminus residues on the domain that were not aligned |
| NUMDOM | Yes | No | Integer | 4 | Number of total domains mapped to this protein |

MySQL

| **Field** | **Type** | **Null** | **Default** | **Column_Definition** |
|---|---|---|---|---|
| rowid | int(11) | No | | Auto incremented id |
| gi | int(11) | No | 0 | Sequence identifier |
| cddid | int(11) | No | 0 | CDD ID (domain ID from CDD) |
| domid | char(12) | No | | Domain ID from primary database (Pfam, SMART, COG, KOG or cd) |
| rfrom | int(11) | No | 0 | First a.a. position aligned to this domain |
| align_len | int(11) | No | 0 | Length of alignment b/w protein and domain |
| score | int(11) | No | 0 | RPS-BLAST score |
| evalue | decimal(15,8) | Yes | NULL | Base 10 log of RPS-BLAST E-value |

| | | | | |
|---|---|---|---|---|
| bitscore | decimal(15,8) | Yes | NULL | RPS-BLAST bit score |
| missing_n | int(11) | No | 0 | The length of N-terminus residues on the domain that were not aligned |
| missing_c | int(11) | No | 0 | The length of C-terminus residues on the domain that were not aligned |
| numdom | int(11) | No | 0 | Number of total domains mapped to this protein |

MySQL Indexes

| **Keyname** | **Type** | **Field** |
|---|---|---|
| irps_rowid | INDEX | rowid |
| irps_gi | INDEX | gi |
| irps_cddid | INDEX | cddid |
| irps_domid | INDEX | domid |
| irps_len | INDEX | align_len |
| irps_numdom | INDEX | numdom |
| irps_gi_e | INDEX | gi<br>evalue |

**Source db:** SeqHound redundant table
**Source program:** RPS-BLAST results
**Parser :** rpsdb.h/c in *seqhound/rps*

*****gi*****
**description:** Primary sequence identifier assigned at NCBI
**Default value :** 0

**source:** GI's are collected from Seqhound redund table. Proteins that were not annotated in this table were the hypothetical ORF from RefSeq (XP_xxxxxx) and SWISS-PROT proteins. These proteins are not present in SeqHound (no Bioseq) although their GI's are in redund table. In each redundant group the first GI was used for computing RPS-BLAST (ordinal 1). These proteins are considered to be the best representative of the redundant group. However, some redundant groups may not have the first GI in SeqHound, in those cases the program collects ordinal 2 or higher. The redundant list is collected from redund table using "*redundlist*" program (*seqhound/rps*).

**API:** `SHoundGetGisByDomainIdAndEvalue`
`SHoundGetGisByDomainId`
`SHoundGetGisByNumberOfDomains`

**Comment:** There are two functions in the C version that use Codebase relational query. They should not be used and are there for experimental purposes only.

**More info:** *seqhound/rps/rpsdb_README.txt*

*****cddid*****

**description:** Conserved Domain Database unique identifier.

**Default Value:** none

**Source (ASN.1) :** CddIdPtr, can also be collected from CddHitPtr cdd_id field.

**Parser :** rpsdb

**Function:** `RPSDBSHoundRedund2ResultsCallback`

**More info:** *seqhound/rps/rpsdb_README.txt*

*****domid*****

**Description:** Domain identifier from the primary database of origin. These correspond to either Pfam or SMART string identifiers.

**Default Value:** Null

**source:** Definition field in CddHitPtr structure.
**Function:** `RPSDBSHoundRedund2ResultsCallback`

*****rfrom*****
**Description:** The index position of the first amino acid in the protein that is aligned with this domain.
**Default value:** 0
**source:** Start field in CddHitPtr structure
**Function:** `RPSDBSHoundRedund2ResultsCallback`

*****align_len*****
**Description:** The length of sequence alignment between the protein and the domain.
**Default value :** 0
**source:** stop- start field values in CddHitPtr.
**Function:** `RPSDBSHoundRedund2ResultsCallback`

*****score*****
**Description :** RPS-BLAST score parameter
**Default value:** 0
**source:** score field in CddHitPtr
**Function:** `RPSDBSHoundRedund2ResultsCallback`

*****evalue*****
**Description :** Base 10 log of RPS-BLAST evalue score
**Default value:** 0
**Source:** evalue field in CddHitPtr
**Function:** `RPSDBSHoundRedund2ResultsCallback`

*****bitscore*****

**Description:** RPS-BLAST bit score
**Default :** 0
**source:** bitscore field in CddHitPtr
**Function:** `RPSDBSHoundRedund2ResultsCallback`

*****missing_n*****
**Description:** The number of residues on the domain's N-terminus that were not aligned with the protein. The missing length on the N-terminus of the domain.
**Default:** 0
**source:** It is collected from DenseDegPtr which is part of SeqAlign structure. This structure is filled up by the RPS-BLAST engine. It contains the collection of aligned segments between the domain and the protein.
**Function:** `RPSDBSHoundRedund2ResultsCallback`

*****missing_c*****
**Description:** The number of missing residues not aligned in the domain's C-terminus.
**Default:** 0
**source:** Same as MISSING_N
**Function:** `RPSDBSHoundRedund2ResultsCallback`

*****numdom*****
**Description:** The total number of domains aligned with the protein.
**Default:** 0
**source:** The number of entries for the query GI in the rpsdb..
**Function:** `SLRICddCountSeqAligns` in rpsdb

**API:** The above fields are all accessed through a set of calls that retrieve the domain annotation based on different requirements.

```
SHoundGetDomainsFromGi
SHoundGetDomainsFromGiWithEvalue
SHoundGetDomainsFromGiListWithEvalue
```

**Molecular Interaction (MI) module**

**MI-BIND parser**

Last updated October 1, 2004

**purpose:**

The Molecular Interaction module is meant to consolidate the interaction data, and associated annotation, from disparate source interaction databases(e.g. BIND, IntAct, MINT, etc). The source data is parsed out of their own unique formats and placed into the MI module tables' data model. This data model has been designed to provide maximum flexibility in terms of the complexity of queries that can be made to it. Additionally, the module adds value to the data by cross-referencing distinct records, regardless of their source databases, to provide information on molecular object redundancy and interaction similarity. The MI module's set of parsers takes records from source interaction modules, parse out their data, and insert that data into the MI tables. Currently, there exists only one such parser, for parsing BIND XML records; parsers for other interaction databases will be developed in the future.

**Logic:**

**MI-BIND parser:**

This parses the BIND XML records, available on the BIND ftp site. It uses the SAX XML parsing API, in order to achieve maximum parsing speed. In order to foster code reusability, the parser is broken down into three components: The first component parses out the BIND XML records interaction data and places it into a general MI data structure. This data structure is then passed to another component, which is responsible for placing the contents into the MI tables in the database. Another component is then called to do the cross-referencing and redundancy/similarity analysis on the data just processed, and places that additional annotation into the database. This break-down is convenient, because it means that developers of MI parsers for other source interaction databases will only need to replace the first component, the one which parses the data out of the source record, which they can then pass to the already written data feed and cross-referencing components. The parser was written in the Java programming language to take advantage of Java's mature XML processing capabilities, and because a great deal of java source code was available from the open source BIND project for processing BIND XML records.

**input files:**

The MI-BIND parser processes BIND records in their native XML format. These are available from the BIND ftp site, in a number of different partitions, each of which can be used interchangeable. In order to import all of BIND into the MI module, one would download the “Divisions” partition from
*ftp://ftp.blueprint.org/pub/BIND/data/divisions/xml/*.xml*

and then process this list of input files using the MI-BIND parser.
**tables altered:**

MI_complex2ints
MI_complex2subunits
MI_complexes
MI_dbases
MI_exp_methods
MI_ints
MI_mol_type
MI_obj_dbases
MI_obj_labels
MI_objects
MI_record_types
MI_refs
MI_refs_db
MI_source
source code location:
The source is contained in the following seqhound java packages:
*org.bluprint.seqhound.parsers.mi*
*org.bluprint.seqhound.parsers.mi.bind*
**config file dependencies:**

MI.properties file

This file must be present in the same directory as where the MI-BIND parser is being invoked, and must contain the entries:

```
dbDriverName=myDatabaseDriversName
dbUserName=myDatabaseUserName
dbPassWord=myDatabasePassword
dbURL=myDatabaseConnectionURL
```

These contain the settings, which the parser will use to connect to the database management system, which manages the MI data tables. An example entry follows:

```
dbDriverName=com.mysql.jdbc.Driver
dbUserName=johnsmith
dbPassWord=johmsmithspassword
dbURL=jdbc:mysql://dbhostname:dbportnumber/MIdbname
```

**library dependencies:**

Along with the standard java runtime environment, the MI-BIND parser requires one third party java library; this is the open source xerces2 XML parser implementation, available for free from the apache foundation(see *http://xml.apache.org/xerces2-j/download.cgi* for free download instructions).

The xerces jar files *xercesImpl.jar* and *xmlParserAPIs.jar* must be in classpath when executing the parser.

The MI-BIND parser has been tested only with xerces2 java version 2.6.2, but may work with other versions.

**command line parameters:**

The MI-BIND parser takes one command line argument: a file containing a list of filenames of files for the parser to process.
**example use:**

**`java org.blueprint.seqhound.parsers.mi.bind.bmdParse BINDXMLFileList.txt`**
Where ***`BINDXMLFileList.txt`*** is a text file containing a newline delimited list of the names of files containing the BIND XML records to be processed; these BIND XML files must be in the same directory. Note that the compiled bind module parser files, as well as the xerces jars, must be in classpath in order for the above command to function.

**associated scripts:**

none
**error and run-time logs:**

runtime and error information is printed to standard output and standard error, respectively. This will likely be changed in a future release, to print to a standard log file.
troubleshooting:
**additional info:**

**MI_source table**

Last updated October 4, 2004

**Database:** MI
**Table:** MI_source
**Module:** Molecular Interaction(MI)
**Definition:** Contains information about the source of an interaction record

MySQL

| Field | Type | Null | Default | Column Definition |
|---|---|---|---|---|
| uid | Int(11) | No | | Internal MI identifier for record |
| intcompid | Int(11) | No | 0 | Internal MI identifier of the interaction, complex or pathway this record refers to |
| db | Smallint(6) | Yes | NULL | Internal MI identifier of the source db which this record comes room, corresponds to db column of MI_dbases |
| acc | Varchar(10) | Yes | Null | Source db accession of this record, if it exists |
| id | Int(11) | Yes | Null | Source db ID of this record, if it exists |
| type | Smallint(6) | No | Null | Type of this record, either interaction(1), complex(2) or pathway(3) |
| descr | Text | Yes | Null | Text description of this record from the source db |
| data_blob | Longblob | Yes | Null | Binary version of original record from source db, if it exists |
| data_clob | Longtext | Yes | Null | Text version of original record |

| | | | | |
|---|---|---|---|---|
| | | | | from source db, if it exists |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| Primary | Primary | uid |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

*****uid*****
**description:**
**example:**
**default value**
**ASN.1 structure:**
**parser:**
**function:**
**API:**
**more info:**

**MI_ints table**

Last updated October 4, 2004

**Database:** MI
**Table:** MI_ints
**Module:** MI
**Definition:** Contains information about individual interactions

MySQL

| Field | Type | Null | Default | Column Definition |
|---|---|---|---|---|
| intid | Int(11) | No | | Internal MI id of this interaction |
| objAid | Int(11) | No | 0 | Internal MI id of the first object in this interaction |
| objBid | Int(11) | No | 0 | Internal MI id of the second object in this interaction |
| rig | Int(11) | No | 0 | Internal MI id of the redundant interaction group to which this interaction belongs |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| Primary | Primary | intid |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

**MI_objects table**

Last updated October 4, 2004

**Database:** MI
**Table:** MI_objects
**Module:** MI
**Definition:** Contains information about the individual objects involved in interactions, complexes and pathways

MySQL

| Field | Type | Null | Default | Column Definition |
|---|---|---|---|---|
| objid | Int(11) | No | | Internal MI identifier for the object which this row describes |
| type | Smallint(6) | No | 0 | Internal MI identifier for the molecule type of this object; corresponds to column type of MI_mol_type |
| db | Smallint(6) | No | 0 | Internal MI identifier for the source db of this object; corresponds to column db of MI_obj_dbases |
| id | Int(11) | Yes | Null | Source db id of this object |
| tax | Int(11) | Yes | Null | NCBI taxonomy id of this object, if applicable |
| acc | Varchar(20) | Yes | Null | Source db accession of this object |
| rog | Int(11) | No | 0 | Internal MI id of the redundant object group to which this object belongs |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| Primary | Primary | objid |

| | |
|---|---|
| **Observation:** | |
| **Source org:** | Blueprint |
| **Source file:** | BIND division files |
| **FTP script:** | N/A |
| **Parser:** | MI-BIND |

**MI_obj_dbases table**

Last updated October 4, 2004

**Database:** MI
**Table:** MI_obj_dbases
**Module:** MI
**Definition:** Table of objects source databases

MySQL

| Field | Type | Null | Default | Column Definition |
|---|---|---|---|---|
| db | Smallint(6) | No | | Internal MI identifier for the source db |
| db_name | Varchar(30) | No | | The name of the object source db |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| Primary | Primary | db |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

**MI_mol_types table**

Last updated October 4, 2004

**Database:** MI
**Table:** MI_mol_types
**Module:** MI
**Definition:** Molecular types of objects

MySQL

| Field | Type | Null | Default | Column Definition |
|---|---|---|---|---|
| type | Smallint(6) | No | | Internal MI identifier for molecules of this type |
| type_name | Varchar(15) | No | | Natural language name for this molecule type |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| Primary | Primary | type |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

**MI_dbases table**

Last updated October 4, 2004

**Database:** MI
**Table:** MI_dbases
**Module:** MI
**Definition:** Table of source databases for interaction records

MySQL

| Field | Type | Null | Default | Column Definition |
|---|---|---|---|---|
| db | Smallint(6) | No | | Internal MI identifier for this source interaction database |
| db_name | Varchar(30) | No | | Natural language name for this source interaction database. |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| Primary | Primary | db |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

**MI_record_types table**

Last updated October 4, 2004

**Database:** MI
**Table:** MI_record_types
**Module:** MI
**Definition:** Table of types for interaction records

MySQL

| Field | Type | Null | Default | Column Definition |
|---|---|---|---|---|
| type | Smallint(6) | No | | Internal MI identifier for this record type |
| type_name | Varchar(20) | No | | Natural language name for this record type(by default, either interaction, complex or pathway). |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| Primary | Primary | type |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

**MI_complexes table**

Last updated October 4, 2004

**Database:** MI
**Table:** MI_complexes
**Module:** MI
**Definition:** Table of complex and pathway records

MySQL

| Field | Type | Null | Default | Column Definition |
|---|---|---|---|---|
| compid | Int(11) | No | | Internal MI identifier for this complex record |
| numsubunits | Int(11) | No | 0 | Number of subunits in this complex |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| Primary | Primary | compid |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

**MI_complex2ints table**

Last updated October 4, 2004

**Database:** MI
**Table:** MI_complex2ints
**Module:** MI
**Definition:** Mapping of complexes to their component interactions

MySQL

| Field | Type | Null | Default | Column Definition |
|---|---|---|---|---|
| compid | Int(11) | No | 0 | Internal MI identifier for this complex |
| intid | Int(11) | No | 0 | Internal MI identifier for an interaction which is a component of this complex |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| | | |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

**MI_complex2subunits table**

Last updated October 4, 2004

**Database:** MI
**Table:** MI_complex2subunits
**Module:** MI
**Definition:** Mapping of complexes to subunits

MySQL

| Field | Type | Null | Default | Column Definition |
|---|---|---|---|---|
| compid | Int(11) | No | 0 | Internal MI identifier for this complex |
| objid | Int(11) | No | 0 | Internal MI identifier for the subunit object which belongs to this complex |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| | | |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

**MI_complex2subunits table**

Last updated October 4, 2004

**Database:** MI
**Table:** MI_complex2subunits
**Module:** MI
**Definition:** Mapping of complexes to subunits

MySQL

| Field | Type | Null | Default | Column Definition |
|---|---|---|---|---|
| compid | Int(11) | No | 0 | Internal MI identifier for this complex |
| objid | Int(11) | No | 0 | Internal MI identifier for the subunit object which belongs to this complex |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| | | |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

**MI_refs table**

Last updated October 6, 2004

**Database:** MI
**Table:** MI_refs
**Module:** MI
**Definition:** Mapping of MI records to literature references which support it

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| uid | Int(11) | No | 0 | Internal MI identifier for the interaction record which this reference is a part of |
| db | Smallint(6) | No | 0 | Internal MI identifier for the reference database which this reference is from (eg pubmed or medline) |
| acc | Varchar(15) | Yes | Null | Accession of this reference from source reference database |
| id | Int(11) | Yes | Null | ID of this reference from the source reference database |
| method | Smallint(6) | No | 0 | Internal MI identifier for the experimental method used in the referenced experiment |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| | | |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A

**Parser:** MI-BIND

**MI_refs_db table**

Last updated October 6, 2004

**Database:** MI
**Table:** MI_refs_db
**Module:** MI
**Definition:** Mapping of internal MI reference database Ids to source reference databases

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| db | Smallint(6) | No | | Internal MI identifier for this reference database |
| db_name | Varchar(15) | Yes | Null | The natural language name of the reference source database |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| Primary | Primary | db |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

**MI_exp_methods table**

Last updated October 6, 2004

**Database:** MI
**Table:** MI_exp_methods
**Module:** MI
**Definition:** Mapping of internal experimental method identifiers to their descriptions

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| method | Smallint(6) | No | | Internal MI identifier for this experimental method |
| method_descr | Varchar(40) | Yes | Null | Natural language name of the experimental method |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| Primary | Primary | method |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

**MI_obj_labels table**

Last updated October 6, 2004

**Database:** MI
**Table:** MI_obj_labels
**Module:** MI
**Definition:** Mapping of molecular objects to their free form labels

MySQL

| Field | Type | Null | Default | Column_Definition |
|---|---|---|---|---|
| uid | Int(11) | No | 0 | Internal MI identifier for the interaction/complex/pathway record which assigns this label to this object |
| objid | Int(11) | No | 0 | Internal MI identifier for the molecular object being labeled |
| label | Text | Yes | Null | Free form label given to this molecular object by this interaction/complex/pathway record |

MySQL Indexes

| Keyname | Type | Field |
|---|---|---|
| | | |

**Observation:**
**Source org:** Blueprint
**Source file:** BIND division files
**FTP script:** N/A
**Parser:** MI-BIND

## Text mining module

### Overview:

The SeqHound text mining module helps researchers locate mentions and co-mentions of biologically related entities in the scientific literature.
At the time of writing this is limited to finding protein mentions in PubMed abstracts. The module however has been designed to be extensible to small molecules, complexes and even biological concepts in both abstract and full-text articles. Each of the steps in the process may be scored by multiple methods that can be developed internally or by external developers.

### mother parser

Note that a number of the tables in the text module are created at the same time as the creation of the other core tables (see core.sql) and some of these tables are populated by the mother parser (see table descriptions below). Mother, is used to retrieve protein names and synonyms from the RefSeq database, so these tables are created at the same time as other core module tables. The mother parser is described under the core module section above. Parsers specific to the text module are described below.

**text searcher parser**

last updated February 25th, 2005

**purpose:**

The text update parser and related programs are used to collect bionames, search against a literature database, and then investigate co-mentions of bioentities in the literatures. The co-mentions of bioentities are scored using pattern recognition and statistical machine learning methods to look for potential biophysical interactions between bioentities. The text mining module tables are updated daily.

**logic:**

Most of the update logic is implemented in the Text.pm Perl module and other scoring programs. The text update parser calls the functions in Text.pm and other Perl modules. The text mining module depends on the CORE module to generate and update names of proteins and on the MyMED in house literature database. These resources are updated daily. The steps taken to update the text-mining module are as follows:

Step 1: Collect bioentity names from the lexicon
Step 2: Formulate searches; collect search results and scores
Step 3: Collect co-occurrences of names and scores
Step 4: Summarize evidence for each pair of bioentities and scores

**module: text**

**input files:**

Latest Medline release: *ftp://ftp.ncbi.nih.gov/nlmdata/.medlease/*.xml.gz*

Latest PubMed Central release: *ftp://ftp.ncbi.nlm.nih.gov/pub/pmc/*

Latest Biomed Central release: *ftp://ftp.biomedcentral.com/*

Latest NRC LitMiner SVM release: *http://ii200.iit.nrc.ca/~martinj/*

British National Corpus: *ftp://ftp.itri.bton.ac.uk/bnc/*

Moby project English word list: *http://www.dcs.shef.ac.uk/research/ilash/Moby/*

PubMed help stop word list: *http://www.ncbi.nlm.nih.gov/entrez/query/static/help/pmhelp.html#Stopwords*

Smart English stop word list: *ftp://ftp.cs.cornell.edu/pub/smart/english.stop*

**tables altered:**

text_bncorpus, text_db, text_doc, text_docscore, text_doctax, text_englishdict, text_evidence, text_evidencescore, text_method, text_namepair, text_namepairresult, text_organism, text_pattern, text_point, text_pointscore, text_result, text_resultscore, text_rng, text_rngscore, text_search, text_searchscore, text_stopword

**source code location:**

*slri/seqhound/text/text_update.pl*

**config file dependencies:**

*slri/seqhound/text/text.ini*

**command line parameters:**

Typing "**`./text_update.pl -`**" or "**`perl text_update.pl -`**" at the command line while in the directory where text_update.pl resides will return a list of command line parameters and default settings.

```
text_update.pl   arguments:

      -r  redo all name searches against new insertions from MyMED using time stamp [T/F] optional

      -t  taxnomy ids for organism to be searched, seperated by comma. If specified in command line, only provided
      organism(s) will be searched. Otherwise, a default list of taxids stored in text.ini file will be searched.
      Optional

      -u update target table only, default is all. Optional
```

**example use:**

For example:

```
>./text_update.pl -r F –t 4932,10090,9606 -u text_searchscore
```

**associated scripts:**

*slri/seqhound/text/text.sql* Data Definition file for text mining module tables.

*slri/seqhound/text/text_dump.sh* Mysql dump script for portable tables.

*slri/seqhound/text/text_create.sh* Script used to create Text database, the starting point.

*slri/seqhound/text/text_regex.pl* Script used to score evidence using regex patterns.

*slri/seqhound/text/Text.pm* contains most functions that will be using for update.

*slri/seqhound/text/Pattern.pm* Perl module used to represent regular expression objects.

*slri/seqhound/text/Tee.pm* Perl module used to branch the output to different outputs.

*slri/seqhound/text/text_updatecron.sh* Text module daily update cron script.

*slri/seqhound/text/myeutils.pl* Entrez eutil script used for comparing results between MyMED and entrez searches.

**error and run-time logs:**

Errors and runtime logs will be directed to file specified in text.ini , current default log file name is text_update.log

Daily update log will also be send to email account specified in text.ini file

**troubleshooting:**

Check the email message sent by text_update.pl to see if there is any error during update. Consult update log file to look for detail problem.

**additional info:**

All text mining module tables are in small cases, and are prefixed with "text_". Tables with auto incremented rowid have a primary key "id" as default. When referencing primary key in other table, the field name in the referencing table will be the referenced table name plus id.

**yeastnameparser.pl parser**

Last updated September 27, 2004

**purpose:**

The yeastnameparser extracts names from the SGD file *SGD_features.tab*. Only names that belong to yeast records that are already in RefSeq are added, as determined using the DBXRef module. This means that this parser MUST be run after the DBXRef parsers.
It is not necessary to run this parser, if yeast names are not desired.

**logic:**

The yeastnameparser reads through each record in *SGD_features.tab*. It searches for a refseq cross reference for each record. If one is found, then the parser gets the relevant bioentityid and checks all names for that bioentityid.
If the name does not already exist in the database, then it is added and the db field is set to "sgd" and the access field is set to the SGDID. The action field is set to 1, ADD and the current data is written to actiondate.
Existing names in the database are also compared to the file. Names which are no longer present in the yeast file are marked as deleted (action =2) and the current data is written to actiondate. If the name already exists in refseq, then a SECONDREFS record is filled out for the yeast record.
module: names

input files:

*SGD_features.tab* from
*ftp://genome-ftp.stanford.edu/pub/yeast/data_download/chromosomal_feature/*

**tables altered:**

bioentity, bioname, secondrefs

**source code location:**

*slri/seqhound/names/yeastnameparser.pl*

**config file dependencies:**

The relevant configuration files are:

*.intrezrc and .odbc.ini* should be set up as described above for seqhound. The values will be read by *shconfig.pm*, which should be located in the same directory as *yeastnameparser.*

**command line parameters:**

None.

**example use:**

```
perl yeastnameparser.pl
```

**associated scripts:**

The program *yeastnamecron.pl* can be used for both the initial read of *SGD_features.tab* and updates of the file. *yeastnamecron.pl* checks whether *SGD_features.tab* needs updating, downloads it and calls *yeastnameparser.pl. SGD_features.tab* is updated weekly by SGD.

**error and run-time logs:**

*yeastnameparser* writes errors to a file called *yeastname.log*. Updates are written to a file called *yeastupdate.log* as a tab delimited file where the fields are: name, sgdid, bionameid and field. Additions are written to a file called *yeastadd.log* as a tab delimited file where the fields are:name, sgdid bioentityid and field.

**troubleshooting:**

**additional info:**

**text_bioentity table**

Last updated Febuary 15, 2004

| | |
|---|---|
| **Database:** | SeqHound |
| **Table:** | text_bioentity |
| **Module:** | text (note mother parser is part of the core module) |
| **Definition:** | A bioentity refers to any biological object with names that may be used in the literature to refer to these objects. Currently, all bioentities are proteins from RefSeq. This table tells us which database contains the primary record for this bioentity, the accession and the field which refers to this bioentity. At the moment, all bioentities are obtained from RefSeq. RefSeq was chosen because it represents a high quality database of non-redundant records. The intention of this part of the core is to collect a non-redundant list of biological objects and the names that are used in written language to refer to them by. |
| **Source file:** | **.bna.gz* from *ftp://ftp.ncbi.nih.gov/refseq/release/complete* |
| **FTP script:** | *asnftp.pl* |
| **Parser:** | mother |

text_bioentity table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | no | | Auto incremented id. A unique identifier for this bioentity. | 1 | mother parser autoincrements this field | SHoundBioentityIdFromGi<br>SHoundBioentityIdFromAcc<br>SHoundBioentityIdListFromBionameAndTaxId |
| bioentitytypeid | int(11) | No | 0 | Bioentity type (for example, molecule type). Id from the bioentitytype table. | 1 | mother parser (see GetType()) parsing and see bioseq->mol | SHoundBioentityFromBioentityId |
| db | varchar(15) | No | | The primary database where this bioentity was found. | ref | mother parser inserts "ref" | SHoundBioentityFromBioentityId |
| access | varchar(20) | No | | Accession in the primary database. Any alphanumeric identifier used by the primary database. | NP_858066 | mother parser (see FillBionameDB()) and see bioseq-->seqid | SHoundBioentityFromBioentityId |
| identifier | int(11) | Yes | | Numeric identifier for this bioentity in the primary database; for example an NCBI Gene Info identifier (GI). This field is not required. | 31982991 | mother parser (see GetGI) see bioseq-->seqid (choice 12)). | SHoundBioentityFromBioentityId |
| fieldtypeid | int(11) | No | | A number that represents the field from which this bioentity was derived. This is the id from the fieldtype table. For example, 1 indicates the ASN.1 path "seqentry/seqset/bioseq" | 1 | mother parser (see ASN.1 path) | SHoundBioentityFromBioentityId |

text_bioentity indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | access |
| ibioe_id | INDEX | id |
| ibioe_type | INDEX | bioentitytypeid |
| ibioe_identifier | INDEX | identifier |

**text_bioname table**

Last updated February 15, 2005

| | |
|---|---|
| **Database:** | SeqHound |
| **Table:** | text_bioname |
| **Module:** | text (note that the mother parser is part of the core module) |
| **Definition:** | This table holds names for bioentities. A Bioname is some "name" applied to some bioentity. |
| **Source org:** | NCBI |
| **Source file:** | **.bna.gz from ftp://ftp.ncbi.nih.gov/ncbi/refseq/release/complete* |
| **FTP script:** | *asnftp.pl* |
| **Parser:** | mother |

text_bioname table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | A unique identifier for this bioentity-name pair. | 1 | mother parser auto increments this column | SHoundBionameListFromBioentityId |
| timestamp | datetime | Yes | NULL | | | mother parser yeastnameparser | |
| bioentityid | int(11) | No | 0 | The id of the bioentity to which this name refers. | 1 | mother parser yeastnameparser | SHoundBionameListFromBioentityId |
| name | text | No | | The name. | 2-isopropylmalate synthase | mother parser yeastnameparser | SHoundBionameListFromBioentityId |
| nametypeid | int(11) | No | 0 | Type of name. For example, protein name (1) or gene name (2). This is the id from the nametype table. | 1 | mother parser yeastnameparser | SHoundBionameListFromBioentityId |
| db | varchar(15) | No | | The database in which this name was found. | ref | mother parser yeastnameparser | SHoundBionameListFromBioentityId |
| access | varchar(20) | No | | The accession of the record in which this name was found. | NP_047187 | mother parser yeastnameparser | SHoundBionameListFromBioentityId |
| identifier | int(11) | Yes | NULL | The identifier of the record in which this name was found; for example a Gene Info identifier (GI). | 10954458 | mother parser yeastnameparser | SHoundBionameListFromBioentityId |
| fieldtypeid | int(11) | No | 0 | The field of the record in which this name was found. This is the id from the fieldtype table; for example, 5 indicates the ASN.1 path "seqentry/seqset/bioseq/descr-title/" | 5 | mother parser yeastnameparser | SHoundBionameListFromBioentityId |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| official | int(11) | Yes | 0 | Is this an official name? 1=Yes, 2=N0 | 1 | yeastnameparser | SHoundBionameListFromBioentityId |
| deprecated | int(11) | Yes | 0 | Has this name been deprecated? Not used at present. | 0 | | SHoundBionameListFromBioentityId |
| datedeprecated | datetime | Yes | 0000000000 00000 | The date the name was deprecated. | 0000000000 000 | mother parser yeastnameparser | SHoundBionameListFromBioentityId |
| ruleid | int(11) | Yes | NULL | What rule was used to construct this name? This is the id from the rules table. For example, 1 indicates that A gene name is being used to refer to a protein. | 1 | mother parser yeastnameparser | SHoundBionameListFromBioentityId |
| action | char(1) | Yes | A | What was the last action taken on this record. A=ADD, D=DELETE. | | mother parser yeastnameparser | |
| actiondate | datetime | Yes | 0000000000 00000 | Date of the last action. | 2004-08-20 01:30:08 | mother parser yeastnameparser | |

text_bioname indices

| **Keyname** | **Type** | **Field** |
|---|---|---|
| ibioname_id | INDEX | id |
| ibioname_identifier | INDEX | identifier |
| ibioname_access | INDEX | access |
| ibioname_bioentityid | INDEX | bioentityid |
| ibioname_nametypeid | INDEX | nametypeid |
| ibioname_official | INDEX | official |
| ibioname_deprecated | INDEX | deprecated |
| ibioname_ruleid | INDEX | ruleid |
| ibioname_action | INDEX | action |
| ibioname_actiondate | INDEX | actiondate |

**text_secondrefs table**

Last updated February 15, 2005

| | |
|---|---|
| **Database:** | SeqHound |
| **Table:** | text_secondrefs |
| **Module:** | core |
| **Definition:** | Additional references for sources of bionames. |
| **Source org:** | SGD |
| **Source file:** | *SGD_features.tab* from ftp://genome-ftp.stanford.edu/pub/yeast/data_download/chromosomal_feature/ |
| **FTP script:** | *yeastnamecron.pl* |
| **Parser:** | *yeastnameparser.pl* |

text_secondrefs table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | id of the second reference. Mysql auto-increment column. | 1 | yeastnameparser will Auto-increment this column | |
| timestamp | datetime | Yes | NULL | | | yeastnameparser | |
| bionameid | int(11) | No | 0 | id of the name that this reference refers to. | 1 | yeastnameparser retrieves this from text_bioname table | |
| db | varchar(15) | No | | Database in which this reference is found. | sgd | yeastnameparser (see AddSeconfRef()) | |
| access | varchar(20) | Yes | NULL | Accession of the record that refers to the name. | S000033 | yeastnameparser (see AddSeconfRef()) | |
| fieldtypeid | int(11) | No | 0 | Identifies the field in the record where this name was found. | 101 | yeastnameparser (see AddSeconfRef()) | |

text_secondrefs indices

| Keyname | Type | Field |
|---|---|---|
| isecondrefs_id | INDEX | id |
| isecondrefs_bionameid | INDEX | bionameid |
| isecondrefs_dbsearch | INDEX | access, db |
| isecondrefs_field | INDEX | field |

**text_bioentitytype table**

Last updated February 15, 2005

**Database:** SeqHound

**Table:** text_bioentitytype

**Module:** text (note that this table is currently defined when the core module is created)

**Definition:** Look up table that stores bioentity types.

**Source org:** Blueprint

**Source file:** *core.sql*

**FTP script:** NA

**Parser:** NA

text_bioentitytype table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Identifier for a bioentitytype. Mysql auto-increment column. | 1 | core.sql | |
| type | varchar(80) | No | | The molecule type. | protein | core.sql | |

text_bioentitytype indices

NA

**text_fieldtype table**

Last updated February 15, 2005

**Database:** SeqHound

**Table:** text_fieldtype

**Module:** text (note that this table is defined when the core module is created)

**Definition:** Look up table that stores the field that contains the name.

**Source org:** Blueprint

**Source file:** This is a look up table that is filled by *core.sql*

**FTP script:** *NA*

**Parser:** NA

text_fieldtype table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Identifier for a fieldtype. | 1 | core.sql | |
| pathtofield | varchar(80) | No | | The field that contains the name. For an ASN.1 record, this is the ASN.1 "path" to the field that contains the name. For a flat file, this is of the form "Column #:Column Name". | `seqentry/seqset/bioseq/seq-annot/seqfeat-gene/syn` | core.sql | |

text_fieldtype indices

NA

**text_nametype table**

Last updated February 15, 2005

**Database:** SeqHound

**Table:** text_nametype

**Module:** text (note that this table is defined when the core module is created)

**Definition:** Look up table that stores name types.

**Source org:** Blueprint

**Source file:** This is a look up table that is filled by *core.sql*

**FTP script:** *NA*

**Parser:** NA

text_nametype table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Identifier for a nametype. Mysql auto-increment column. | 1 | core.sql | |
| type | varchar(880) | No | | The type of name. | protein | core.sql | |

text_nametype indices

NA

**text_rules table**

Last updated September 30, 2004

**Database:** SeqHound

**Table:** text_rules

**Module:** text (note that this table is defined when the core module is created)

**Definition:** Look up table that stores rules for generating names.

**Source org:** Blueprint

**Source file:** This is a look up table that is filled by *core.sql*

**FTP script:** *NA*

**Parser:** NA

text_rules table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Identifier for a rule. Mysql auto-increment column. | 1 | core.sql | |
| type | varchar(80) | No | | The rule. | Use gene name for protein. | core.sql | |

text_rules indices

NA

**text_db table**

Last updated February 15, 2005

**Database:** seqhound

**Table:** text_db

**Module:** text

**Definition:** Lookup table that lists biomedical literature databases used by the text module.

**Source file:**

**Source org:** Blueprint

**FTP script:** NA

**Parser:** NA

text_db table

| Field | Type | Null | Default | Column Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| dbid | int(11) | No | | Auto incremented id | 1 | text.sql | |
| name | varchar(80) | No | | name of database | PubMed | text.sql | |

text_db indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | dbid |

**text_doc table**

Last updated February 16, 2005

| | |
|---|---|
| **Database:** | seqhound |
| **Table:** | text_doc |
| **Module:** | text |
| **Definition:** | This table lists the accession ids from each literature database and assigns them an internal document id. |
| **Source file:** | *ftp://ftp.nlm.nih.gov/nlmdata/.medlease/medline*.xml.gz*<br>*ftp://ftp.ncbi.nlm.nih.gov/pub/pmc/* |
| **Source org:** | NLM MEDLINE and other biomedical literature databases |
| **FTP script:** | *slri/medline/updates/updatecron.sh*<br>*slri/medline/pubmedcentral/pmc_updatecron.sh* |
| **Parser:** | text_update.pl |

text_doc table

| Field | Type | Null | Default | Column Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| docid | int(11) | No | | auto incremented identifier | 1077882 | | |
| dbid | int(11) | No | 0 | literature database id | 1 | | |
| accession | int(11) | No | 0 | accession in literature database such as a PubMed identifier (PMID) | 1077882 | Medline Xpath: "/MedlineCitation/PMID" Or PMC Xpath: /art/ui[@type="pmid"]' | |
| status | char(10) | Yes | NULL | insert, delete or update | NULL | | |

text_doc indices

| Keyname | Type | Field |
|---|---|---|
| id | PRIMARY | id |
| dbid | INDEX | dbid |
| accession | INDEX | accession |

**text_docscore table**

Last updated September 28, 2004

| | |
|---|---|
| **Database:** | seqhound |
| **Table:** | text_docscore |
| **Module:** | text |
| **Definition:** | This table lists scores for documents. Multiple scores (from different scoring methods) may be listed for each document. |
| **Source file:** | |
| **Source org:** | NRC |
| **FTP script:** | *wget –P ~/nrc -m http://ii200.iit.nrc.ca/~martinj/slri/text/nrc.sh* |
| **Program:** | LitMiner :*http://textomy.iit.nrc.ca/cgi-bin/bindpresent.cgi?qry=10747882* |
| **Notes:** | The current method for scoring a document is an SVM (support vector machine) classifier implemented by National Research Council's Joel Martin and Berry deBruijn. Detailed information can be found in the prebind publication: *http://www.pubmedcentral.nih.gov/articlerender.fcgi?tool=pubmed&pubmedid=12689350* |

text_docscore table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | foreign key from doc table. See docid | 25 | | |
| methodid | int(11) | No | | scoring method identifier. See the text_method table. For example, 1 indicates an SVM trained to recognize papers describing interaction data. | 1 | | |
| score | double | No | 0 | score | -0.852876574 | *http://ii200.iit.nrc.ca/~martinj/* | |

text_docscore indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | (docid, methodid, score) |
| methodid | INDEX | methodid |
| score | INDEX | score |

text_**evidence** table
Last updated February 16, 2004

**Database:** seqhound

**Table:** text_evidence

**Module:** text

**Definition:** This table assigns a unique identifier to each co-occurrence of two bionames in the same document. A bioname points to a specific name bioentity pair in the bioname table (this pair is repeated here). This is to be distinguished from a pair of names that co-occur in a document; this pair of names is identified by a namepairid and does not make any reference to a specific pair of bioentities. This evidence is in support of some point and is based on some name pair.

**Program:**

text_evidence table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | A unique identifier for this piece of evidence. | 1 | Auto incremented identifier | |
| docid | int(11) | No | 0 | the document identifier where this evidence occurs | 325387 | | |
| resultidA | int(11) | No | 0 | search result identifier for bioname A | 2200 | | |
| bioentityida | int(11) | No | 0 | identifier for bioentity A | 107564 | | |
| nama | char(80) | No | | name referring to A | LEU1 | | |
| resultidB | int(11) | No | 0 | search result identifier for bioname B | 9513 | | |
| bioentityidb | int(11) | No | 0 | identifier for bioentity B | 109911 | | |
| namb | char(80) | No | | name referring to B | HIS4 | | |
| pointid | int(11) | Yes | NULL | POtential INTeraction between two bioentites that this evidence supports | 2 | | |
| namepairid | int(11) | Yes | NULL | corresponding namepairid on which this evidence is based | 10634 | | |
| state | smallint(6) | Yes | NULL | book keeping | 0 | | |

text_evidence indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | evidenceid |
| docid | INDEX | docid |
| resultida | INDEX | resultidA |
| resultidb | INDEX | resultidB |

**text_evidencescore table**

Last updated February 16, 2005

**Database:** seqhound

**Table:** text_evidencescore

**Module:** text

**Definition:** This table assigns a score to a piece of evidence. See evidence table. Multiples cores may be assigned to one evidence if different methods were used. Currently, this table stores potential protein-protein interaction scores for each co-occurrence of bionames. The current scoring method uses a set of manually collected regular expression patterns to identity interactions. Detailed information can be found at: *ftp://ftp.blueprint.org/pub/BIND/PreBIND/README*

**Program:**

text_evidencescore table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| evidenceid | int(11) | No | 0 | see text_evidence table | 8 | | |
| methodid | int(11) | No | 0 | scoring method identifier (see text_method table); for example, 2 indicates a method that uses regular expressions to detect bioentities that are physically interacting | 2 | | |
| score | double | No | 0 | the score | 0.63 | | |

text_evidencescore indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | (evidenceid, methodid, score) |
| methodid | INDEX | methodid |
| score | INDEX | score |

**text_method table**

Last updated March 15, 2005

| | |
|---|---|
| **Database:** | seqhound |
| **Table:** | text_method |
| **Module:** | text |
| **Definition:** | This table assigns a unique identifier to each of the multiple scoring schemes used in the SeqHound text mining module. |
| **Source:** | This file is hand-edited. |
| **Source Org.** | Blueprint |

text_method table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | 0 | Auto incremented identifier | 1 | | |
| type | varchar(30) | No | | This field describes the type of score that is generated by the method. It will be one of searchscore, docscore, resultscore, evidencescore or pointscore. | searchscore | | |
| hypothid | int(11) | Yes | 0 | corresponding hypothesis identifier. See the text_hypoth table. | 23 | | |
| hypoth | text | Yes | NULL | a hypothesis that this method attempts to support or refute. | This document describes biophysical interaction data for some molecule(s). | | |
| | | | | | | | |
| method | text | Yes | NULL | a more detailed description of the method with pointers to more details about the method and its performance. | A support vector machine was trained to recognize abstracts containing biophysical interaction data. See PubMed Identifier 12689350 for more details. | | |
| positive | text | Yes | NULL | the value (range) of scores corresponding to the hypothesis being found TRUE | >0 | | |
| negative | text | Yes | NULL | the value (range) of scores corresponding to the hypothesis being found FALSE | <0 | | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| undecided | text | Yes | NULL | the value (range) of scores corresponding to the hypothesis being found UNDECIDED | 0 | | |
| implemented | enumerated | Yes | NULL | has this method been implemented | NO | | |
| assume | text | Yes | NULL | the score value that can be assumed if the method has been implemented but no score is found | >0 | | |
| script | text | Yes | NULL | the script or program that implements the method | text_search.pl | | |

text_method indices

| **Keyname** | **Type** | **Field** |
|---|---|---|
| methodid | PRIMARY | methodid |

**text_point table**

Last updated February 16, 2005

**Database:** seqhound

**Table:** text_point

**Module:** text

**Definition:** A POINT represents two bioentities for which some POtential INTeraction may occur in the literature. Each POINT may be supported by multiple pieces of evidence in the evidence table.

**Program:**

text_point table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | auto incremented identifier | 1 | | |
| bioentityidA | int(11) | No | 0 | bioentity identifier | 110070 | | |
| bioentityidB | int(11) | No | 0 | bioentity identifier | 1268438 | | |
| state | small int | Yes | NULL | book keeping | 0 | | |

text_point indices

| Keyname | Type | Field |
|---|---|---|
| tid | PRIMARY | id |
| bioentityida | INDEX | bioentityida |
| bioentityidb | INDEX | bioentityidb |

**text_pointscore table**

Last updated February 16, 2005

**Database:** seqhound

**Table:** text_pointscore

**Module:** text

**Definition:** This table lists scores for potential interactions. These scores may be viewed as a summary of the scores for all the pieces of evidence that support this POINT. A POINT may have multiple scores that are generated by multiple methods.

**Program:**

text_pointscore table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| pointid | int(11) | No | 0 | a unique identifier for some POINT (see text_point table) | 11 | | |
| methodid | int(11) | No | 0 | an identifier for the method used to generate this score for the POINT (see text_method table). | 3 | | |
| score | double | No | 0 | the score | 0.63 | | |

text_pointscore indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | (pointid, methodid, score) |
| methodid | INDEX | methodid |
| score | INDEX | score |
| pointid | INDEX | pointid |

**text_result table**

Last updated February 16, 2004

**Database:** seqhound

**Table:** text_result

**Module:** text

**Definition:** This table stores all the search results (document ids) for performed searches (see text_search table). Position default is 0, which means that the bioname appears somewhere in the document without specifying exactly where or how many times.

**Program:**

text_result table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | auto incremented identifier | 1 | | |
| searchid | int(11) | No | 0 | identifies the search that generated this result | 1 | | |
| docid | int(11) | No | 0 | the document identifier where the name was found | 7874750 | | |
| positionid | int(11) | No | 0 | the postion id in the document where the name appears (0 indicates no specified position) | 0 | | |
| state | smallint(6) | Yes | NULL | book keeping | 0 | | |

text_result indices

| Keyname | Type | Field |
|---|---|---|
| tid | PRIMARY | id |

| | | |
|---|---|---|
| searchid | INDEX | searchid |
| docid | INDEX | docid |
| positioned | INDEX | positionid |

**text_resultscore table**

Last updated February 16, 2005

**Database:** seqhound

**Table:** text_resultscore

**Module:** text

**Definition:** This table holds scores for search results; i.e., is the searched-for bioentity really mentioned in the document. This table might be used to store disambiguation scores for search results. Because a bioname can refer to many different bioentities, an algorithm (some method) )may be used to determine which bioentity a name occurrence refers to. This table might also hold the results of methods that disambiguate bioentities that have English words as names.

**Program:**

text_resultscore table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | 0 | Auto incremented identifier | 1 | | |
| methodid | int(11) | No | 0 | identifier for the method used to score this result (see text_method table) | 3 | | |
| score | double | No | 0 | the score | -1 | | |

text_resultscore indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | (resultid, methodid, score) |
| resultid | INDEX | resultid |
| methodid | INDEX | methodid |
| score | INDEX | score |

**text_search table**

Last updated February 16, 2004

**Database:** seqhound

**Table:** text_search

**Module:** text

**Definition:** This search table is generated using the text_bioname table. A search is minimally composed of a name that is used to look for some bioentity (listed in this table) using some method. Currently all bioname items with `nametypeid=2` and a taxid that can be found in the taxgi table and are inserted into this search table for MyMedline searching.

**Program:**

text_search table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | auto incremented identifier | 1 | | |
| bioentityid | int(11) | No | 0 | bioentity being searched for | 106945 | | |
| bionameid | int(11) | No | 0 | bionameid used to search for bioentity | 414737 | | |
| name | char(80) | No | | name used to find mention of bioentity | AI1 | | |
| taxid | int(11) | No | 0 | taxonomy identifier for bioentity (if applicable) | 4932 | | |
| rngid | int(11) | Yes | NULL | redundant name group identifier | 70513 | | |
| methodid | int(11) | No | | method used to search for the bioentity mention using name | 1 | | |
| searched | datetime | No | 0000-00-00 00:00:00 | date and time that search was last performed | 2004-12-01 10:12:22 | | |
| results | int(11) | Yes | NULL | number of search results returned | 17 | | |

text_search indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | searchid |
| bioentityid | INDEX | bioentityid |
| bionameid | INDEX | bionameid |
| taxid | INDEX | taxid |

| | | |
|---|---|---|
| searched | INDEX | searched |

**text_searchscore table**

Last updated February 16, 2004

**Database:** seqhound

**Table:** text_searchscore

**Module:** text

**Definition:** This table holds some score that may be used to determine if a given search strategy WILL BE informative if performed or its results are likely TO BE informative if examined. This score might also be used to determine whether a search strategy is to be performed at all or if some search strategy is best left until more informative searches have been informed. For example, if the name to be used is an English word, the search may be scored so as to skip this search. Multiple methods (and their scores) may be applied to a single search.

**Program:**

text_searchscore table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| searchid | int(11) | No | 0 | identifies a search strategy (see text_search table) | 1 | | |
| methodid | int(11) | No | 0 | identifies the method used to score the search strategy | | | |
| score | double | No | 0 | the score | | | |

text_searchscore indices

| Keyname | Type | Field |
|---|---|---|
| PRIMARY | PRIMARY | (searchid, methodid, score) |
| searchid | INDEX | resultid |
| methodid | INDEX | methodid |
| score | INDEX | score |

**text_rng table**

Last updated February 16, 2004

**Database:** seqhound

**Table:** text_rng (redundant name group)

**Module:** text

**Definition:** This table groups together bionames that have equivalent names (i.e. homonyms). This table facilitates searching by reducing the eliminating redundant searches for the same string in the document collection. It is thus an intermediate table in the process of creating the text_result table.

**Program:**

text_rng table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | auto incremented identifier. This is a unique identifier for the redundant name group identifier. | 8 | | |
| name | char(80) | No | | the homonym represented by this group | SRB8 | | |
| searched | datetime | No | 0000-00-00 00:00:00 | when this name was last used to search | 2004-12-01 12:02:23 | | |
| results | | Yes | NULL | the number of documents returned by this search | 0 | | |
| status | char(20) | Yes | NULL | book keeping | searched | | |

text_rng indices

| Keyname | Type | Field |
|---|---|---|
| Id | PRIMARY | id |
| Name | Unique | Name |
| Searched | INDEX | Searched |
| Results | INDEX | Results |
| Status | INDEX | status |

**text_rngresult table**

Last updated February 16, 2004

| | |
|---|---|
| **Database:** | seqhound |
| **Table:** | text_rngresult |
| **Module:** | text |
| **Definition:** | This table is an intermediate step in one method for searching for mentions of protein names in text. The table stores search results for redundant name groups. These results are combined with the text_doctax table to generate the final text_results table. |
| **Program:** | |
| **Note:** | This is an intermediate table and is not distributed as part of SeqHound. |

text_rngresults table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Auto incremented identifier. | 1 | | |
| rngid | int(11) | No | 0 | a redundant name group identifier. See the text_rng table. | 2 | | |
| docid | int(11) | Yes | NULL | a document identifier where this name appears | 45549 | | |
| pmid | int(11) | Yes | NULL | the corresponding PubMed identifier where this name appears | 45549 | | |
| state | int(11) | No | 0 | book keeping | 0 | | |

text_rngresults indices

| Keyname | Type | Field |
|---|---|---|
| Id | PRIMARY | Id |
| Rngid | INDEX | Rngid |
| Docid | INDEX | Docid |
| Pmid | INDEX | Pmid |
| State | INDEX | State |

**text_doctax table**

Last updated February 16, 2004

**Database:** seqhound

**Table:** text_doctax

**Module:** text

**Definition:** This table keeps a list of the organisms (by taxon identifiers) that are described in a document.

**Program:**

text_doctax table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Auto incremented identifier. A unique identifier. | 1 | | |
| docid | int(11) | No | 0 | document identifier (see text_doc table). | | | |
| taxid | int(11) | No | 0 | organism described in this document (listed by NCBI taxonomy database identifier) | | | |

text_doctax indices

| Keyname | Type | Field |
|---|---|---|
| Id | PRIMARY | Id |
| Docid | INDEX | Docid |
| Taxid | Index | taxid |

**text_organism table**

Last updated February 16, 2004

| | |
|---|---|
| **Database:** | seqhound |
| **Table:** | text_organism |
| **Module:** | text |
| **Definition:** | This table keeps a list of the MESH terms that are used to identify the presence of an organism in a PubMed abstract. |
| **Program:** | |
| **Source Org:** | Blueprint |
| **Source file:** | |
| **Note:** | |

text_organism table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | auto incremented identifier | 1 | | |
| taxid | int(11) | No | 0 | NCBI taxonomy identifier | 4932 | | |
| mesh | timestamp | No | | mesh term found in abstracts that describe this organism | Saccharomyces cerevisiae | | |
| searched | timestamp | Yes | CURRENT_TIMESTAMP | time that this search was last completed | 2005-02-15 15:58:38 | | |
| results | int(11) | Yes | NULL | number of documents returned | NULL | | |
| bioentities | int(11) | Yes | NULL | number of bioentities for this organism | NULL | | |
| bionames | int(11) | Yes | NULL | number of names for this organism | NULL | | |
| maxbionameid | int(11) | Yes | NULL | maximum bioname identifier | NULL | | |
| lastupdate | timestamp | Yes | 0000-00-00 00:00:00 | time that all all updates were last completed | 0000-00-00 00:00:00 | | |

text_organism indices

| Keyname | Type | Field |
|---|---|---|
| Id | PRIMARY | Id |
| | | |
| | | |
| | | |

**text_englishdict table**

Last updated February 16, 2004

**Database:** seqhound

**Table:** text_englishdict

**Module:** text

**Definition:** This table holds an English Dictionary from Moby project *http://www.dcs.shef.ac.uk/research/ilash/Moby/*

**Program:**

**Organization:** Oxford University

**File:**

text_englishdict table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Auto incremented identifier. Aunique identifier for this word-pos combination. | 1 | | |
| word | char(16) | Yes | NULL | the word | the | | |
| pos | char(10) | Yes | NULL | part of speech | Det | | |
| freq | int(11) | Yes | NULL | frequency in the bnc per million words | 61847 | | |
| count | int(11) | Yes | NULL | how many bioname identifiers does this word refer to | 1 | | |
| source | char(10) | Yes | NULL | pubmed = this word is in th pubmed stopword list<br>stop = present in other stopword lists<br>other possibilities | pubmed | | |

text_englishdict indices

| Keyname | Type | Field |
|---|---|---|
| Id | PRIMARY | Id |
| Word | Index | Word |
| Pos | Index | Pos |
| Freq | Index | Freq |
| Count | Index | count |

**text_bncorpus table**

Last updated February 16, 2004

| | |
|---|---|
| **Database:** | seqhound |
| **Table:** | text_bncorpus |
| **Module:** | text |
| **Definition:** | This table holds the British National Corpus. |
| **Parser:** | |
| **Organization:** | Oxford University (http://www.natcorp.ox.ac.uk/) |
| **File:** | *ftp://ftp.itri.bton.ac.uk/bnc/* |
| **Note:** | this file is not distributed with SeqHound |

text_bncorpus table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | auto incremented identifier. A unique identifier for this word. | 1 | | |
| word | char(160) | No | | the word | the | | |
| freq | int(11) | No | 0 | frequency in the corpus | 6187267 | | |
| pos | char(16) | No | | part of speech | at0 | | |
| files | int(11) | No | 0 | number of files (out of 4120) that this word appears in | 4120 | | |

text_bncorpus indices

| Keyname | Type | Field |
|---|---|---|
| Id | Primary | Id |
| Word | Index | Word |
| Freq | Index | Freq |

**text_pattern table**

Last updated February 16, 2004

| | |
|---|---|
| **Database:** | seqhound |
| **Table:** | text_pattern |
| **Module:** | text |
| **Definition:** | This table holds a list of regular expressions used to detect mentions of biophysical interactions between two given names that appear in a sentence. |
| **Program:** | |
| **Source Org:** | Blueprint |
| **Source File:** | |
| **Note:** | |

text_pattern table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | varchar(8) | No | | a unique identifier for this regular expression. | 9920 | | |
| parentid | varchar(8) | Yes | NULL | the parent identifier if this expression is derived from another. | 99 | | |
| class | int(11) | No | 0 | does this expression identify an interaction (1) or the absence of an interaction (-1). | 1 | | |
| score | double | Yes | NULL | score for this regex | 0.85 | | |
| regex | text | Yes | NULL | the regular expression | A(\S*\s+){0,4}\S*B(\S*\s+){0,4}\S*heterodimer | | |

text_pattern indices

| Keyname | Type | Field |
|---|---|---|
| Id | Primary | Id |
| Parentid | Index | Parentid |

**text_stopword table**

Last updated February 16, 2004

**Database:** seqhound

**Table:** text_stopword

**Module:** text

**Definition:** This table contains a complete list of stopwords.
1.*http://www.ncbi.nlm.nih.gov/entrez/query/static/help/pmhelp.html#Stopwords*
2.*ftp://ftp.cs.cornell.edu/pub/smart/english.stop*
3. Manually collected from bioname table

**Program:**

**Source Org:** Various (see definition)

**Source file:**

**Note:**

text_stopword table

| Field | Type | Null | Default | Column_Definition | Example | Source | API |
|---|---|---|---|---|---|---|---|
| id | int(11) | No | | Auto incremented identifier | 1 | | |
| word | char(16) | No | | the stop word | a | | |
| source | char(16) | Yes | | Source of this stop word | PubMed help | | |

text_ indices

| Keyname | Type | Field |
|---|---|---|
| Id | Primary | Id |
| Word | Index | word |

# 6. Developing for SeqHound.

## Open source development.

SeqHound code is developed on a cvs tree internal to the Samuel Lunenfeld Research Institute by the members of the Blueprint Initiative Development team. The most stable current release is available at
*ftp://ftp.blueprint.org/pub/SeqHound/*
External developers are encouraged to discuss major additions or modifications to the system with the Project Manager at *seqhound@blueprint.org*.
Minor additions or corrections may also submitted to *seqhound@blueprint.org*.

## Code organization.

Note: The following section is under revision and will be updated shortly.

This document summarizes the contents in the directories under *slri/seqhound* and *slri/nblast* as of June of 2003. The contents of directories are first stated and then the purpose of the contents is given.
Under the current directory hierarchy, the seqhound directory contains the following directories (/) and files (*):

*asn/*

*bioperl/*
*build/*
*cgi/*
*config/*
*db2/*
*domains/*
*examples/*
*genomes/*

*go/*
*html/*
*include/*
*include_cxx*
*java/*
*lib/*
*locuslink/*
*parsers/*

*perl/*
*rps/*
*scripts/*
*shreadme/*

*shreadme_cxx/*
*src/*
*src_cxx/*
*taxon/*
*tindex/*
*updates/*
*yeast/*

*seqhound .mk**
*seqhound_cb.mk**
*seqhound_db2.mk**
*seqhound_odbc.mk**
*seqhound_rem.mk**
*shreadme**
*shreadme_cxx**

| | |
|---|---|
| **asn/ :** | contains the asn specifications (**.asn*) for various objects used in seqhound, auxiliary files used by datatool & asntool (**.def*), and the scripts used by asntool and datatool to autogenerate the objects in unix (**.sh*) and windows (**.bat*) platforms. |
| **bioperl/:** | contains the files used in the SeqHound bioperl module |
| **build/:** | contains a directory structure used to store the executables. As executables get compiled, they will be moved into their relevant directories inside the build directory. Executables using Codebase will be moved to *cb/*, db2 executables are moved to *db2/*, and odbc executables to *odbc/*. The appropriate directories will get created as the need arises. |
| **cgi/:** | contains the source code for the cgi and web services. |
| **config/:** | the configuration files used in seqhound remote & local applications. |
| **db2/:** | scripts to create the tables in db2 and redund for db2. |
| **domains/:** | source code for the domain module. |
| **examples/:** | source code showing how to use some of the code in seqhound, ex the asn structures and functions, the C++ remote library. |
| **genomes/:** | source code for the complete genome module. |
| **go/:** | source code for the gene ontology module. |
| **html/:** | documentation for SeqHound API, and some scripts for converting the documentation to html |
| **include/:** | the **.h* files for SeqHound |
| **include_cxx/:** | the include files for the C++ remote library |
| **java/:** | source code for the SeqHound Java remote library |
| **lib/:** | libraries for SeqHound are copied here once compiled. |
| **locuslink/:** | source code for the locuslink module. |
| **parsers/:** | source code for various parsers (mother, cbmmdb, cddb, redund, mmdbloc) |
| **perl/:** | the SeqHound perl module (deprecated in favor of bioperl) |
| **rps/:** | source code for the rps module (domname, rpsdb) |
| **scripts/:** | various scripts to retrieve flatfiles from NCBI, and to build SeqHound |
| **src/:** | source code for SeqHound (includes db layers for GO, HIST, LOCUSLINK, NBR, rpsdb, taxdb& core modules), the C remote API |
| **src_cxx/:** | source code for the remote C++ library. |
| **taxon/:** | source code for the taxon module parser. |
| **tindex/:** | source code for the text indexer. |
| **updates/:** | source code for the daily updates & histparser. |
| **yeast/:** | source code for importing yeast GO into Seqhound (never completed). |

| | |
|---|---|
| ***.mk:** | various auxiliary files used by SeqHound makefiles. |
| **shreadme*:** | readme files for C & C++ SeqHound |

Under the current directory hierarchy, the *nblast* directory contains the following directories(*/*) and files(*****):

*asn/*
*db/*
*docs/*
*lib/*
*msvc/*
*scripts/*
*src/*

*nblast.mk**
*nblastflags.mk**

| | |
|---|---|
| *asn/:* | contains the ASN specifications for nblast. |
| *db/:* | source code for nblast Codebase layer. |
| *docs/:* | instructions for compiling nblast. |
| *lib/:* | source code for the ASN nblast object. |
| *msvc/:* | files for Microsoft Visual C++ project. |
| *scripts/:* | various scripts for retrieving NCBI Blast flatfiles & setting up NBlast. |
| *src/:* | core source code for nblast. |
| **.mk:* | auxiliary makefile for nblast applications. |

## Adding/Modifying a remote API function to SeqHound.

> Note: This section is included for historical purposes and is being rewritten for a future release (5.0)

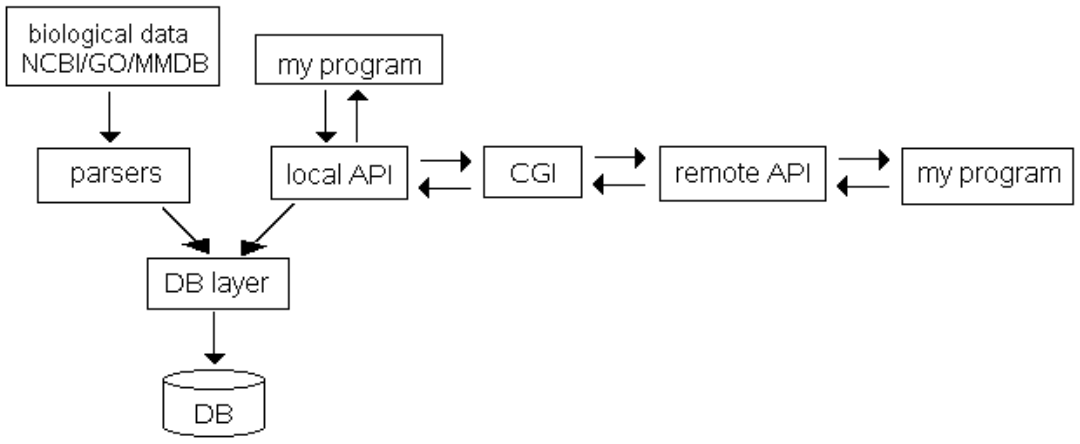
Overall steps:

1. open a new Bugzilla report
2. create the database search functionality
3. create the local API call
4. create the CGI call
5. add the remote calls (C/C++/Java/Bioperl/Perl)
6. test the new functionality in each of the layers
7. write/update documentation
8. inform technical writer
9. inform tester
10. update seqrem and local library in production server
11. In some rare cases, modifications may have to be made to the underlying data table structure, then SeqHound must be rebuilt in test and production environments before code is checked into cvs.
12. check in the new source code
13. update API website
14. close Bugzilla report

> This document only goes over steps 2-5 in detail.

**Overall architecture of the SeqHound system.**

*The diagram shows how the various code layers in SeqHound.*



2. Create the Database Search Functionality

   If adding a new data file, you will need to write the database search functions, one for each data file. Database Search functions are found in '*slri/seqhound/src/*_cb.c*' files.

   '*' is the name of the module that the searched table belongs to like 'GO' or 'intrez'. 'cb' refers to the database engine that the function talks to like CodeBase (cb) or ODBC compliant databases (odbc).

   Functions that search data tables are typically called `SearchXXX`. New data files require you to define the ASN structure, typically each field in the data file corresponds to an ASN field.

   Most of the existing databases already have search functions so you should not have to write these yourself. If they don't exist, then you should consult the instructions under Creating a new SeqHound module first. The details below are here to help you understand the database layer and to use Search functions in your API function.

   ```
   Boolean LIBCALL SearchACCDB (StAccdbPtr PNTR ppac)
   ```

   The search functions should find **ALL** instances of a key in the database and return them through the ASN pointer. Each ASN structure is a linked list, so multiple records can be retrieved. Pseudo code for the typical search function:

   ```
   Boolean SearchXXX(ASNLinkList Pointer)
   {
        foreach record that matches key in Pointer
            create a new ASNLinkList Node;
            fill node with record fields;
            join node to Pointer;
        end foreach

        return TRUE if key found
        else return FALSE;
   }
   ```

   As an example, the function

   ```
   Boolean LIBCALL SearchACCDB (StAccdbPtr PNTR ppac)
   ```

   finds records in the accdb table for an ODBC compliant database engine. This function is located in *slri/seqhound/src/intrez_odbc.c*. The corresponding function for a CodeBase database engine has the same name but is found in *slri/seqhound/src/intrez_cb.c*. The ASN structure that StAccdbPtr points to is defined in *slri/seqhound/asn/slristruc.asn* (search for StAccdb) and the corresponding C structure is defined in *slri/seqhound/include/objslristruc.h*. You need to know this when you use a database search function in your local API function.

3. Create The Local API Function

   You will need to change one of three files in order to add new functionality to SeqHound.

   a) *go_query.c* : to add functionality to gene ontology module API functions

   b) *ll_query.c* : to add to locuslink module API functions

   c) *intrez.c* : to add new functionality to the other data tables.

Declare function prototype in *slri/seqhound/include/seqhound.h*. Try to group the functions logically in the *.c* and *.h* files.

The API functions follow a general logic. You should try to stick to that logic. Typical example of an API function:

```
Int4 LIBCALL SHoundFindAcc(CharPtr pcAcc)
{
   Int4 gi = 0;
   StAccdbPtr pac = NULL, pachead = NULL;
   Int2 res = 0;

   if ((pcAcc == NULL) || (strcmp(pcAcc, "n/a") == 0))
   {
      ErrPostEx(SEV_ERROR,0,0,"SHoundFindAcc: No accession.");
      return 0;
   }

   pac = StAccdbNew();

   pachead = pac;
   pac->access = StrSave(pcAcc);
   res = SearchACCDB(&pac);

   if (res == FALSE)
   {
      ErrPostEx(SEV_ERROR,0,0,"SHoundFindAcc: Search failed.");
      StAccdbFree(pachead);
      return 0;
   }else if(res == TRUE){
      gi = pac->gi;
      pac = pac->next;
   }
   StAccdbFree(pachead);
   return gi;
}
```

Input integrity check

Each data table has specific asn structure.

Set the key in the asn structure

database layer to search for the key. The asn structure will hold all the records that match the key.

Failed search. Free structure and return

Successful search - extract what you need and return it.

4. Step 4. Create the CGI Function

Definitions:

**CGI (Common Gateway Interface):**

a program that allows 2 computers connected to the internet to communicate with each other.

**HTTP (Hypertext Transfer Protocol):**

a way of passing messages between the 2 computers. Is used for web services, eg CGI, servlets … Format of HTTP:

*http://server_name/path*/to/cgi/cgi_name?key1=value1&key2=value2&….

**Query string:**

The portion of the HTTP call that is used to pass parameters to the CGI. Format of query strings: ?param1=value1&param2=value2….

**SeqHound's CGI**

is slri/seqhound/cgi/seqrem.c.

**Remote users**

can call seqrem on our servers using HTTP calls. Format of a HTTP call:

*http://seqhound.blueprint.org/cgi-bin/seqrem?fnct=SeqHoundFindAcc&acc=AA73235*

2 parts to edit in *seqrem.c*

1. `if` statement in function: `ProcessFnctRequest(CharPtr pfnct);`
2. Add a corresponding CGI function call that calls the local API

---

There is currently an `if-else` statement in the `ProcessFnctRequest` function. It needs to be modified to check if the first field of the query string contains your new function name. If so, it will call a CGI function that calls your local API function.

---

```
SLRI_ERR ProcessFnctRequest(CharPtr pfnct)
{
   if(SeqHoundInit() == SLRI_FAIL) {
       MemFree(pfnct);
       return 1;
   } else if (strcmp(pfnct, "SeqHoundFindAcc") == 0) {
       if(SeqHoundFindAcc() == SLRI_FAIL) {
       MemFree(pfnct);
       return 1;
       }
   } ...

   } else if(strcmp(pfnc, "YourNewFunction" ..
       if(SeqHoundYourNewFunction() ...
   }
}
```

Calling internal CGI function … see below

Your new function gets called here

Next you need to define a function with the prototype

```
SLRI_ERR SeqHoundYourNewFunction(void)
```

This function will extract the remaining keys in the query string portion of the HTTP call, and call the local API function you defined in step 3, then output the HTTP response to be sent back to the user.

```
http://seqhound.blueprint.org/cgi-bin/seqrem?fnct=SeqHoundFindAcc&acc=AA73235
```

Internal CGI function that calls the local API

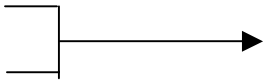
```
SLRI_ERR SeqHoundFindAcc(void)
{
   Int4 gi = 0;
   Int4 IndexArgs = -1;

   printf("Content-type: text/html\r\n\r\n");
   if ((IndexArgs = WWWFindName(ginfo,"acc")) >= 0)
   {
      pcThis = WWWGetValueByIndex(ginfo,IndexArgs);
      pacc = StringSave(pcThis);
   }
   if ((pacc == NULL) || (strlen(pacc) == 0))
   {
      ErrPostEx(SEV_ERROR,0,0, " Failed to get parameter value.");
      fprintf(stdout, "SEQHOUND_ERROR Failed to get parameters.");
      return SLRI_FAIL;
   }
   gi = SHoundFindAcc(pacc);
```

Output the HTTP headers

Extract the remaining fields from the CGI

Calling the local API

```
    fprintf(stdout, "SEQHOUND_OK\n");
    fprintf(stdout, "%ld\n", (long) gi);
    MemFree(pacc);
    return SLRI_SUCCESS;
}
```



Send output back to remote users using HTTP

5. Step 5. Create the Remote Calls

We have programs available in most of the widely used languages that allow SeqHound users to write programs in their favorite language, accessing SeqHound data without having to understand how everything works. Our remote programs in effect constructs the HTTP calls (described above), sends the HTTP calls to the server and then parses the server's return value and sends this back to the user's program.
Our remote interfaces are:

1. *slri/seqhound/src/seqhoundapi.c*
2. *slri/seqhound/src_cxx/Seqhound.cpp*
3. *slri/seqhound/java/SeqHound.java*
4. *slri/seqhound/perl/SeqHound.pm*
5. *slri/seqhound/bioperl/SeqHound.pm*

```
Int4 LIBCALL SHoundFindAcc(CharPtr pcAcc)
{

  Char fpath[PATH_MAX];
  Int4 gi = 0;

  if(pcAcc == NULL)
  {
      ErrPostEx(SEV_ERROR,0,0, "Invalid parameter.");
      return 0;
  }

  sprintf(fpath,"%s?fnct=SeqHoundFindAcc&acc=%s", slri_cgipath, pcAcc);

  ErrPostEx(SEV_INFO,0,0, "SeqHoundFindAcc request: %s.\n", fpath);

  if(SHoundWWWGetfile(slri_sername, fpath) == 0)
  {
      ErrPostEx(SEV_ERROR,0,0, "SHoundWWWGetfile failed.");
      return 0;
  }
  gi = ReplyBSGetInteger();
  if (gi == 0)
  {
      ErrPostEx(SEV_INFO,0,0, "SeqHoundFindAcc returned zero.");
      return 0;
  }
  return gi;
}
```

Making the HTTP call. Contains the server name, path to CGI,

Send the HTTP call

Get the return value. A family of ReplyBSGetXXX exists for

Similar logic is used in the remote C++, Java, and Perl libraries.

## Adding a new module to SeqHound

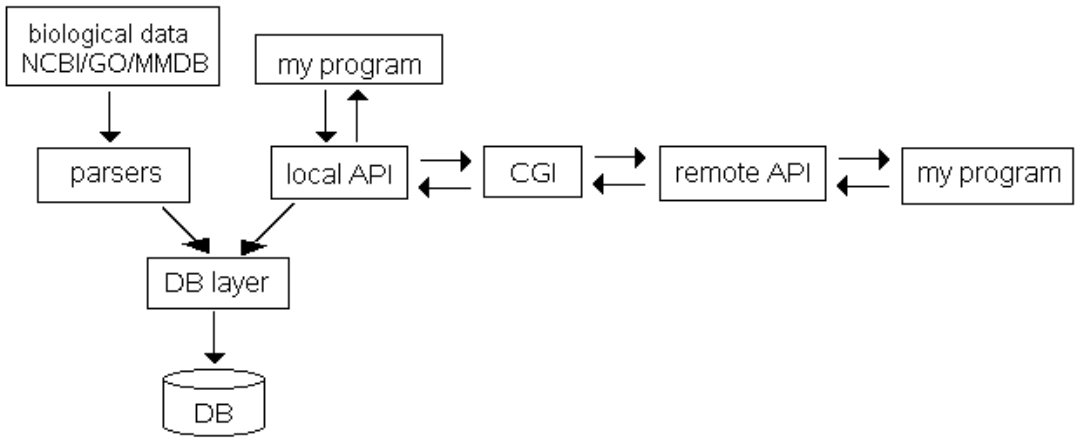
> Note: This section is included for historical purposes and is being rewritten for a future release (5.0)

This section describes how to go about adding a new module to SeqHound from the developer's point of view. It is basically a description of the different files that have to be written for a new module and where they should go in the code tree. So this section may be used as a guide for looking at existing modules to find out what files are expected and where they are. However, historically, several programmers have added modules to SeqHound and have used different code organization schemes; therefore, historical modules may be organized differently. Going forward (as of November 2003) all modules will have the components that are organized in the way described below.

1. Start a new module project plan

   Creating a new module begins with starting a new project plan (see Format for project reports). This should contain a clearly stated *"Need"* and *"Objective"* as well as a *"General approach"* to developing the module; this may include background information on the data resource being incorporated into SeqHound. The *"Detailed planning"* section will contain a section on *"Data table design"* and *"Code Organization"* that will be described further. See the DBXREF (Database cross-reference) module Project Plan as an example (***./slri/seqhound_priv/dbxref/dbxref_module_desc.txt***).

   The components of a new module are summarized in the diagram below. The rest of this section describes the creation of each of these components and their organization. File names in ***bold italics*** indicate files that may be looked at as examples.



**Database layer**

2. Design the data table structure

   The module's project description should contain a description of the final table design. See the example in the DBXREF (Database cross-reference) module Project Plan as an example.

3. Write the script file that creates the data table.

   You must modify the existing script file that creates the SeqHound data tables (this step is only for ODBC SeqHound). This file is called *seqhound.sql* and is located in

   ./slri/seqhound/sql/seqhound.sql

   Add the line

   ```
   DROP TABLE SEQHOUND.DBXREF_tablename;
   ```

   near the top of the file. Every time this script is run, it will destroy any pre-existing data tables that belong to the module.

   Add the lines that describe the table(s) that are a part of the module so the script creates the new tables belonging to the module. See the example file "*seqhound.sql*".

   Note that CodeBase tables to not require a script to be made; these tables are created by the function InitCodeBase in the <*module_name*>*_cb.c* file.

4. Write ASN.1 structure(s) that corresponds to data table descriptions.

   The file ***./slri/seqhound/asn/slristruc.asn*** must be modified to contain a description of tables in the module. See the example structure StDbXref in the slristruc.asn file.

   The shell script "***./slri/seqhound/asn/makeasn***" calls asntool which auto generates *slristruc.h*, *objsslristruc.h* and *objslristruc.c* files. These files contain functions that allow one to allocate and free memory for a structure corresponding to a database record. See the makeasn file.

5. Step 5: Design new functions for the Database code layer

   The DB layer contains C functions that create and retrieve records from tables in the module. In the case of the DBXREF module, the tables are populated by a parser written in PERL so there are no functions listed that write to the tables. The requirement for a certain Perl modules is however noted in the project plan; these modules allow Perl to converse with a database.

   The DB layer will have three files that were auto generated from the preceding step.

   *a) ./slri/seqhound/include/slristruc.h*

   *b) ./slri/seqhound/include/objsslristruc.h*

   *c) ./slri/seqhound/src/objsslristruc.c*

   These files will be placed in this location by the *makeasn* script.

   In addition, DB layer will require that two new files be made.

   *a) ./slri/seqhound/include/<module_name>_odbc.h*

   This will contain function prototypes and comments for functions in

*b) ./slri/seqhound/src/<module_name>_odbc.c*

This will contain at least one functions called "`Search<module_name>` that retrieves records from the database. Other functions that read or write to the database may be included in this file.

The example function "`SearchDBXREF`" (see *dbxref_odbc.h* and *dbxref_odbc.c*) takes as input a pointer to a structure called StDbXref. This structure has the same fields as the DBXREF table. This structure is described in ASN.1 and functions to allocate and free memory for this structure are auto generated using ASNtool. Any row in a DBXREF table that contains field values matching anyone of the field values passed to "`SearchDBXREF`" will be returned in a linked list of Valnodes that contain pointers to StDBXref structures.

6. Make changes to existing code to accommodate changes to the database code layer.

   You must modify the existing function called `InitCodeBase` so that it handles tables that are new to the module. This function is found in two locations:

   a) ***./slri/seqhound/src/intrez_cb.c*** is the file that supports a CodeBase database backend to SeqHound. `InitCodeBase()` needs to be changed to open the code base data files that belong to the new module. See the example *intrez_cb.c* file.

   b) ***./slri/seqhound/src/intrez_odbc.c*** is the file that supports a supports an ODBC database backend to SeqHound. `InitCodeBase()` need to contain the necessary code to establish a connection to the Database Server. See the example *intrez_odbc.c* file.

   The function `InitCodeBase()` under *intrez_odbc.c* has a function call:

```
GetAppParam(intrez", "datab", "db2alias", NULL,
(Char*)dsn, sizeof(char) * 10) <= 0 )
```

   that retrieves database connection information from the ***./slri/seqhound/config/.intrezrc*** configuration file.

**Parser layer**

7. Design the parser layer.

   Parsers are generally written in C or Perl. A separate script is written to download some file from an external ftp site. The parser takes this file as input and uses it to populate a set of data tables belonging to the module.

   Pseudocode for parsers should be documented in the project plan.

   Parser layer code is located in

   ./slri/seqhound/<module_name>/[parser_name]

   for example

   ***./slri/seqhound/dbxref/dbxref_parser_sp.pl***

   Finally, by project end, all parsers must be documented according to the examples given in the SeqHound manual. See the example parser description for "mother".

**Local API layer (Query layer)**

8. Design the Local API layer

   Design the local API local query layer. This layer will consist of three files

   a) ./slri/seqhound/src /[Module name]_query.c

      This file contains all of the API functions that query the module's tables as well as auxiliary functions (if any). Note that this naming convention is not followed by API calls that belong to the core module of SeqHound; code for these local API calls that query core module tables is in *./slri/seqhound/src/intrez.c*.

   b) ./slri/seqhound/include/[Module name]_query.h

      This file contains function prototypes and comments for auxiliary functions (if any) that may be used by the module's parsers, API functions or other applications specific to the module.

   c) ./slri/seqhound/include/seqhound.h

      This is where all publicly available API functions are defined. Note that the local and the remote API's use the same header file. ALL API functions for ALL modules are defined in this header. This file already exists and must be simply modified.

   Examples are:

   ***./slri/seqhound/src /dbxref_query.c***

   ***./slri/seqhound/include/dbxref_query.h***

   ***./slri/seqhound/include/seqhound.h***

   An example of an API function is a function(s) to retrieve data base cross-references given a source record (`SHoundDBXREFGetDBXrefListBySourceRecord`). See the example in the *dbxref_query.c* file. This is a local API call. Notice the naming convention: 'Shound' followed by the module name 'GODB' followed by the actual API function name.

   In the example function note the line

   ```
   if(!SHoundModule("godb"))
   ```

   This checks the SeqHound configuration file to make certain that the build of SeqHound actually includes this module. All API function calls must have an analogous check.

   ---

   Note that this function calls a database layer function called `SearchDBXREF`.

   ---

**CGI layer**

9. Design the CGI layer

   The SeqHound cgi layer that supports the remote API is contained in only one file

   ***./slri/seqhound/cgi/seqrem.c***

   There is no header file for *seqrem.c* since all functions are defined before "`Main()`" and `Main` only calls functions in this file.

This file must be edited to include cgi support for the remote API calls for the new module. See the examples in the *seqrem.c* file. See the example function `SeqHoundDBXREFGetDBXrefListBySourceRecord`.

Note the naming convention: SeqHound followed by the module name followed by the same function name used by the local API function.

**Remote API layer**

10. Design the remote API layer

    The remote API for SeqHound supports 4 languages. So there are four files that must be modified to include new API functions for the new module.

| | |
|---|---|
| For C: | ***./slri/seqhound/src/seqhoundapi.c*** |
| For C++: | ./slri/seqhound/src_cxx/SeqHound.c |
| For Java: | ./slri/seqhound/java/SeqHound.java |
| For Perl: | ./slri/seqhound/perl/SeqHound.pm |

    The function names will be exactly the same as those listed in the local API layer (for example; `SHoundDBXREFGetDBXrefListBySourceRecord`).

    Examples for the C remote API are given in the *seqhoundapi.c* file.

11. Modify the seqhound config file.

    New modules require that another entry be made in the *.intrezrc* file. This setting allows the SeqHound administrator to indicate whether any given SeqHound module has been built. The function `SHoundModule()` will look at these config file settings every time a local API call is made to determine if the module is present.

    Modify the ***./slri/seqhound/config/intrezrc*** according to the example. Analogous additions must be made to the *./slri/seqhound/config/intrez.ini* file for Windows platforms.

    Modify the `ShoundModule()` function in ***./slri/seqhound/src/intrez_cfg.c*** file to support the new module. Follow the example in this file.

12. Modify/create make files to support the new module.

    Modify the following files.

    ***./slri/seqhound/seqhound_odbc.mk***

    SEQH_SRC_ODBC

    SEQH_OBJ_OODBC

    ***./slri/seqhound/seqhound.mk***

    SEQH_SRC_COM

    SEQH_OBJ_COM

    SEQH_ODBC_COM

***./slri/seqhound/seqhound_rem.mk***

***./slri/seqhound/seqhoundrem.mk??***

***./slri/seqhound/src/make.shoundlocllib***

***./slri/seqhound/src/make.shoundremlib***

Create the following make files for any parsers written in C.

./slri/seqhound/<module_name>/make.[parser_name]

see the example in

***./slri/seqhound/locuslink/make.llparser***

13. Design regression tests

    Regression tests are based on the CuTest C Unit Testing Framework.
    (see *http://cutest.sourceforge.net/*).

    One file must be modified to support tests for the new module. Follow the examples in:

    ***./slri/seqhound/test/regresion/main.c***

    And a new file must be created that contains the actual test functions. See the examples in the test driver for the database layer for the DBXREF module:

    ***./slri/seqhound/test/regresion/dbxref_odbc_driver.c***

    Examples of some test cases Function calls.

    ```
    void testDBXREF_GetObjectIDbyAcc(CuTest *tc){...}
    ```

    Another driver contains test functions for the

    *./slri/seqhound/test/regresion/dbxref_query_driver.c*

    Finally, the following file must be modified to accommodate the new module test drivers. Follow the examples in:

    ***./slri/seqhound/test/regresion/make.test_driver***

14. Design test cases

    These test cases refer to tests of the local and remote API functions relevant to the module.

15. Code test and debug
16. Finish documentation
17. Compile SeqHound code in test environment
18. Build SeqHound db in test environment
19. Check in code
20. Pass the project on to delivery team (Test Dev/Systems Dev/Software Training)
21. Build module in production (SEQHOUND ADMIN)
22. Update data tables (SEQHOUND ADMIN)

23. Update seqrem (SEQHOUND ADMIN)
24. Update docs (SEQHOUND ADMIN)
25. Update website (SEQHOUND ADMIN)

# 7. Appendices

## Example GenBank record

```
Seq-entry ::= set {
  class nuc-prot ,
  descr {
    title "Vairimorpha necatrix largest subunit of RNA polymerase II
(RPB1)
 gene, complete cds." ,
    source {
      org {
        taxname "Vairimorpha necatrix" ,
        db {
          {
            db "taxon" ,
            tag
              id 6039 } } , <==========================TAXGI/taxid
        orgname {
          name
            binomial {
              genus "Vairimorpha" ,
              species "necatrix" } ,
          lineage "Eukaryota; Fungi; Microsporidia; Burenellidae;
Vairimorpha" ,
          gcode 1 ,
          mgcode 1 ,
          div "INV" } } } ,
    create-date
      std {
        year 1998 ,
        month 12 ,
        day 10 } ,
    pub {
      pub {
        sub {
          authors {
            names
              std {
                {
                  name
                    name {
                      last "Hirt" ,
                      first "R" ,
                      initials "R.P." } } ,
                {
                  name
                    name {
                      last "Healy" ,
                      first "B" ,
                      initials "B." } } } ,
            affil
              std {
                affil "The Natural History Museum" ,
                div "Zoology" ,
                city "London" ,
                country "UK" ,
                street "Cromwell Road" ,
                postal-code "SW7 5BD" } } ,
          medium email ,
          date
            std {
              year 1998 ,
              month 4 ,
              day 16 } } } } ,
    update-date
      std {
        year 1999 ,
        month 2 ,
        day 4 } ,
    pub {
      pub {
        article {
```

```
          title {
            name "Microsporidia are related to Fungi: evidence from the
    largest subunit of RNA polymerase II and other proteins." } ,
          authors {
            names
              std {
                {
                  name
                    name {
                      last "Hirt" ,
                      initials "R.P." } } ,
                {
                  name
                    name {
                      last "Logsdon" ,
                      initials "J.M." ,
                      suffix "Jr." } } ,
                {
                  name
                    name {
                      last "Healy" ,
                      initials "B." } } ,
                {
                  name
                    name {
                      last "Dorey" ,
                      initials "M.W." } } ,
                {
                  name
                    name {
                      last "Doolittle" ,
                      initials "W.F." } } ,
                {
                  name
                    name {
                      last "Embley" ,
                      initials "T.M." } } } ,
            affil
              str "Department of Zoology, The Natural History Museum,
    London
     SW7 5BD, United Kingdom." } ,
          from
            journal {
              title {
                iso-jta "Proc. Natl. Acad. Sci. U.S.A." ,
                ml-jta "Proc Natl Acad Sci U S A" ,
                issn "0027-8424" ,
                name "Proceedings of the National Academy of Sciences
    of the
     United States of America." } ,
              imp {
                date
                  std {
                    year 1999 ,
                    month 1 ,
                    day 19 } ,
                volume "96" ,
                issue "2" ,
                pages "580-585" ,
                language "eng" } } ,
          ids {
            pubmed 9892676 ,
            medline 99110933 } } ,
        muid 99110933 ,
        pmid 9892676 } } } ,
  seq-set {
<==================================beginning of bioseq
<==========================look down for end of bioseq(see ASNDB/asn1)
    seq {
      id {
        genbank{<==============================ACCDB/DB
          name "AF060234" ,<================= ======ACCDB/name
```

```
          accession "AF060234" ,<====================ACCDB/accession
          version 1 } ,<============================ACCDB/version
        gi 4001823 } , <==========================Many tables/GI
      descr {
        molinfo {
          biomol genomic } } ,
      inst {
        repr raw ,
        mol dna ,
        length 5019 ,
        seq-data
          ncbi2na
'171B6C0C434EFC0FBDC301F7E3FFFF3F396FF3FD7FFFF355C03BF8E03EC
10020DDB4350F6BF3FDD48203080352EDB5030D4578053A00EAF57037AEBF0C8FC00EA4
71202A7
FFCEF4D7B8008C3FF7E57AD3FE944F83C1C250EF53BEBC4E18034200DFA0EEFEFFCFBDC
87C03CB
1000DF0808FE0FFB3A0CFDC21C02EFE60AE03EA803ABF129EE80C2497B0C00082838BF8
C9FF380
A208202E3AC0B0FF83A2022F4C33DE0823EC0E08E7BBFFABFE3482FC70978BA7CFF87BD
FF2F5D7
5F7B0A5CB3ED3A0A0EF889208E3F874C0FA48CCB009C31F37C203383C82A917AD3B2C2A
3CE043C
750FD33E510E3E10E130BA5051291F4802EA657F0024FDE761E029020A98B5AA03F0EA0
02AC8FD
2E52B7B0F1978D60CFDEC820B68BD7D223E608D447F5480F3075FF0CF8597C701FB740E
A5038B1
56A983CEC3080E1A1020C87C0FD0CAA233C2F2082BCECB622113908688ECBFCFC32105F
7F1100E
24E3A74FFB58B4E829007FC8703FB7EEDD95CC19A3FE1AA180E0DF44E5902F104B0A683
C820F3B
F2C2C042CF0B510DC3014B0EA8CB1084BF049DC21FFC4F188F4FFF8DB22010E43CF33DE
C0CF0C3
CE2FC78F6D80F0F3874E3874FEB0C3F131E0837D033CE00CF03F549CFDF35C203EE87AC
040DF0B
C4FF140C43F30E80370E244182087E803B608F7C6D30F203A6037C2E83CF842027B6AD0
4429AFC
3D130F90387FAD7848B87EFDFE38E748038E0DFCFD9C430197FDCFA0FAE190C92102010
E2D0B10
20B32012702042C0E034CB4091000301C808F14ACED0E22227F80B42C0F13FE0C050884
FDE99B4
9F4037F8BFFB0C138A18EB5E928D00A74FCC0CFD10B449FBF2B4100EC828008357F6BFC
3CC8DFC
513FCB0268F3DEA037228FEC8032F3B00A0F1D7820F7DFD39CEA2B220ADC3E33E73C012
4804A33
3D020872C0243A08E71ED1DF8C8DEC228923A3F3F3433831A208EBFE3947FFC80E40038
74E386E
9C702386EDFF003F93F2C84EFC48FE0FD90C000803BC48D03F103CF871E3B03F1200FF3
38E0FE2
EBC0E00EC000CE000E0CF9CB53B0FD40830C0FC98FCC0FE3EC802884FD56CFC3FC8C7F0
00FC320
0FC50F083F3C3E033C300CC3F3630228FF0383303CD3C827CC3E8FF0080F03F00FF00D0
C3F7503
80EB291FE9A7437B2A81494540E1FC0C7F53F24A2CD240CF18EA2C508F0080F303BE600
33C21D7
ECE08FCFC02353F0C01FC80E9C200D40B83C83FD233002DDEE0FCB80FCF3857B8C8211F
7300823
023FEF4A0CFF8FD5E3813F23FCB00E5C0FCD308F003E120F03EB0B003F80F200CFB002F
C4E297F
5C33FD4CC3C8D238032D20FC30C20C23B3F4DFE0C30EC833CC3F10CC00CCF03F023CEAF
30C0342
02FFCC2E08C08408E2EB3F12123A2FECC22033DDD3503B20A13FAC1F70E3F0380CB20BF
CA0C827
9C888437E0E0F87F2F321A03A0BCED0D329134971E9E3B8E10E0A8C5F12B304213A2E0C
0BA8FEA
E47019934FE0807BA33FC721927F2C920033B0402BCC488330E3A845C957FAA12832805
E7FE8EC
2C0F230273147F70148330F3820BE3194FCC44B52ED2005E2CC24BA01E895A7CFCB20A0
3633994
0042FCCF75862561F32D4189504CCB5462541332D4109507C495842541F32D4189585C7
4504D94
DB32D610B58BC4B5042562F12D4109589CCB5042D4DF3254109537C4B504D16DF12D413
```

```
    45B7C4B
    504256DF32D41095B7CCB504256DF32D41B18C38600801C3280600A024300CF0CB0000F
    C00FFFF
    FFEC03FFCCD035CCF8DCCBFC33C030304'H } ,
          annot {
            {
              data
                ftable {
                  {
                    data
                      gene {
                        locus "RPB1" } ,
                      location
                        int {
                          from 100 ,
                          to 4917 ,
                          id
                            gi 4001823 } } } } } } ,
<==============================the first bioseq ends here
see ASNDB/asn1
<==============================next bioseq begins here
         seq {
           id {
             genbank {
               accession "AAD12604" ,
               version 1 } ,
             gi 4001824 } ,
           descr {
             molinfo {
               biomol peptide ,
               tech concept-trans-a } ,
             title "largest subunit of RNA polymerase II; RPO21 [Vairimorpha
     necatrix]" } ,
           inst {
             repr raw ,
             mol aa ,
             length 1605 ,
             topology not-set ,
             seq-data
               ncbieaa
    "MFDEIVTKRISSIQFGLFSPEEIRKSSVVQIIHPETMENGFPKSGGLIDLKMGTTERAF
    LCSSCEKDNFSCPGHFGHIELTKPMFHVGYMTKIKKILECVCFYCSRLKISTKNLKKDLNFVWNISKTKSV
    CEGEIGE
    NGFTGCGNKQPVIKKEGMSLIAFMKGEEESDGKVILNGERVHNILKKIVNEDAVFLGFDQKFTKPEWLILT
    VLLVPPP
    SVRPSIVMEGMLRAEDDLTHKLADIVKANTYLKKYELEGAPGHVVRDYEQLLQFHIATMIDNDISGQPQAL
    QKSGRPL
    KSISARLKGKEGRVRGNLMGKRVDFSARSVITPDPNISVEEVGVPSEIAKIHTFPEIITPFNIDRLTKLVS
    NGPNEYP
    GANYVIRNDGQRIDLNFNRGDIKLEEGYVVERHMQDGDVVLFNRQPSLHKMSMMAHFVRVMEGKTFRLNLS
    CVSPYNA
    DFDGDEMNLHMPQSYNSKAELEELCLVSKQVLSPQSNKPVMGIVQDSLTALRLFTLRDSFFDRRETMQLLY
    SVNINNY
    EFTDSSKLIMTHDDSFGNNLHTEESSNIMKILNFPAISYPKKLWTGKQILSYILPNTIYNGKSNEHNEEDL
    ENVEDSY
    VIIRNGEILSGIIDKKAVGSTQGGLIHIIANDFGPDRVTCFFDDAQKMMNLYFATINAFSIGIGDAIADKE
    TMSQVQR
    SIETAKEQVNEIIVKAQKNKLERLPGMSMRESFESQVNYILNKPRDISGASASKSLSFCNNMRTMVLAGSK
    GSFINIS
    QVTACLGQQNVEGKRIPFGFNYRSLPHFSKADYSGKSRGFVENSYVKGITPEEFFFHAMGGREGLIDIAIK
    TAETGYI
    QRRLVKAMEDATVTLDRSVRGADGFIYQYEYGEDGFDATFLEMQKMTHDDVATKDDVSFKNLHLVDMFTDL
    NFAIKKE
    NVTDQIYKLLTTDVNLQKILYDEFEWLNENVKKYEKMNIASPCNFQRIINLAIYKFDCRKGDISPYLILDT
    LKNLIEN
    LPIKNLLIEILIKYNLSIKRILNEYKLSLEAYNWILKEIKFKILKSIISPNEMVGTLAAQSVGEPATQMTL
    NTFHLAG
    VSANITMGVPRLKEIINVAKNIKTPCMKIYLKDPFNKTLEMAKKIQSELEFSDIKSLCEFSEIYYDPVIED
    TSIKEDK
    DFVQEYFDFPDEHLDFSKMPKFIIRLKIDRIKLVSKNLKLENIVKSLHEAFPNIFHIIRSDENSQNLIIRI
    RCISSLN
```

```
NNVEYYNLQYKNILNLKIMGYNKIKKVFISEDKDKDEWYLQTDGVCIREIFSHPNVEGHLVTSNDLNEIVE
VLGIEAA
RETILNELTLVIDGNGSYVNHRHISLLADVMTMKGYLTGITRHGVNKVGFGCTKRASFEETVDILLDAALV
AEKYVTK
GYTENIMMGHLAPLGTGIGNLLLDVSKLDKAIPLSKPEYNYEEVDTPFIHSPVSENLSISSGNWSPAYLVE
GNRYAPK
TSLYSPTSPTYSPTSPTYSPTSPTYSPTSPTYSPTSPTYSPTSPTYSPTSPSYSPTSPSYSPTSPSYSPTS
PSYSPTS
PSYSPTSPSYSPTSPSYSPTSPSYSPTSPSYSPTSPSYSPTYDNDEKKTNRKRKGKQ" } ,
      annot {
        {
          data
            ftable {
              {
                data
                  prot {
                    name {
                      "largest subunit of RNA polymerase II" ,
                      "RPO21" } } ,
                location
                  int {
                    from 0 ,
                    to 1604 ,
                    strand plus ,
                    id
                      gi 4001824 } } } } } } ,
  annot {
    {
      data
        ftable {
          {
            data
              cdregion {
                frame one ,
                code {
                  id 1 } } ,
            product
              whole
                gi 4001824 ,
            location
              int {
                from 100 ,
                to 4917 ,
                strand plus ,
                id
                  gi 4001823 } } } } }
```

## Example SwissProt record

```
Seq-entry ::= seq {
  id {
    swissprot {
      name "RPB1_YEAST" ,<============================ACCDB/name
      accession "P04050" } ,<=========================ACCDB/accession
    gi 2507347 } ,
  descr {                                  <======ACCDB/title
    title "DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT (B220)." ,
    comment "-----------------------------------------------------------
-------
--~This SWISS-PROT entry is copyright. It is produced through
a~collaboration
 between the Swiss Institute of Bioinformatics and~the EMBL outstation
- the
 European Bioinformatics Institute.~The original entry is available
from
 http://www.expasy.ch/sprot~and
 http://www.ebi.ac.uk/sprot~-----------------------------------------
-------
----------------" ,
    comment "[FUNCTION] DNA-DEPENDENT RNA POLYMERASE CATALYZES THE
 TRANSCRIPTION OF DNA INTO RNA USING THE FOUR RIBONUCLEOSIDE
TRIPHOSPHATES AS
 SUBSTRATES." ,
    comment "[CATALYTIC ACTIVITY] N NUCLEOSIDE TRIPHOSPHATE = N
PYROPHOSPHATE
 + RNA(N)." ,
    comment "[SUBUNIT] RNA POLYMERASE II CONSISTS OF 12 DIFFERENT
SUBUNITS.
 THIS SUBUNIT IS THE LARGEST COMPONENT OF RNA POLYMERASE II." ,
    comment "[SUBCELLULAR LOCATION] NUCLEAR." ,
    comment "[PTM] THE TANDEM 7 RESIDUES REPEATS CAN BE HIGHLY
PHOSPHORYLATED.
 THE PHOSPHORYLATION ACTIVATES POL2." ,
    comment "[MISCELLANEOUS] THREE DISTINCT ZINC-CONTAINING RNA
POLYMERASES
 ARE FOUND IN EUKARYOTIC NUCLEI: POLYMERASE I FOR THE RIBOSOMAL RNA
PRECURSOR,
 POLYMERASE II FOR THE MRNA PRECURSOR, AND POLYMERASE III FOR 5S AND
TRNA
 GENES." ,
    comment "[SIMILARITY] BELONGS TO THE RNA POLYMERASE BETA' CHAIN
FAMILY." ,
    sp {
      class standard ,
      extra-acc {
        "Q12364" ,
        "Q92315" } ,
      seqref {
        gi 4397 ,
        gi 4398 ,
        gi 1419218 ,
        gi 1419221 ,
        gi 1431216 ,
        gi 1431217 ,
        gi 886080 ,
        gi 886082 ,
        gi 2144431 } ,
      dbref {
        {
          db "SGD" ,
          tag
            str "L0001744" } ,
        {
          db "PFAM" ,
          tag
            str "PF00623" } ,
```

```
        {
          db "PROSITE" ,
          tag
            str "PS00115" } } ,
      keywords {
        "Transferase" ,
        "DNA-directed RNA polymerase" ,
        "Transcription" ,
        "Zinc" ,
        "Repeat" ,
        "DNA-binding" ,
        "Nuclear protein" ,
        "Phosphorylation" ,
        "Zinc-finger" } ,
      created
        std {
          year 1986 ,
          month 11 ,
          day 1 } ,
      sequpd
        std {
          year 1997 ,
          month 11 ,
          day 1 } ,
      annotupd
        std {
          year 1999 ,
          month 7 ,
          day 15 } } ,
    create-date
      std {
        year 1986 ,
        month 11 ,
        day 1 } ,
    update-date
      std {
        year 1999 ,
        month 7 ,
        day 15 } ,
    source {
      org {
        taxname "Saccharomyces cerevisiae" ,
        common "baker's yeast" ,
        db {
          {
            db "taxon" ,
            tag
              id 4932 } } ,
        orgname {
          name
            binomial {
              genus "Saccharomyces" ,
              species "cerevisiae" } ,
          lineage "Eukaryota; Fungi; Ascomycota; Saccharomycotina;
 Saccharomycetes; Saccharomycetales; Saccharomycetaceae; Saccharomyces"
,
          gcode 1 ,
          mgcode 3 ,
          div "PLN" } } } ,
    molinfo {
      biomol peptide ,
      completeness complete } ,
    pub {
      pub {
        gen {
          serial-number 1 } ,
        muid 85282617 ,
        article {
          title {
            name "Extensive homology among the largest subunits of
eukaryotic
 and prokaryotic RNA polymerases." } ,
```

```
            authors {
              names
                std {
                  {
                    name
                      name {
                        last "Allison" ,
                        initials "L.A." } } ,
                  {
                    name
                      name {
                        last "Moyle" ,
                        initials "M." } } ,
                  {
                    name
                      name {
                        last "Shales" ,
                        initials "M." } } ,
                  {
                    name
                      name {
                        last "Ingles" ,
                        initials "C.J." } } } } ,
            from
              journal {
                title {
                  iso-jta "Cell" ,
                  ml-jta "Cell" ,
                  issn "0092-8674" ,
                  name "Cell." } ,
                imp {
                  date
                    std {
                      year 1985 ,
                      month 9 } ,
                  volume "42" ,
                  issue "2" ,
                  pages "599-610" ,
                  language "eng" } } ,
            ids {
              pubmed 3896517 ,
              medline 85282617 } } ,
          pmid 3896517 } ,
        comment "SEQUENCE FROM N.A.~STRAIN=A364A" } ,
      pub {
        pub {
          gen {
            serial-number 2 } ,
          muid 97127826 ,
          article {
            title {
              name "Analysis of a 26,756 bp segment from the left arm of
yeast
 chromosome IV." } ,
            authors {
              names
                std {
                  {
                    name
                      name {
                        last "Wolfl" ,
                        initials "S." } } ,
                  {
                    name
                      name {
                        last "Hanemann" ,
                        initials "V." } } ,
                  {
                    name
                      name {
                        last "Saluz" ,
                        initials "H.P." } } } ,
```

```
            affil
              str "Hans-Knoll-Institut fur Naturstoff-Forschung,
Department of
 Cell and Molecular Biology, Jena, Germany." } ,
            from
              journal {
                title {
                  iso-jta "Yeast" ,
                  ml-jta "Yeast" ,
                  issn "0749-503X" ,
                  name "Yeast (Chichester, England)" } ,
                imp {
                  date
                    std {
                      year 1996 ,
                      month 12 } ,
                  volume "12" ,
                  issue "15" ,
                  pages "1549-1554" ,
                  language "eng" } } ,
            ids {
              pubmed 8972577 ,
              medline 97127826 } } ,
          pmid 8972577 } ,
        comment "SEQUENCE FROM N.A.~STRAIN=S288C / FY1679" } ,
      pub {
        pub {
          gen {
            serial-number 3 } ,
          muid 95377607 ,
          article {
            title {
              name "The gene encoding the biotin-apoprotein ligase of
 Saccharomyces cerevisiae." } ,
            authors {
              names
                std {
                  {
                    name
                      name {
                        last "Cronan" ,
                        initials "J.E." ,
                        suffix "Jr." } } ,
                  {
                    name
                      name {
                        last "Wallace" ,
                        initials "J.C." } } } ,
              affil
                str "Department of Microbiology, University of Illinois,
Urbana
 6180, USA." } ,
            from
              journal {
                title {
                  iso-jta "FEMS Microbiol. Lett." ,
                  ml-jta "FEMS Microbiol Lett" ,
                  issn "0378-1097" ,
                  name "FEMS microbiology letters." } ,
                imp {
                  date
                    std {
                      year 1995 ,
                      month 8 ,
                      day 1 } ,
                  volume "130" ,
                  issue "2-3" ,
                  pages "221-229" ,
                  language "eng" } } ,
            ids {
              pubmed 7649444 ,
              medline 95377607 } } ,
```

```
        pmid 7649444 } ,
      comment "SEQUENCE OF 1669-1733 FROM N.A.~STRAIN=S288C" } } ,
  inst {
    repr raw ,
    mol aa ,
    length 1733 ,
    seq-data
      ncbieaa
"MVGQQYSSAPLRTVKEVQFGLFSPEEVRAISVAKIRFPETMDETQTRAKIGGLNDPRLGSIDR
NLKCQTCQEGMNECPGHFGHIDLAKPVFHVGFIAKIKKVCECVCMHCGKLLLDEHNELMRQALAIKDSKKR
FAAIWTL
CKTKMVCETDVPSEDDPTQLVSRGGCGNTQPTIRKDGLKLVGSWKKDRATGDADEPELRVLSTEEILNIFK
HISVKDF
TSLGFNEVFSRPEWMILTCLPVPPPPVRPSISFNESQRGEDDLTFKLADILKANISLETLEHNGAPHHAIE
EAESLLQ
FHVATYMDNDIAGQPQALQKSGRPVKSIRARLKGKEGRIRGNLMGKRVDFSARTVISGDPNLELDQVGVPK
SIAKTLT
YPEVVTPYNIDRLTQLVRNGPNEHPGAKYVIRDSGDRIDLRYSKRAGDIQLQYGWKVERHIMDNDPVLFNR
QPSLHKM
SMMAHRVKVIPYSTFRLNLSVTSPYNADFDGDEMNLHVPQSEETRAELSQLCAVPLQIVSPQSNKPCMGIV
QDTLCGI
RKLTLRDTFIELDQVLNMLYWVPDWDGVIPTPAIIKPKPLWSGKQILSVAIPNGIHLQRFDEGTTLLSPKD
NGMLIID
GQIIFGVVEKKTVGSSNGGLIHVVTREKGPQVCAKLFGNIQKVVNFWLLHNGFSTGIGDTIADGPTMREIT
ETIAEAK
KKVLDVTKEAQANLLTAKHGMTLRESFEDNVVRFLNEARDKAGRLAEVNLKDLNNVKQMVMAGSKGSFINI
AQMSACV
GQQSVEGKRIAFGFVDRTLPHFSKDDYSPESKGFVENSYLRGLTPQEFFFHAMGGREGLIDTAVKTAETGY
IQRRLVK
ALEDIMVHYDNTTRNSLGNVIQFIYGEDGMDAAHIEKQSLDTIGGSDAAFEKRYRVDLLNTDHTLDPSLLE
SGSEILG
DLKLQVLLDEEYKQLVKDRKFLREVFVDGEANWPLPVNIRRIIQNAQQTFHIDHTKPSDLTIKDIVLGVKD
LQENLLV
LRGKNEIIQNAQRDAVTLFCCLLRSRLATRRVLQEYRLTKQAFDWVLSNIEAQFLRSVVHPGEMVGVLAAQ
SIGEPAT
QMTLNTFHFAGVASKKVTSGVPRLKEILNVAKNMKTPSLTVYLEPGHAADQEQAKLIRSAIEHTTLKSVTI
ASEIYYD
PDPRSTVIPEDEEIIQLHFSLLDEEAEQSFDQQSPWLLRLELDRAAMNDKDLTMGQVGERIKQTFKNDLFV
IWSEDND
EKLIIRCRVVRPKSLDAETEAEEDHMLKKIENTMLENITLRGVENIERVVMMKYDRKVPSPTGEYVKEPEW
VLETDGV
NLSEVMTVPGIDPTRIYTNSFIDIMEVLGIEAGRAALYKEVYNVIASDGSYVNYRHMALLVDVMTTQGGLT
SVTRHGF
NRSNTGALMRCSFEETVEILFEAGASAELDDCRGVSENVILGQMAPIGTGAFDVMIDEESLVKYMPEQKIT
EIEDGQD
GGVTPYSNESGLVNADLDVKDELMFSPLVDSGSNDAMAGGFTAYGGADYGEATSPFGAYGEAPTSPGFGVS
SPGFSPT
SPTYSPTSPAYSPTSPSYSPTSPSYSPTSPSYSPTSPSYSPTSPSYSPTSPSYSPTSPSYSPTSPSYSPTS
PSYSPTS
PSYSPTSPSYSPTSPSYSPTSPSYSPTSPSYSPTSPAYSPTSPSYSPTSPSYSPTSPSYSPTSPSYSPTSP
NYSPTSP
SYSPTSPGYSPGSPAYSPKQDEQKHNENENSR" ,
    hist {
      replaces {
        date
          std {
            year 1997 ,
            month 10 ,
            day 9 } ,
        ids {
          gi 133330 } } } } ,
  annot {
    {
      data
        ftable {
          {
            data
              region "Zinc finger region" ,
            comment "C2H2-TYPE (POTENTIAL)." ,
            location
              int {
                from 66 ,
```

```
      to 82 ,
      id
        gi 2507347 } ,
  exp-ev not-experimental } ,
{
  data
    region "Domain" ,
  comment "CARBOXYL-TERMINAL 7-RESIDUE REPEATS." ,
  location
    int {
      from 1543 ,
      to 1718 ,
      id
        gi 2507347 } ,
  exp-ev experimental } ,
{
  data
    region "Variant" ,
  comment "MISSING (IN STRAIN A364A)." ,
  location
    int {
      from 1652 ,
      to 1658 ,
      id
        gi 2507347 } ,
  exp-ev experimental } ,
{
  data
    region "Conflict" ,
  comment "A -> V (IN REF. 1)." ,
  location
    pnt {
      point 1513 ,
      id
        gi 2507347 } ,
  exp-ev experimental } ,
{
  data
    region "Conflict" ,
  comment "G -> A (IN REF. 1)." ,
  location
    pnt {
      point 1523 ,
      id
        gi 2507347 } ,
  exp-ev experimental } ,
{
  data
    region "Conflict" ,
  comment "T -> M (IN REF. 1)." ,
  location
    pnt {
      point 1600 ,
      id
        gi 2507347 } ,
  exp-ev experimental } ,
{
  data
    gene {
      locus "RPB1" ,
      syn {
        "RPO21" ,
        "RPB220" ,
        "SUA8" ,
        "YDL140C" ,
        "D2150" } } ,
  location
    int {
      from 0 ,
      to 1732 ,
      id
        gi 2507347 } } ,
```

```
{
  data
    prot {
      name {           <=============ACCDB/title
        "DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT" } ,
      ec {
        "2.7.7.6" } } ,
  location
    int {
      from 0 ,
      to 1732 ,
      id
        gi 2507347 } } } } } }
```

## Example EMBL record

```
Seq-entry ::= set {
  level 1 ,
  class nuc-prot ,
  descr {
    pub {
      pub {
        gen {
          cit "Unpublished" ,
          authors {
            names
              std {
                {
                  name
                    name {
                      last "Drebot" ,
                      initials "M.A." } } ,
                {
                  name
                    name {
                      last "Jansma" ,
                      initials "D." } } ,
                {
                  name
                    name {
                      last "Himmelfarb" ,
                      initials "H.J." } } ,
                {
                  name
                    name {
                      last "Friesen" ,
                      initials "J.D." } } } } ,
          title "Suppressors of yeast RNA polymerase II mutations
belong to a
 family of gene products that interact with a protein kinase" } } } ,
    pub {
      pub {
        sub {
          authors {
            names
              std {
                {
                  name
                    name {
                      last "Jansma" ,
                      initials "D." } } } ,
            affil
              str "David Jansma, Genetics, Hospital for Sick Children,
555
 University, Avenue, Toronto, Ontario, M5G 1X8, Canada" } ,
          medium other ,
          date
            std {
              year 1992 ,
              month 7 ,
              day 28 } } } } ,
    create-date
      std {
        year 1992 ,
        month 12 ,
        day 11 } ,
    update-date
      std {
        year 1993 ,
        month 3 ,
        day 12 } ,
    source {
      org {
        taxname "Saccharomyces cerevisiae" ,
```

```
          common "baker's yeast" ,
          db {
            {
              db "taxon" ,
              tag
                id 4932 } } ,
          orgname {
            name
              binomial {
                genus "Saccharomyces" ,
                species "cerevisiae" } ,
            mod {
              {
                subtype isolate ,
                subname "Mating type a" } } ,
            lineage "Eukaryota; Fungi; Ascomycota; Saccharomycotina;
   Saccharomycetes; Saccharomycetales; Saccharomycetaceae; Saccharomyces"
  ,
            gcode 1 ,
            mgcode 3 ,
            div "PLN" } } ,
        subtype {
          {
            subtype chromosome ,
            name "7" } } } } ,
    seq-set {
      seq {
        id {
          embl {
            name "SCSPM2" ,<==============================ACCDB/name
            accession "Z14128" ,<=======================ACCDB/accession
            version 1 } ,<================================ACCDB/version
          gi 287914 } ,
        descr {
          title "S.cerevisiae spm2+ gene for spm2+ protein" ,
          embl {
            div fun ,
            creation-date
              std {
                year 1992 ,
                month 12 ,
                day 11 } ,
            update-date
              std {
                year 1993 ,
                month 3 ,
                day 12 } ,
            keywords {
              "CDC68/SPT16 protein" ,
              "spm2+ gene" ,
              "spm2+ protein" } ,
            xref {
              {
                dbname
                  name "SGD" ,
                id {
                  str "L0001891" ,
                  str "SIP2" } } ,
              {
                dbname
                  code swissprot ,
                id {
                  str "P34164" ,
                  str "SIP2_YEAST" } } } } ,
          molinfo {
            biomol genomic } } ,
        inst {
          repr raw ,
          mol dna ,
          length 2032 ,
          seq-data
            ncbi2na
```

```
'00F965EC6C171E0103E3BFD06B54022FC17F9A55FFCDD14FFD770607B4E
0107C933066C7C4C8C8F0323053933470724DB4E0C91BF973183E69693ADFF33E757E85
8B023F1
7E6FF68DB4037FCA80A303114423D7A80E00B3780C3EE7FE82AC78892E0BF73AB1C610B
4D49500
024041000BB6E45CD38B86F2200152439D0A798164203A39EE24202F1E0789F0303BD23
D50866A
925F42A2A373C50000361BCF9E6E38A18951CE502737BCE8079EE847877AB7DB71C98E3
822A233
CF9521848950908E52D78E38D9D294F7D952228A841240C6E50209F6A2B50B80D089D3C
3AF56E8
8C2BA490AEBD00BF1B84A74F4503A28038DAFE3178F78430E9D3F4EE09C29E7D4A444C8
F48FCCB
A30E27C8BCB8FD7951241E348EA01F6D0F1320B4A4148000541C180230AD428248F5398
5D51498
D8D743E77903EB0A35218FFAE1A3310AFD38237B45485D6FA0CC41213D596EFC7856DED
3A0631C
F317E8DB4902431E31B4E9E114550F175D2FA20EF37E0C0C739464214BD062041D299DE
54F5814
EEB9F051FAF1CB24F0910C47FBB25D4DBD8CC0480CED1523DFCC654C8B5DB0D6A3D71FF
C0A6CFB
333FFA49CE911C3F73F50FCBB0922332093304C38FC70EA74B1DD0E7CFBCD1014631C31
5A0B66E
37FFFFF6803883651FF706020CF80DF0CFAE208A0C02C9C222D1A8700AC00BD273D41FC
75FDE33
E45FDB81E9F6ECFC2E0CE'H ,
        hist {
          replaces {
            date
              std {
                year 1993 ,
                month 6 ,
                day 11 } ,
            ids {
              gi 4525 } } } } ,
      annot {
        {
          data
            ftable {
              {
                data
                  pub {
                    pub {
                      muid 92017853 ,
                      article {
                        title {
                          name "CDC68, a yeast gene that affects
regulation of
 cell proliferation and transcription, encodes a protein with a highly
acidic
 carboxyl terminus." } ,
                        authors {
                          names
                            std {
                              {
                                name
                                  name {
                                    last "Rowley" ,
                                    initials "A." } } ,
                              {
                                name
                                  name {
                                    last "Singer" ,
                                    initials "R.A." } } ,
                              {
                                name
                                  name {
                                    last "Johnston" ,
                                    initials "G.C." } } } ,
                          affil
                            str "Department of Microbiology, Dalhousie
 University, Halifax, Nova Scotia, Canada." } ,
```

```
                        from
                          journal {
                            title {
                              iso-jta "Mol. Cell. Biol." ,
                              ml-jta "Mol Cell Biol" ,
                              issn "0270-7306" ,
                              name "Molecular and cellular biology." }
,
                            imp {
                              date
                                std {
                                  year 1991 ,
                                  month 11 } ,
                              volume "11" ,
                              issue "11" ,
                              pages "5718-5726" ,
                              language "eng" } } ,
                        ids {
                          pubmed 1833637 ,
                          medline 92017853 } } ,
                      pmid 1833637 } } ,
                location
                  int {
                    from 1282 ,
                    to 2031 ,
                    id
                      gi 287914 } } ,
              {
                data
                  gene {
                    locus "spm2+" } ,
                location
                  int {
                    from 398 ,
                    to 1645 ,
                    id
                      gi 287914 } } } } } } ,
    seq {
      id {
        embl {
          accession "CAA78503" ,
          version 1 } ,
        gi 287915 } ,
      descr {
        title "spm2+ [Saccharomyces cerevisiae]" ,
        molinfo {
          biomol peptide } } ,
      inst {
        repr raw ,
        mol aa ,
        length 415 ,
        seq-data
          ncbieaa
"MGTTTSHPAQKKQTTKKCRAPIMSDVREKPSNAQGCEPQEMDAVSKKVTELSLNKCSDS
QDAGQPSREGSITKKKSTLLLRDEDEPTMPKLSVMETAVDTDSGSSSTSDDEEGDIIAQTTEPKQDASPDD
DRSGHSS
PREEGQQQIRAKEASGGPSEIKSSLMVPVEIRWQQGGSKVYVTGSFTKWRKMIGLIPDSDNNGSFHVKLRL
LPGTHRF
RFIVDNELRVSDFLPTATDQMGNFVNYIEVRQPEKNPTNEKIRSKEADSMRPPTSDRSSIALQIGKDPDDF
GDGYTRF
HEDLSPRPPLEYTTDIPAVFTDPSVMERYYYTLDRQQSNTDTSWLTPPQLPPQLENVILNKYYATQDQFNE
NNSGALP
IPNHVVLNHLVTSSIKHNTLCVASIVRYKQKYVTQILYTPIESS" ,
        hist {
          replaces {
            date
              std {
                year 1993 ,
                month 6 ,
                day 11 } ,
            ids {
              gi 4526 } } } } ,
```

```
        annot {
          {
            data
              ftable {
                {
                  data
                    prot {
                      name {
                        "spm2+" } ,
                      activity {
                        "Wild-type version of SPM2,a dominant extragenic
 suppressor of some temperature-sensitve mutations in RPO21 and PRP4."
} } ,
                  location
                    whole
                      gi 287915 } } } } } ,
      seq {
        id {
          embl {
            accession "CAA78504" ,
            version 1 } ,
          gi 4388554 } ,
        descr {
          title "CDC68 /SPT16 [Saccharomyces cerevisiae]" ,
          molinfo {
            biomol peptide ,
            completeness partial } } ,
        inst {
          repr raw ,
          mol aa ,
          length 1 ,
          seq-data
            ncbieaa "M" } ,
        annot {
          {
            data
              ftable {
                {
                  data
                    prot {
                      name {
                        "CDC68 /SPT16" } } ,
                  partial TRUE ,
                  location
                    whole
                      gi 4388554 } } } } } } ,
    annot {
      {
        data
          ftable {
            {
              data
                cdregion {
                  frame one ,
                  code {
                    id 1 } } ,
              product
                whole
                  gi 287915 ,
              location
                int {
                  from 398 ,
                  to 1645 ,
                  id
                    gi 287914 } ,
              dbxref {
                {
                  db "SWISS-PROT" ,
                  tag
                    str "P34164" } } } ,
            {
              data
```

```
  cdregion {
    frame one ,
    code {
      id 1 } } ,
partial TRUE ,
product
  whole
    gi 4388554 ,
location
  int {
    from 2029 ,
    to 2031 ,
    id
      gi 287914 ,
    fuzz-to
      lim gt } ,
cit
  pub {
    muid 92017853 } } } } } }
```

## Example PDB record

```
Seq-entry ::= set {
  class pdb-entry ,
  descr {
    pdb {
      deposition
        std {
          year 1992 ,
          month 4 ,
          day 3 } ,
      class "Isomerase(Intramolecular Oxidoreductse)" ,
      compound {
        "D-Xylose Isomerase (E.C.5.3.1.5) Mutant With Glu 186 Replaced
By Gln
 (E186Q) Complex With Xylose And Mn" } ,
      source {
        "(Actinoplanes missouriensis) E186Q Mutant Gene Expressed In
 (Escherichia coli)" } ,
      exp-method "X-Ray Diffraction" } ,
    comment "Revision History:~JUL 15 93 Initial Entry" ,
    pub {
      pub {
        sub {
          authors {
            names
              std {
                {
                  name
                    name {
                      last "Janin" ,
                      full "J.Janin" ,
                      initials "J." } } } } ,
          date
            std {
              year 1992 ,
              month 4 ,
              day 3 } } } } ,
    pub {
      pub {
        muid 92304915 ,
        article {
          title {
            name "Protein engineering of xylose (glucose) isomerase
from
 Actinoplanes missouriensis. 1. Crystallography and site-directed
mutagenesis
 of metal binding sites." } ,
          authors {
            names
              str {
                "J.Jenkins" ,
                "J.Janin" ,
                "F.Rey" ,
                "M.Chiadmi" ,
                "H.van Tilbeurgh" ,
                "I.Lasters" ,
                "M.De Maeyer" ,
                "D.Van Belle" ,
                "S.J.Wodak" ,
                "M.Lauwereys" ,
                "P.Stanssens" ,
                "N.T.Mrabet" ,
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                "G.Matthyssens" ,
                "A.-M.Lambeir" } } ,
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              title {
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                "P.Stanssens" ,
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                "H.van Tilbeurgh" ,
                "G.Matthyssens" ,
                "I.Lasters" ,
                "M.De Maeyer" ,
                "S.J.Wodak" ,
                "J.Jenkins" ,
                "M.Chiadmi" ,
                "J.Janin" } } ,
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                {
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                      last "Jenkins" ,
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                    {
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                        name {
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              month 4 ,
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### Example Biostruc

An example of the ASN biostruc. Some data has been removed for the sake of brevity.

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    pdb-comment "remark   3: Authors                    Westhof,Dumas,Moras" ,
    pdb-comment "remark   3: R Value                    0.163" ,
    pdb-comment "remark   3: Free R Value               0.252" ,
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    pdb-comment "remark   3: Resolution Range       8.0 - 2.25 Angstroms" ,
    pdb-comment "remark   3: Data Cutoff                2.0    Sigma(F)" ,
    pdb-comment "remark   3: Number Of Protein Atoms
                         0" ,
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                   488" ,
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                        33" ,
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    pdb-comment "remark   3: Sigma, In Parentheses, Are The Input Estimated" ,
    pdb-comment "remark   3: Standard Deviations That Determine The Relative" ,
    pdb-comment "remark   3: Weights Of The Corresponding Restraints)" ,
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                full "D.S.Goodsell" ,
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                initials "M.L." } } ,
          {
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          month 12 ,
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                initials "R.E." } } } } ,
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               {
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          residue-id 12 ,
          atom-id 1 } } } } ,
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            div "SYN" } } } } ,
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              residue-id 1 ,
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              residue-id 2 ,
              atom-id 1 } } ,
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              residue-id 11 ,
              atom-id 9 } ,
            atom-id-2 {
              molecule-id 2 ,
              residue-id 12 ,
              atom-id 1 } } } } ,
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            name "  58 " ,
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        descr {
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        atom-id-2 {
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          residue-id 1 ,
          atom-id 1 } } ,
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          residue-id 9 ,
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          residue-id 1 ,
          atom-id 1 } } } ,
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            name " C5 " ,
            iupac-code {
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            element c } ,
          {
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            name " C6 " ,
            iupac-code {
              " C6 " } ,
            element c } } ,
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            atom-id-2 17 ,
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          {
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            atom-id-2 18 ,
            bond-order unknown } } } ,
      {
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      iupac-code {
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          name " C1 " ,
          iupac-code {
            " C1 " } ,
          element c } ,
        {
          id 5 ,
          name " C2 " ,
          iupac-code {
            " C2 " } ,
          element c } ,
        {
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          atom-id-2 3 ,
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          atom-id-2 14 ,
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          atom-id-2 31 ,
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      descr {
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      atoms {
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          name "MG  " ,
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            "MG  " } ,
          element mg } ,
        {
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          name " O1 " ,
          iupac-code {
            " O1 " } ,
          element o } ,
        {
          id 3 ,
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          iupac-code {
            " O2 " } ,
          element o } ,
        {
          id 4 ,
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            iupac-code {
              " O3 " } ,
            element o } } ,
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            atom-id-2 2 ,
            bond-order unknown } ,
          {
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            atom-id-2 3 ,
            bond-order unknown } ,
          {
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            atom-id-2 4 ,
            bond-order unknown } } } ,
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        iupac-code {
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        atoms {
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        pdb-method "X-Ray Diffraction" ,
        pdb-comment "FEB 27 95 Initial Entry" } ,
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        thermal-factor-units b } ,
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      19853 ,
      20375 ,
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      34632 ,
      33233 ,
      30694 } ,
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      22605 ,
      8518 ,
      -2033 ,
      26343 } } ,
  temperature-factors
    isotropic {
      scale-factor 1000 ,
      b {
        23239 ,
        24930 } } } } } } } }
```

**GO background material**

Please see*: http://www.geneontology.org/doc/GO.doc.html*}