Sample application: SimplePDBBrowser

Overview of the application

SimplePDBBrowser will be a relatively simple gateway to access Protein Data Bank data. It will allow to search by codes, and for textual data included in PDB headers like, description, techniques used, resolution, source or author. Results of the search will give basic information about the PDB entry and link to the appropriate web pages in the main PDB web site.

Input data. *Nature and origin (user input, replicated database, calculation results, etc.). Input validation if necessary. User control, etc.*

User input: User should fill a web form including either a PDB id or some information. Fields available would be:

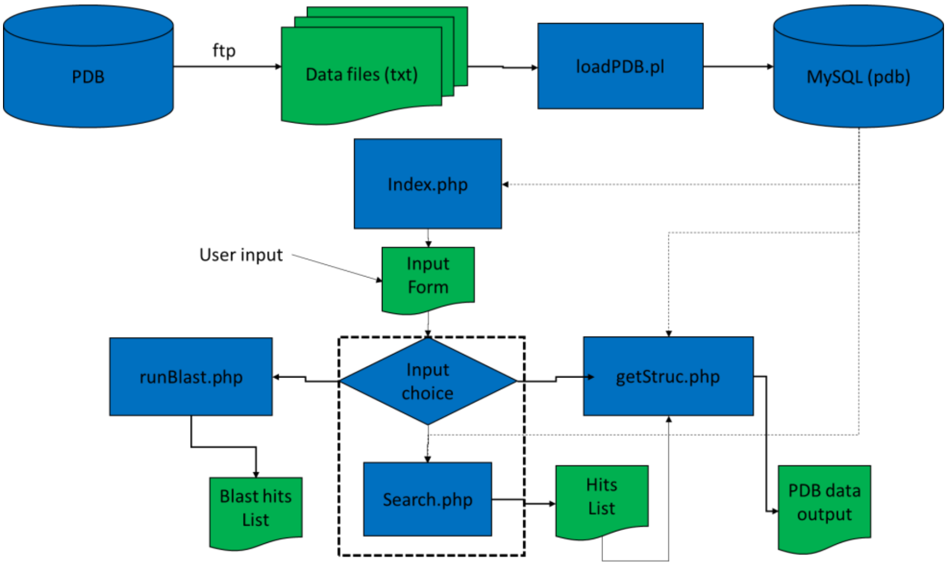
- PDB code (4 letter code). Will direct to a single entry if available
- Search Fields
    - Description, headers, authors, source (text search)
    - Resolution (numeric input)
    - Technique used (selection of possibles, X Ray, NMR, etc)
    - Type of molecule (selection of protein, nucleic acid, complex)
    - Year of submission (numeric input)
- Sequence search: PDB entries will be obtained through a Standard Blast search. Sequence can be provided as text or uploaded file

Data input: Data will be obtained off-line by parsing the index files provided at Protein Data Bank Ftp (/derived_data), and stored in the a database with the appropriate structure.

Output. *Data, way of presentation (web/email).*

Search/blast search outputs: Output of a search would be a list of the found hits, showing a limited amount of information just to identify the hit: PDB Id, entry description, type of molecule, source. List items will have links to entries data.

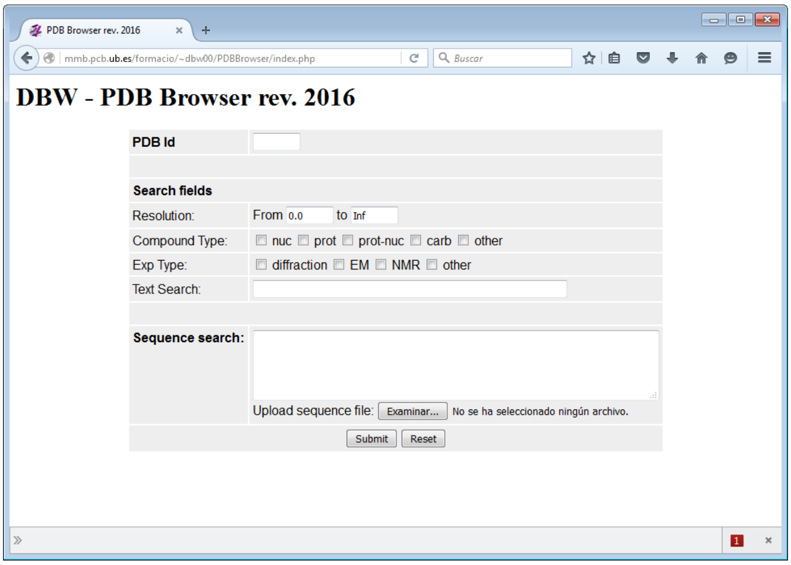
Entry data: Complete information available about the entry, links to the PDB main site, and to other related sites with structural information.



Globals.inc.php

(to be included by any .php script)

```
<?php
/*
 * globals.inc.php
 * Global variables and settings
 */
// Base directories
#$baseDir = $_SERVER['DOCUMENT_ROOT'].'/PDBBrowser';
$baseDir = '/home/dbw00/public_html/PDBBrowser';
$baseURL = dirname($_SERVER['SCRIPT_NAME']);

// Temporal dir, create if not exists
$tmpDir = "$baseDir/tmp";
if (!file_exists($tmpDir))
    mkdir($tmpDir);

// Blast details, change to adapt to local settings
$blastHome = "/home/dbw00/blast";
$blastDbsDir = "$blastHome/dbs";
$blastExe = "$blastHome/bin/blastall";
$blastDbs = array("SwissProt" => "sprot", "PDB" => "pdb_seqres.txt");
$blastCmdLine = "$blastExe -d $blastDbsDir/" . $blastDbs['PDB'] . " -p blastp  -e 0.001 -v 100 -b 0 ";

// Include directory
$incDir = "$baseDir/include";

// Load accessory routines
include_once "$incDir/bdconn.inc.php";
include_once "$incDir/libDBW.inc.php";

// Load predefined arrays
// Fulltext search fields
$textFields = Array('e.header', 'e.compound', 'a.author', 's.source', 'sq.header');

// Compounds
$rs = mysql_query("SELECT * from comptype") or print mysql_error();
while ($rsF = mysql_fetch_array($rs))
    $compTypeArray[$rsF['idCompType']] = $rsF;

//expTypes
$rs = mysql_query("SELECT * from expType") or print mysql_error();
while ($rsF = mysql_fetch_array($rs))
    $expTypeArray[$rsF['idExpType']] = $rsF;

//expClasses
$rs = mysql_query("SELECT * from expClasse") or print mysql_error();
while ($rsF = mysql_fetch_array($rs))
    $expClasseArray[$rsF['idExpClasse']] = $rsF;

// Start session to store queries
session_start();
```



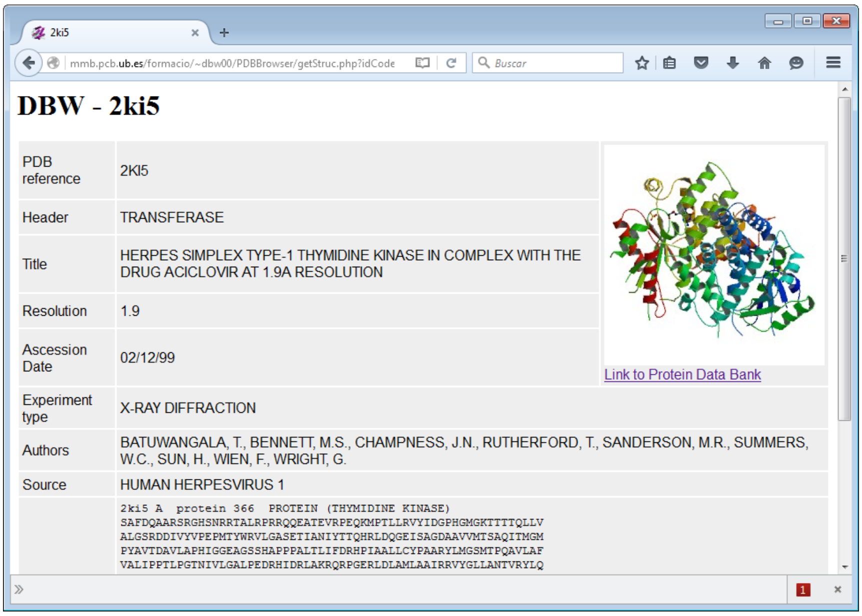
DBW - PDB Browser rev. 2016

PDB Id	
Search fields	
Resolution:	From 0.0 to Inf
Compound Type:	□ nuc □ prot □ prot-nuc □ carb □ other
Exp Type:	□ diffraction □ EM □ NMR □ other
Text Search:	
Sequence search:	Upload sequence file: Examinar... No se ha seleccionado ningún archivo.
Submit Reset	

Index.php

Main entry for the application. Uses default values from $_SESSION to reload pass choices

```
<?php
/*
 * index.php
 * main form
 */
# Loading global variables and DB connection
include "globals.inc.php";

// $_SESSION['queryData'] array holds data from previous forms, if empty it should be
// initialized to avoid warnings, and set defaults
// also a ...?new=1 allow to clean it from the URL.
if (isset($_REQUEST['new']) or ! isset($_SESSION['queryData'])) {
   $_SESSION['queryData'] = array(
      'minRes' => '0.0',
      'maxRes' => 'Inf',
      'query' => ''
   );
}
# All HTML settings and CSS is loaded from headerDBW
print headerDBW("PDB Browser rev. 2016");

#Main Form follows
?>
<form name="MainForm" action="search.php" method="POST" enctype="multipart/form-data">
   <table border="0" cellspacing="2" cellpadding="4" align="center">
      <tbody>
         <tr>
            <td><b>PDB Id</b></td>
            <td><input type="text" name="idCode" value="" size="5" maxlength="4"/></td>
         </tr>
         <tr>
            <td colspan="2">&nbsp;</td>
         </tr>
         <tr>
            <td colspan="2"><b>Search fields</b></td>
         </tr>
         <tr>
            <td>Resolution:</td>
            <td>
               From <input type="text" name="minRes" value="<?php print $_SESSION['queryData']['minRes'] ?>" size="5">
               to <input type="text" name="maxRes" value="<?php print $_SESSION['queryData']['maxRes'] ?>" size="5" />
            </td>
        </tr>
        <tr>
            <td>Compound Type:</td>
            <td>
                <?php
                /* We obtain the possible fields from the comptype table,
                 * alternatively this could be done in globals.inc.php and stored as $compTypeArray
                 * Then here we will use $compTypeArray instead
                 *
                 *  foreach (array_values($compTypeArray) as $c) {
                 *   <input type="checkbox" name="idCompType[<?php print $c ?>]" /> <?php print
                 *       $c['type'] ?>-->
                 * }
                 *
                 * Note that input names build idCompType[] array
                 */
                $rs = mysql_query("SELECT * from comptype");
                while ($rsF = mysql_fetch_array($rs)) {
                    ?>
                    <input type="checkbox" name="idCompType[<?php echo $rsF['idCompType'] ?>]" /> <?php echo $rsF['type'] . "\n"
?>
                <?php } ?>
            </td>
        </tr>
        <tr>
            <td>Exp Type:</td>
            <td>
                <?php
                /* We obtain the possible fields from the expClasse table,
                 * that is a condensed version of expType, alternatively this could be done in
                 * globals.inc.php
                 * as compType
                 * input names build idExpClasse[] array
                 */
                $rs = mysql_query("SELECT * from expClasse  order by ExpClasse");
                while ($rsF = mysql_fetch_array($rs)) {
                    ?>
                    <input type="checkbox" name="idExpClasse[<?php echo $rsF['idExpClasse'] ?>]" /> <?php echo $rsF['expClasse'] .
"\n" ?>
                <?php } ?>
            </td>
        </tr>
        <tr>
            <td>Text Search:</td>
            <td><input type="text" name="query1" value="<?php print $_SESSION['queryData']['query1'] ?>" size="60" /></td>
        </tr>
        <tr>
            <td colspan="2">&nbsp;</td>
        </tr>
        <tr>
            <td valign="top"><b>Sequence search:</b></td>
            <td>
                <textarea name="seqQuery" rows="4" cols="60"></textarea><br>
                Upload sequence file: <input type="file" name="seqFile" value="" width="50" />
            </td>
        </tr>
        <tr>
            <td colspan="2" align="center">
                <input type="submit" value="Submit" />
                <input type="reset" value="Reset" />
            </td>
        </tr>
        </tbody>
    </table>
</form>
<?php
print footerDBW();
```


2ki5
mmb.pcb.ub.es/formacio/~dbw00/PDBBrowser/getStruc.php?idCode
Buscar

DBW - 2ki5

PDB reference	2KI5	Link to Protein Data Bank
Header	TRANSFERASE	
Title	HERPES SIMPLEX TYPE-1 THYMIDINE KINASE IN COMPLEX WITH THE DRUG ACICLOVIR AT 1.9A RESOLUTION	
Resolution	1.9	
Accession Date	02/12/99	
Experiment type	X-RAY DIFFRACTION	
Authors	BATUWANGALA, T., BENNETT, M.S., CHAMPNESS, J.N., RUTHERFORD, T., SANDERSON, M.R., SUMMERS, W.C., SUN, H., WIEN, F., WRIGHT, G.	
Source	HUMAN HERPESVIRUS 1	
	2ki5 A protein 366 PROTEIN (THYMIDINE KINASE) SAFDQAARSRGHSNRRTALRPRRQQEATEVRPEQKMPTLLRVYIDGPHGMGKTTTTQLLV ALGSRDDIVYVPEPMTYWRVLGASETIANIYTTQHRLDQGEISAGDAAVVMTSAQITMGM PYAVTDAVLAPHIGGEAGSSHAPPPALTLIFDRHPIAALLCYPAARYLMGSMTPQAVLAF VALIPPTLPGTNIVLGALPEDRHIDRLAKRQRPGERLDLAMLAAIRRVYGLLANTVRYLQ	

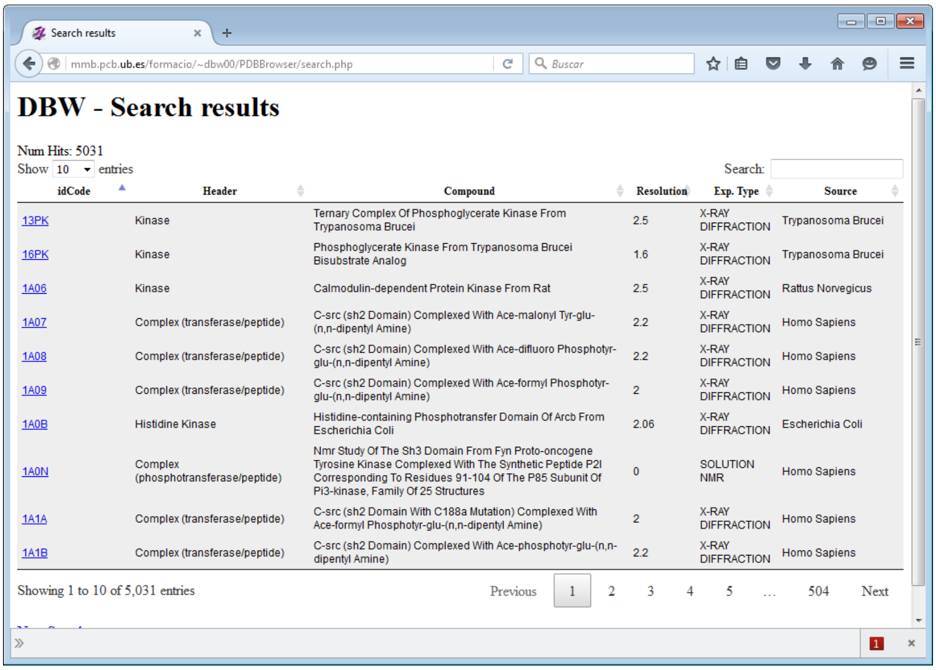
getStruc.php

Output view for PDB data (parameters passed using GET)

```
<?php
/*
 * getStruc.php Shows data for a PDB entry
 */
// load global vars and includes
include "globals.inc.php";

//get data for the structure requested
$sql = "SELECT e.* from entry e where e.idCode='" . $_REQUEST['idCode'] . "'";
$rs = mysql_query($sql) or print mysql_error();
if (!mysql_num_rows($rs)) { //search is empty
   print errorPage('Not Found', 'The requested structure is not available');
} else {
   $data = mysql_fetch_array($rs);
   print headerDBW($_REQUEST['idCode']);
   ?>
   <table border="0" cellspacing="2" cellpadding="4">
      <tbody>
         <tr>
            <td>PDB reference</td>
            <td><?php print $data['idCode'] ?></td>
            <td rowspan="5">
               <a href="http://www.pdb.org/pdb/explore.do?structureId=<?php print $data['idCode'] ?>">
                  <img src="http://www.pdb.org/pdb/images/<?php print strtolower($data['idCode']) ?>_bio_r_250.jpg" border="0"
width="250" height="250"><br>
                  Link to Protein Data Bank</a>
            </td>
         </tr>
         <tr>
            <td>Header</td>
            <td><?php print $data['header'] ?></td>
         </tr>
         <tr>
            <td>Title</td>
            <td><?php print $data['compound'] ?></td>
         </tr>
         <tr>
            <td>Resolution</td>
            <td>
               <?php
```

```
          if ($data['resolution'])
            print $data['resolution'];
          else
            print "N.D.";
          ?>
        </td>
      </tr>
      <tr>
        <td>Ascession Date</td>
        <td><?php print $data['ascessionDate'] ?></td>
      </tr>
      <tr>

        <?php // $expTypeArray is generated in globals.inc.php?>
        <td>Experiment type</td>
        <td colspan="2"><?php print $expTypeArray[$data['idExpType']]['ExpType'] ?></td>
      </tr>
      <tr>
        <td>Authors</td>
        <td colspan="2">
          <?php

          // new DB query to get authors
          $rsA = mysql_query("SELECT * from author a, author_has_entry ae where ae.idCode='" . $data['idCode'] . "' and
a.idAuthor = ae.idAuthor order by a.author") or print mysql_error();
          if (mysql_num_rows($rsA)) {
            $auts = array();
            while ($rsAF = mysql_fetch_array($rsA))
              $auts[] = $rsAF['author'];
            print join(", ", $auts);
          }
          ?>
        </td>
      </tr>
      <tr>
        <td>Source</td>
        <td colspan="2">
          <?php

          // new DB query to get sources
          $rsA = mysql_query("SELECT * from source s, entry_has_source es where es.idCode='" . $data['idCode'] . "' and
s.idSource = es.idSource order by s.source") or print mysql_error();
          if (mysql_num_rows($rsA)) {
            $sources = array();
            while ($rsAF = mysql_fetch_array($rsA))
              $sources[] = $rsAF['source'];
            print join(", ", $sources);
          }
          ?>
        </td>
      </tr>
      <tr>
        <td>Sequence(s)</td>
        <td colspan="2">
          <?php

          // new DB query to get sequences, output in FASTA format
          $rsA = mysql_query("SELECT * from sequence s where s.idCode='" . $data['idCode'] . "' order by s.chain") or print
mysql_error();
          if (mysql_num_rows($rsA)) {
            while ($sq = mysql_fetch_array($rsA)) {
              print "<pre>" . $sq['header'] . "\n" . preg_replace("/(.{60})/", "$1\n", $sq['sequence']) . "</pre>";
            }
```

```
                }
                ?>
            </td>
        </tr>
    </tbody>
</table>
<?php
print footerDBW();
}
```



DBW - Search results

Num Hits: 5031

Show 10 entries

Search:

idCode	Header	Compound	Resolution	Exp. Type	Source
13PK	Kinase	Ternary Complex Of Phosphoglycerate Kinase From Trypanosoma Brucei	2.5	X-RAY DIFFRACTION	Trypanosoma Brucei
16PK	Kinase	Phosphoglycerate Kinase From Trypanosoma Brucei Bisubstrate Analog	1.6	X-RAY DIFFRACTION	Trypanosoma Brucei
1A06	Kinase	Calmodulin-dependent Protein Kinase From Rat	2.5	X-RAY DIFFRACTION	Rattus Norvegicus
1A07	Complex (transferase/peptide)	C-src (sh2 Domain) Complexed With Ace-malonyl Tyr-glu-(n,n-dipentyl Amine)	2.2	X-RAY DIFFRACTION	Homo Sapiens
1A08	Complex (transferase/peptide)	C-src (sh2 Domain) Complexed With Ace-difluoro Phosphotyr-glu-(n,n-dipentyl Amine)	2.2	X-RAY DIFFRACTION	Homo Sapiens
1A09	Complex (transferase/peptide)	C-src (sh2 Domain) Complexed With Ace-formyl Phosphotyr-glu-(n,n-dipentyl Amine)	2	X-RAY DIFFRACTION	Homo Sapiens
1A0B	Histidine Kinase	Histidine-containing Phosphotransfer Domain Of Arcb From Escherichia Coli	2.06	X-RAY DIFFRACTION	Escherichia Coli
1A0N	Complex (phosphotransferase/peptide)	Nmr Study Of The Sh3 Domain From Fyn Proto-oncogene Tyrosine Kinase Complexed With The Synthetic Peptide P2l Corresponding To Residues 91-104 Of The P85 Subunit Of Pi3-kinase, Family Of 25 Structures	0	SOLUTION NMR	Homo Sapiens
1A1A	Complex (transferase/peptide)	C-src (sh2 Domain With C188a Mutation) Complexed With Ace-formyl Phosphotyr-glu-(n,n-dipentyl Amine)	2	X-RAY DIFFRACTION	Homo Sapiens
1A1B	Complex (transferase/peptide)	C-src (sh2 Domain) Complexed With Ace-phosphotyr-glu-(n,n-dipentyl Amine)	2.2	X-RAY DIFFRACTION	Homo Sapiens

Showing 1 to 10 of 5,031 entries

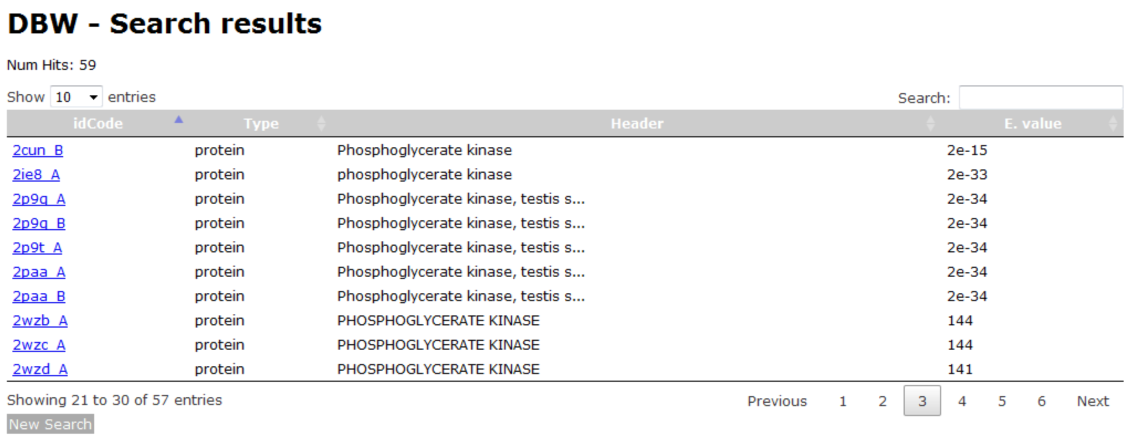
search.php

Search script, includes initial selection of operations

```
<?php

// load global vars and includes
include "globals.inc.php";

// Store input data in $_SESSION to reload initial form if necessary
$_SESSION['queryData'] = $_REQUEST;

// Selection of action to do
// 1. IdCode -> Results page
// 2. Sequence input -> runBlast
// 3. Other -> search on DB

// 1. Redirection to the requested entry if code selected
if ($_REQUEST['idCode']) {
   header('Location: getStruc.php?idCode=' . $_REQUEST['idCode']);

   // 2. Sequence input. If uploaded file, this takes preference
} elseif ($_FILES['seqFile']['name'] or $_REQUEST['seqQuery']) {
   if (($_FILES['seqFile']['tmp_name'])) {
      $_SESSION['queryData']['seqQuery'] = file_get_contents($_FILES['seqFile']['tmp_name']);
   }

   // Redirect to Blast if sequence, data is stored in $_SESSION
   header('Location: runBlast.php');
} else {

   //  3. normal search, Bluiding SQL SELECT from the input form
   //     $ANDConds will contain all sql conditions found in the form
   $ANDconds = Array("True"); // required to fulfill sql syntax if form is empty

   //  Resolution, we consider only cases where user has input something
   if (($_REQUEST['minRes'] != '0.0') or ( $_REQUEST['maxRes'] != 'Inf')) {
      if ($_REQUEST['minRes'] != '0.0') {
         $ANDconds[] = "e.resolution >= " . $_REQUEST['minRes'];
      }
```

```
        if ($_REQUEST['maxRes'] != 'Inf') {
            $ANDconds[] = "e.resolution <= " . $_REQUEST['maxRes'];
        }
    }

    //     Compound type $ORconds holds options selected
    if (isset($_REQUEST['idCompType'])) { //should be isset as idCompType come from checkboxes
        $ORconds = Array();
        foreach (array_keys($_REQUEST['idCompType']) as $k) {
            $ORconds[] = " e.idCompType = " . $k;
        }
        $ANDconds[] = "(" . join(" OR ", $ORconds) . ")";
    }

    //     Classe of experiment
    if (isset($_REQUEST['idExpClasse'])) {//should be isset as idExpClasse come from checkboxes
        $ORconds = Array();
        foreach (array_keys($_REQUEST['idExpClasse']) as $k) {
            $ORconds[] = " et.idExpClasse = " . $k;
        }
        $ANDconds[] = "(" . join(" OR ", $ORconds) . ")";
    }

    //    text query, adapted to use fulltext indexes, $textFields is defined in globals.inc.php and
    // lists all text fields to be searched in.
    if ($_REQUEST['query1']) {
        $ORconds = array();
        foreach (array_values($textFields) as $field) {
            $ORconds[] = "MATCH (" . $field . ") AGAINST ('" . $_REQUEST['query1'] . "' "
                    . "IN BOOLEAN MODE)";
        }
        $ANDconds[] = "(" . join(" OR ", $ORconds) . ")";
    }

    //    text query without fulltext indexes
    //    if ($_REQUEST['query']){
    //        foreach (split (' ',$_REQUEST['query']) as $wd) {
    //            $ANDconds=array();
    //            foreach (array_values($textFields) as $field) {
    //                $ORconds[] = $field." like '%".$wd."%'";
    //            }
    //            $ANDconds[] = "(".join (" OR ", $ORconds).")";
    //        }
    //    }
    //    main SQL string, make sure that all tables are joined, and relationships included
    // SELECT columns FROM tables WHERE Conditions_from_relationships AND Conditions_from_query_Form
    $sql = "SELECT distinct e.idCode,e.header,e.compound,e.resolution,s.source,et.expType FROM
        expType et, author_has_entry ae, author a, source s, entry_has_source es, sequence sq,entry e WHERE
        e.idExpType=et.idExpType AND
        ae.idCode=e.idCode and ae.idAuthor=a.idAuthor AND
        es.idCode=e.idCode and es.idsource=s.idSource AND
        e.idCode = sq.idCode AND " . join(" AND ", $ANDconds);

//    Ordering will be done by the DataTable element using JQuery, if not available can also be done from the SQL

//    switch ($order) {
//        case 'idCode':
//        case 'header':
//        case 'compound':
//        case 'resolution':
//            $sql .= " ORDER BY e." . $order;
//            break;
//        case 'source':
```

```
//             $sql .= " ORDER BY s.source";
//             break;
//         case 'expType':
//             $sql .= " ORDER BY et.expType";
//             break;
//     }
//       $sql .= " LIMIT 50"; // Just to avoid long listings when testing
//     print "<p>$sql</p>";

//      DB query
    $rs = mysql_query($sql) or print mysql_error();
//      We check whether there are results to show
    if (!mysql_num_rows($rs)) {
        print errorPage("Not Found", "No results found.");
    } else {
//         Results table formated with DataTable (jQuery)
        print headerDBW("Search results");
        print "Num Hits: " . mysql_num_rows($rs);
        ?>
        <table border="0" cellspacing="2" cellpadding="4" id="dataTable">
            <thead>
                <tr>
                    <th>idCode</th>
                    <th>Header</th>
                    <th>Compound</th>
                    <th>Resolution</th>
                    <th>Exp. Type</th>
                    <th>Source</th>
                </tr>
            </thead>
            <tbody>
                <?php while ($rsF = mysql_fetch_array($rs)) { ?>
                    <tr>
                        <td><a href="getStruc.php?idCode=<?php print $rsF['idCode'] ?>">
                                <?php print $rsF['idCode'] ?></a></td>
                        <td><?php print ucwords(strtolower($rsF['header'])) ?></td>
                        <td><?php print ucwords(strtolower($rsF['compound'])) ?></td>
                        <td><?php print $rsF['resolution'] ?></td>
                        <td><?php print $rsF['expType'] ?></td>
                        <td><?php print ucwords(strtolower($rsF['source'])) ?></td>
                    </tr>
                <?php } ?>
            </tbody>
        </table>
        <p class="button"><a href="index.php?new=1">New Search</a></p>
        <script type="text/javascript">
        <!-- this activates the DataTable element when page is loaded-->
            $(document).ready(function () {
                $('#dataTable').DataTable();
            });
        </script>
        <?php
        print footerDBW();
    }
}
```



DBW - Search results

Num Hits: 59

Show 10 entries

Search:

idCode	Type	Header	E. value
2cun_B	protein	Phosphoglycerate kinase	2e-15
2ie8_A	protein	phosphoglycerate kinase	2e-33
2p9q_A	protein	Phosphoglycerate kinase, testis s...	2e-34
2p9q_B	protein	Phosphoglycerate kinase, testis s...	2e-34
2p9t_A	protein	Phosphoglycerate kinase, testis s...	2e-34
2paa_A	protein	Phosphoglycerate kinase, testis s...	2e-34
2paa_B	protein	Phosphoglycerate kinase, testis s...	2e-34
2wzb_A	protein	PHOSPHOGLYCERATE KINASE	144
2wzc_A	protein	PHOSPHOGLYCERATE KINASE	144
2wzd_A	protein	PHOSPHOGLYCERATE KINASE	141

Showing 21 to 30 of 57 entries

runBlast.php

Blast search

```
<?php
require "globals.inc.php";

// Take data from $_SESSION, loaded in search.php, if empty back to front page
if (!isset($_SESSION['queryData']) or ! $_SESSION['queryData']['seqQuery'])
   header('Location: index.php');
// prepare FASTA file
// Identify file format, ">" as first char indicates FASTA
$p = strpos($_SESSION['queryData']['seqQuery'], '>');
if (!$p and ( $p !== 0)) { // strpos returns False if not found and "0" if first character in the string
   // When is not already FASTA, add header + new line
   $_SESSION['queryData']['seqQuery'] = ">User provided sequence\n" . $_SESSION['queryData']['seqQuery'];
}

// Set temporary file name to a unique value to protect from concurrent runs
$tempFile = $tmpDir . "/" . uniqId('pdb');

// Open temporary file and store query FASTA
$ff = fopen($tempFile . ".query.fasta", 'wt');
fwrite($ff, $_SESSION['queryData']['seqQuery']);
fclose($ff);

// execute Blast, Command line set in globals.inc.php
exec($blastCmdLine . " -i " . $tempFile . ".query.fasta -o " . $tempFile . ".blast.out");

// Read results file and parse hits onto $result[]
$blast = file($tempFile . ".blast.out");
$i = 0;
while (!preg_match('/Sequences producing/', $blast[$i]) and ( $i < count($blast)))
   $i++;
$i++;
while (!preg_match('/Database:/', $blast[$i]) and ( $i < count($blast))) {
   if ($blast[$i])
      $result[] = $blast[$i];
   $i++;
}
if (!count($result)) {
   print errorPage("Not Found", 'No results found. <p class="button" ><a href="index.php?new=1">New Search</a></p>');
} else {

//       Results table
   print headerDBW("Search results");
   ?>
<p>Num Hits: <?php print count($result) ?> </p>
```

```
    <table border="0" cellspacing="2" cellpadding="4" id="blastTable">
        <thead
            <tr>
                <th>idCode</th>
                <th>Type</th>
                <th>Header</th>
                <th>E. value</th>
            </tr>
        </thead>
        <tbody>
            <?php
            // parsing hit following specific format, note that this format is not standard. It comes from the
            // headers used to generate BLAST databases, this is from PDB
            foreach (array_values($result) as $rr) {
                if (strlen($rr) > 1) {
                    preg_match('/(....)_(.) mol:([^ ]*) length:([0-9]*) ([^0-9]*) *([0-9]*) *([0-9e\-\.]*)/', $rr, $hits);
                    list ($r, $idCode, $sub, $tip, $l, $desc, $sco, $ev) = $hits;
                    ?>
                    <tr>
                        <td>
                            <a href="getStruc.php?idCode=<?php print $idCode ?>"><?php print $idCode . "_$sub" ?></a>
                        </td>
                        <td><?php print $tip ?></td>
                        <td><?php print $desc ?></td>
                        <td><?php print $ev ?></td>
                    </tr>
                    <?php
                }
            }
            ?>
        </tbody>
    </table>
<p class="button"><a href="index.php?new=1">New Search</a></p>
    <?php
    // Cleaning temporary files
    if (file_exists($tempFile . ".query.fasta"))
        unlink($tempFile . ".query.fasta");
    if (file_exists($tempFile . ".blast.out"))
        unlink($tempFile . ".blast.out");
    print footerDBW();
}
?>
<script type="text/javascript">
    $(document).ready(function () {
        $('#blastTable').DataTable();
    });
</script>
```

estil.css

```
body {font-family: Verdana, Arial, sans-serif; font-size: 12px}
th {background-color: #cccccc; color:#ffffff}
.button {padding:2px;display: inline; color:#ffffff; background-color: #aaaaaa}
.button a {color:#ffffff; text-decoration:none}
.button a:hover {font-weight:bold}
```

Include/bdconn.inc.php

```
<?php
/*
 * bdconn.inc.php
 * DB Connection
 */
$host = "localhost";
$dbname = "pdb";
$user = "dbw00";
$password = "master00";
($conn = mysql_connect($host, $user, $password)) or die(mysql_error());
($id = mysql_select_db($dbname)) or die(mysql_error());
```

Include/libDBW.inc.php

```
<?php
function headerDBW($title) {
   return "<html>
<head>
<title>$title</title>
<link rel=\"stylesheet\" type=\"text/css\" href=\"estil.css\">
      <link rel=\"stylesheet\" href=\"DataTable/jquery.dataTables.min.css\"/>
      <script type=\"text/javascript\" src=\"DataTable/jquery-2.2.0.min.js\"></script>
      <script type=\"text/javascript\" src=\"DataTable/jquery.dataTables.min.js\"></script>

</head>
<body bgcolor=\"#ffffff\">
<h1>DBW - $title</h1>
";
}

function footerDBW() {
   return '
</body>
</html>';
}

function errorPage($title, $text) {
   return headerDBW($title) . $text . footerDBW();
}
```

loadPDB.pl

ETL to load database data from PDB text files

```
#!/usr/bin/perl
use DBI;
use strict;
#
require "bdconn.pl";
#
my $dbh=connectDB();
# Clean Tables !!
foreach my $tab ('entry', 'source', 'sequence', 'author', 'author_has_entry', 'expType', 'comptype', 'entry_has_source',
'expClasse') {
  print "Cleaning $tab\n";
  $dbh->do ("DELETE FROM $tab");
}
foreach my $tab ('source','author','expType','comptype','expClasse') {
  $dbh->do ("ALTER TABLE $tab AUTO_INCREMENT=1");
}
#
$dbh->do("SET FOREIGN_KEY_CHECKS=0");
#
print "Authors...";
my %AUTHORS;
my %author_has_entry;
my $sthAuthor=$dbh->prepare ("INSERT INTO author (author) VALUES (?)");
my $sthEntryAuthor=$dbh->prepare("INSERT INTO author_has_entry VALUES (?,?)");
open AUTS, "author.idx";

#author.idx
#IDCODE; AUTHOR
#2NPB ; AACHMANN, F.L.
#2KV1 ; AACHMANN, F.L.

while (<AUTS>) {
  next if !/;/;
  chomp;
  my ($idCode, $author) = split / *; */;
  next if (!$author);
  if ($author && !$AUTHORS{$author}) {
          $sthAuthor->execute ($author);
          $AUTHORS{$author}=$dbh->last_insert_id('','','Author','idAuthor');
  }
  if (!$author_has_entry{"$AUTHORS{$author}-$idCode"}) {
    $sthEntryAuthor->execute ($AUTHORS{$author},$idCode);
    $author_has_entry{"$AUTHORS{$author}-$idCode"}=1;
  }
  print ".";
}
close AUTS;
print "ok\n";
#
#
print "Sources...";
my %SOURCES;
my %Entry_has_source;
my $sthSource =$dbh->prepare("INSERT INTO source (source) VALUES (?)");
my $sthEntrySource = $dbh->prepare("INSERT INTO entry_has_source (idCode,idSource) VALUES (?,?)");
open SOUR, "source.idx";

#source.idx
#IDCODE  SOURCE
#102L      ENTEROBACTERIA PHAGE T4
#102M      PHYSETER CATODON
```

```
while (<SOUR>) {
  chomp;
  my ($idCode,$source) = split ' ', $_, 2;
  next if (!$source) || (length($idCode) != 4);
  foreach my $s (split /; */, $source) {
    if (!$SOURCES{$s}) {
      $sthSource->execute ($s);
             $SOURCES{$s}=$dbh->last_insert_id('','','source','idSource');
    }
    $sthEntrySource->execute($idCode, $SOURCES{$s});
  }
  print ".";
}
close SOUR;
print "ok\n";
#
#
print "Entries...";
open ENTR, "entries.idx";

#entries.idx
# IDCODE, HEADER, ACCESSION DATE, COMPOUND, SOURCE, AUTHOR LIST, RESOLUTION, EXPERIMENT TYPE (IF NOT X-RAY)
#100D	DNA/RNA  12/05/94   CRYSTAL STRUCTURE OF THE HIGHLY DISTORTED CHIMERIC DECAMER R(C)D(CGGCGCCG)R(G)-SPERMINE COMPLEX-SPERMINE
BINDING TO PHOSPHATE ONLY AND MINOR GROOVE TERTIARY BASE-PAIRING			Ban, C., Ramakrishnan, B., Sundaralingam, M.		1.9
	X-RAY DIFFRACTION
#101D	DNA	12/14/94   REFINEMENT OF NETROPSIN BOUND TO DNA: BIAS AND FEEDBACK IN ELECTRON DENSITY MAP INTERPRETATION
	Goodsell, D.S., Kopka, M.L., Dickerson, R.E.  2.25	X-RAY DIFFRACTION

my $sthEntry = $dbh->prepare ("INSERT INTO entry (idCode, header, ascessionDate, compound, resolution) VALUES (?,?,?,?,?)");
my %ExpTypes;
my $sthExpType = $dbh->prepare ("INSERT INTO expType (ExpType) VALUES (?)");
my $sthEntryExpType = $dbh->prepare ("UPDATE entry SET idExpType=? WHERE idCode=?");
my %expTypesbyCode;
while (<ENTR>) {
  chomp;
  my ($idCode, $header, $ascDate, $compound, $source, $authorList, $resol, $expType) = split /\t/;
  next if (length($idCode) != 4);
  $sthEntry-> execute ($idCode,$header, $ascDate, $compound, $resol);
		if (!$ExpTypes{$expType }) {
			$sthExpType->execute($expType);
			$ExpTypes{$expType}=$dbh->last_insert_id('','','ExpType','idExpType');
		}
		$sthEntryExpType->execute($ExpTypes{$expType},$idCode);
		$expTypesbyCode{$idCode}=$expType;
  print ".";
}
close ENTR;
print "ok\n";
#
#
open EXPCL , 'pdb_entry_type.txt';
#pdb_entry_type.txt
#100d	nuc	diffraction
#101d	nuc	diffraction

my %expClasses;
my %compTypes;
my $sthExpClasse=$dbh->prepare('INSERT INTO expClasse (expClasse) VALUES (?)');
my $sthcompType=$dbh->prepare('INSERT INTO comptype (type) VALUES (?)');
my $entryUpdate= $dbh->prepare('UPDATE entry SET idCompType=? WHERE idCode=?');
my $expTypeUpdate=$dbh->prepare('UPDATE expType SET idExpClasse=? where ExpType=?');

while (<EXPCL>) {
  chomp;
```

```
        my ($idCode, $compType, $expClass) = split ' ';
        $idCode =~ tr/a-z/A-Z/;
        if (!$expClasses{$expClass}) {
                $sthExpClasse->execute($expClass);
                $expClasses{$expClass}=$dbh->last_insert_id('','','expClasses','idExpClass');
        }
        if (!$compTypes{$compType}) {
                $sthcompType->execute($compType);
                $compTypes{$compType}=$dbh->last_insert_id('','','compType','idCompType');
        }
        $expTypeUpdate->execute($expClasses{$expClass}, $expTypesbyCode{$idCode});
        $entryUpdate->execute($compTypes{$compType},$idCode);
}
#Sequence
print "Sequences...";
my $codes=[];
my %CODES;
my $sthInsert= $dbh->prepare ("INSERT INTO sequence (idCode,chain,sequence,header) VALUES (?,?,?,?)");
open "SEQS", "pdb_seqres.txt";

#pdb_seqres.txt (FASTA)
#>101m_A mol:protein length:154  MYOGLOBIN
#MVLSEGEWQLVLHVWAKVEADVAGHGQDILIRLFKSHP...
#>...

my $seq;
my $idPdb;
my $chain;
my $header;
while (<SEQS>) {
  chomp;
  if (/^>/) {
        if ($seq) {
                $seq =~ s/\n//g;
                $idPdb =~ tr/a-z/A-Z/;
                $chain =~ s/ //;
                $sthInsert->execute ($idPdb,$chain,$seq, $header) || die $DBI::errstr;
            $seq="";
        }
        /^>([^_]*)_(.*)mol:(\S*) length:(\S*) (.*)/;
        ($idPdb,$chain,$header)=($1,$2,"$1 $2 $3 $4 $5");
        print "$header\n";
  }
  else {$seq .= $_};
};
print "ok\n";
disconnectDB($dbh);
```