My Structures/CSD Editor User Guide

My Structures/CSD-Editor User Guide

2021.2 CSD Release

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Introduction

CSD Editor enables users to manually modify entries from their own deposited structures on My Structures to maintain consistent and up-to-date information.

Installation notes

Currently, CSD Editor is available for:

- Windows - Intel compatible, 64-bit:
- Windows 10
- Linux - Intel compatible, 64-bit:
- RedHat Enterprise 7.6 or higher, and 8
- CentOS 7.6 or higher, and 8

The use of ChemDraw integration within CSD Editor requires a ChemDraw installation – this has been tested using ChemDraw Professional 17.0. ChemDraw is a product of PerkinElmer Informatics, Inc. Copyright 1998-2018 All Rights Reserved, http://www.cambridgesoft.com

We recommend that you do not install directly on top of a previous installation of CSD Editor.

We recommend that you install the latest version of the CSD database files including all CSD update files.

Installation procedure

To install CSD Editor on Windows:

1. Download the `csd-editor-mystructures-windows-installer.exe` Windows installer.
2. Run the `csd-editor-mystructures-windows-installer.exe` file and follow the on-screen instructions to install it.

To install CSD Editor on Linux:

1. Download `csd-editor-mystructures-windows-installer.run` and change directory to the location of the download on your system.
2. Ensure the downloaded file is executable via the command

```
chmod a+x csd-editor-industrial-mystructures-installer.run
```

1. Run the installer with the command

```
./csd-editor-mystructures-windows-installer.run
```

and follow the on-screen instructions to complete the installation.

Managing structures on My Structures

My Structures can be used to manage your CIF files and other supplementary files and to create a database to search in CSDS software.

Adding structures to your My Structures table

Adding new structures

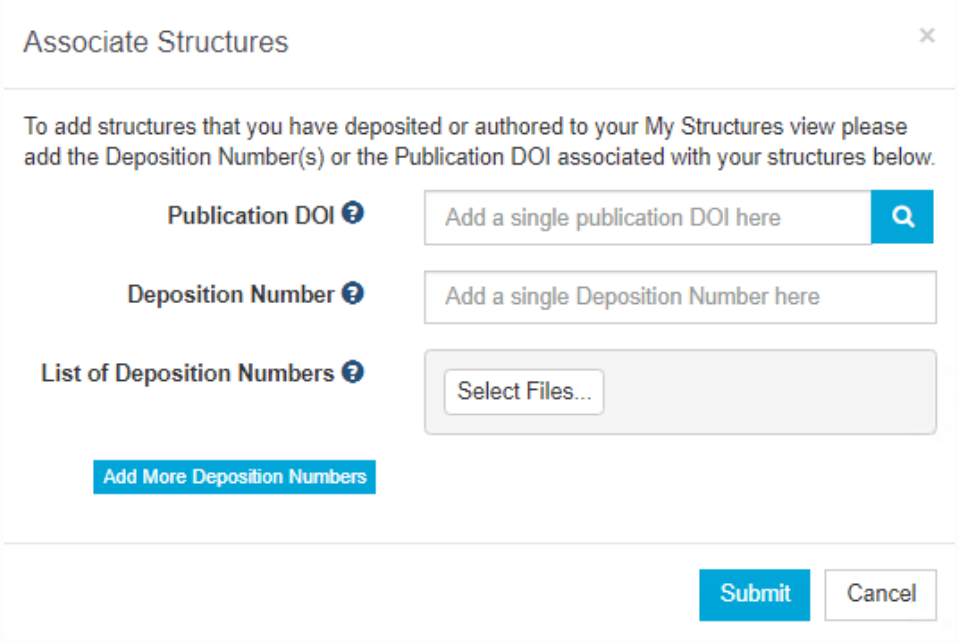
Structures can be added by signing in and depositing them through the deposition service - https://www.ccdc.cam.ac.uk/deposit/upload.

A workshop tutorial giving instructions on all the steps of the process is available on the CCDC website: https://www.ccdc.cam.ac.uk/Community/educationalresources/workshop-materials/csd-community-workshops/CSDC-Deposition.pdf.

Claiming structures already in the system

Existing structures in the system that you have authored or deposited can be added to your My Structures view if you know the Deposition Numbers for the structures or the DOI for the publication that the structures are published in. To do this:

1. Sign in and go to My Structures.
2. Click the **Associate More Structures** button and a **Associate Structures** dialogue will appear.



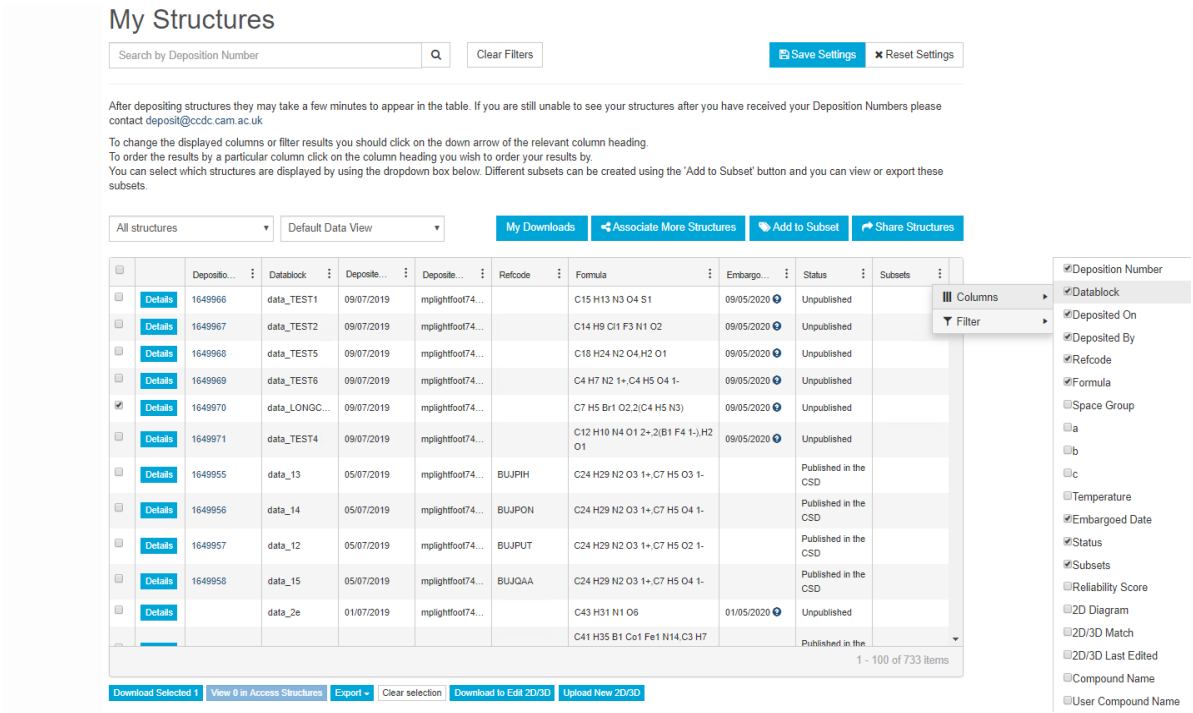
3. Add the Publication DOI for the structures that you would like to add or a list of Deposition Numbers and click **Submit**. You can also add a list of Deposition Numbers from a text file.

This system allows you to see data you have deposited or authored or that have been shared with you by a depositor or author. Ownership of the data will be checked before the structures are added. If the data does not get associated with you after two days, then please contact the original depositor to request that they update the publication details or share the structure with you.

Viewing details about your structures in the My Structures table

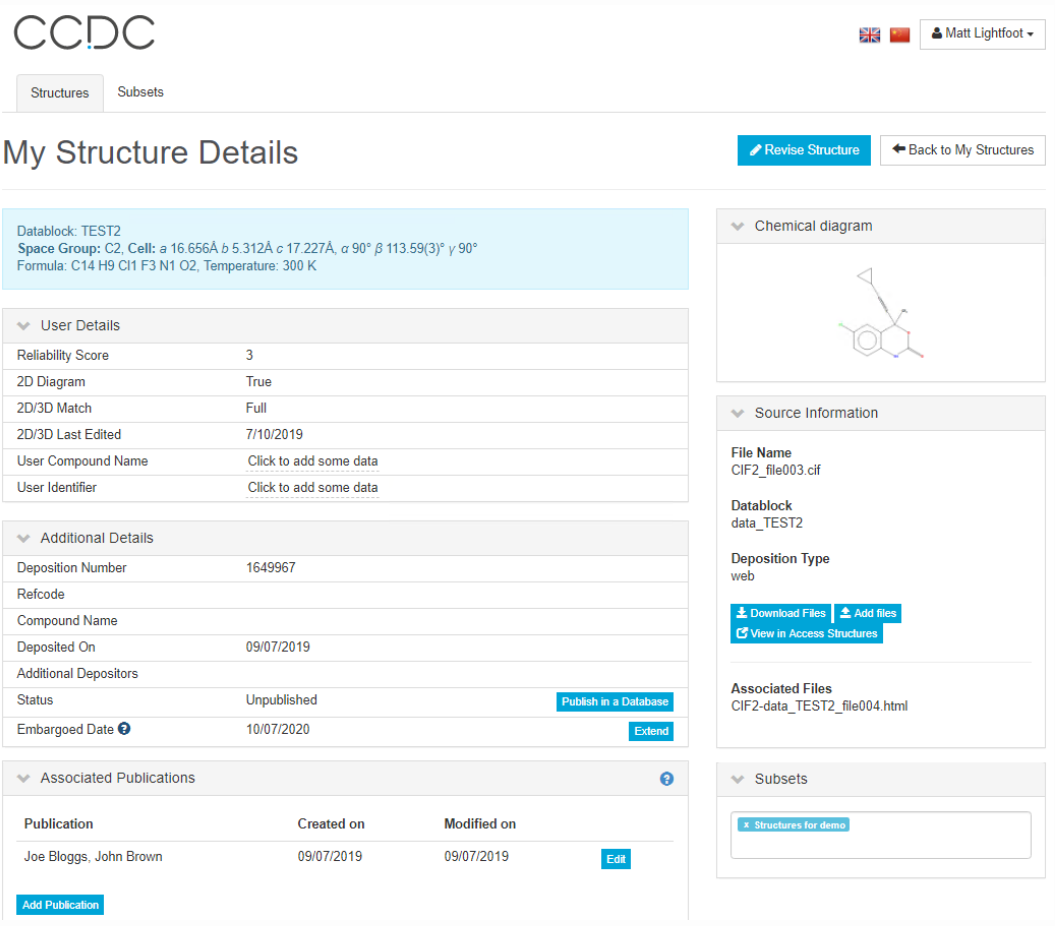
Changing the columns in the table

1. Click the **Three dots** next to one of the column headings
2. Hover over the arrow next to the **Columns** option and the list of possible columns are displayed.
3. Tick the columns that you would like to view



Viewing more details about a structure

Click the **Details** button to display more details about an individual structure.



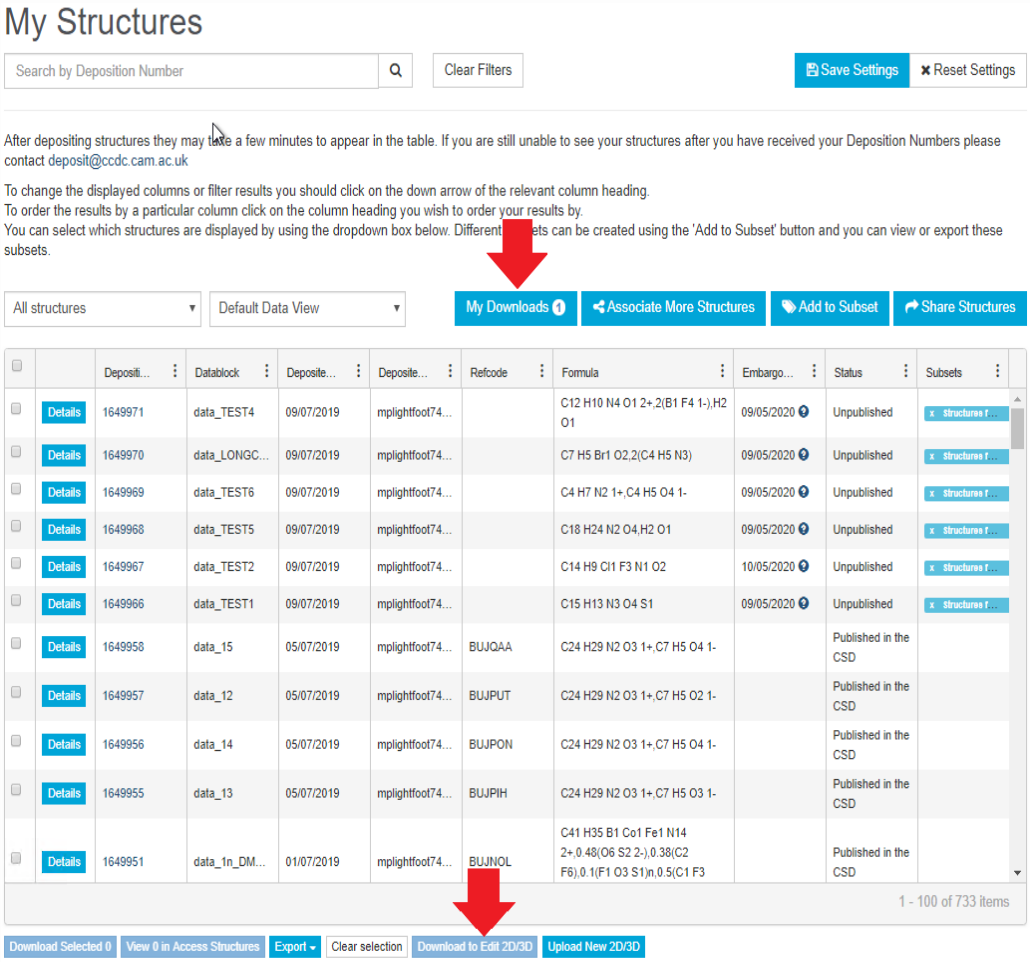
Editing structures in your My Structures table

Editing 2D/3D

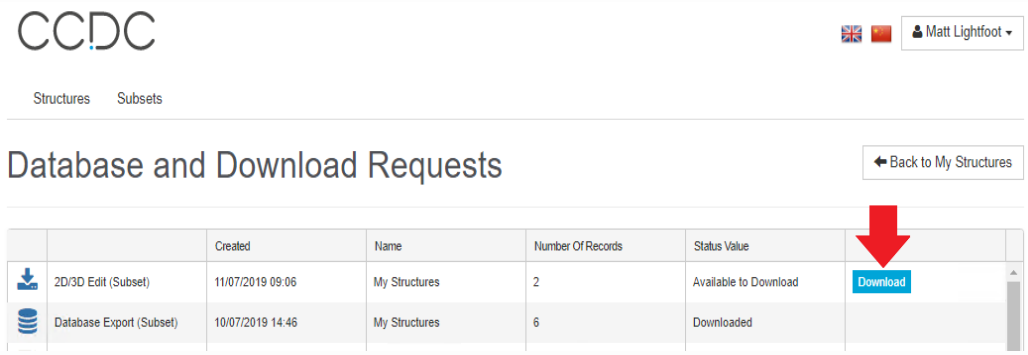
2D/3D editing of structures is done using the CSD Editor desktop program. This will need to be installed on your computer before you start.

1. Select the entries that you want to edit in the **My Structures** table, click the **Download to Edit 2D/3D** button and then click **OK** on the dialogue that appears.

2. Click the **My Downloads** button



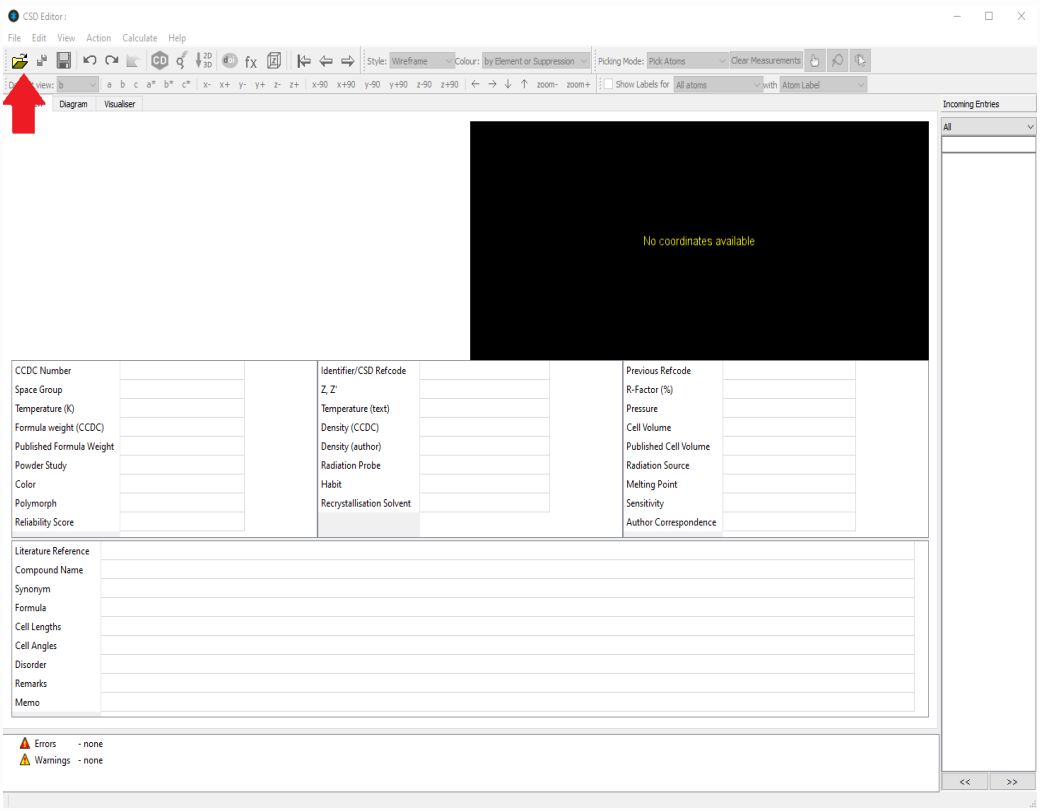
3. This will open a **Database and Download Requests** window and the file with the structures that require editing should be at the top of the table. You should refresh the page until the status for the request goes to **Available to Download** and the **Download** button appears.



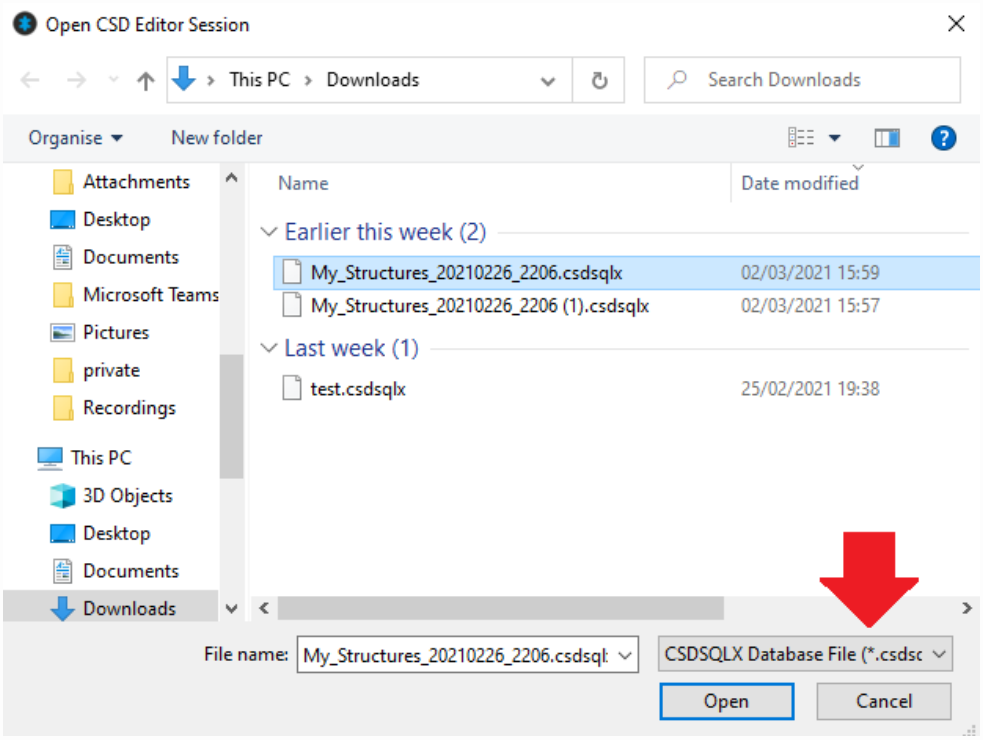
4. Click the **Download** button and save the file on your computer.

5. Open the CSD Editor (`C:\Program Files\CCDC\CSD-Editor-MyStructures\csd_editor.exe`)

6. Click the **Open a new or existing session** button in the CSD Editor

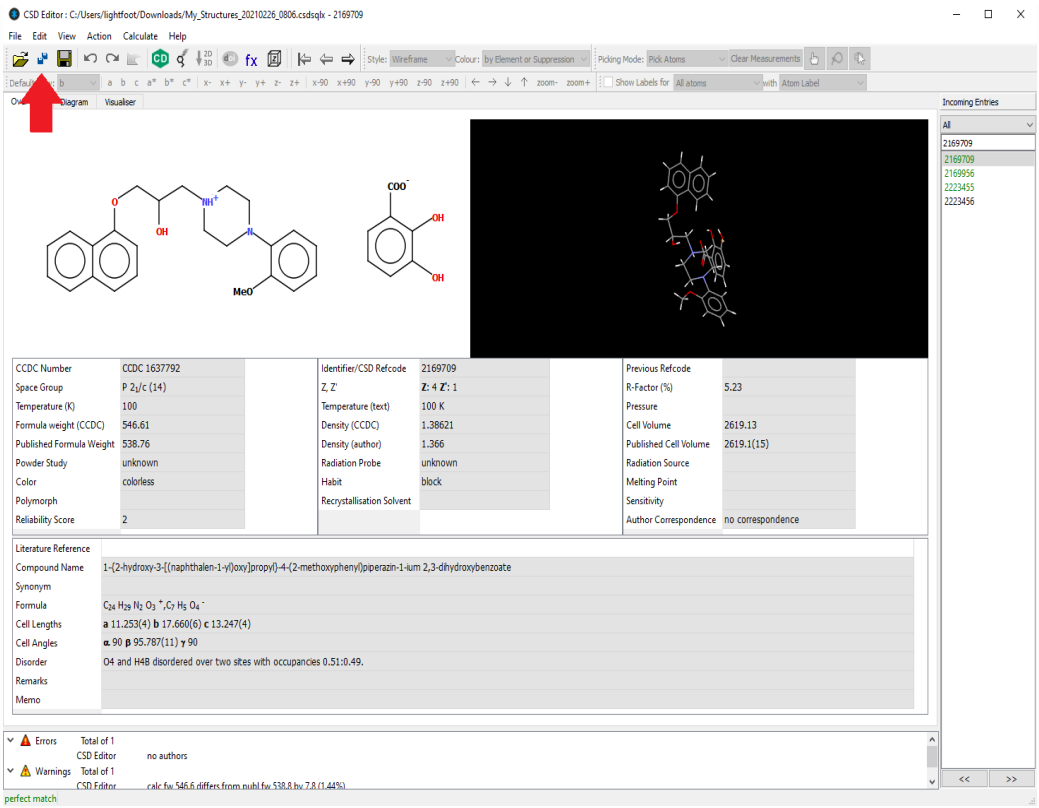


7. A **Open CSD Editor Session** dialogue will open. Check that the CSDSQLX Database File option is selected and then locate the file that you saved in step 4 and click **Open**.

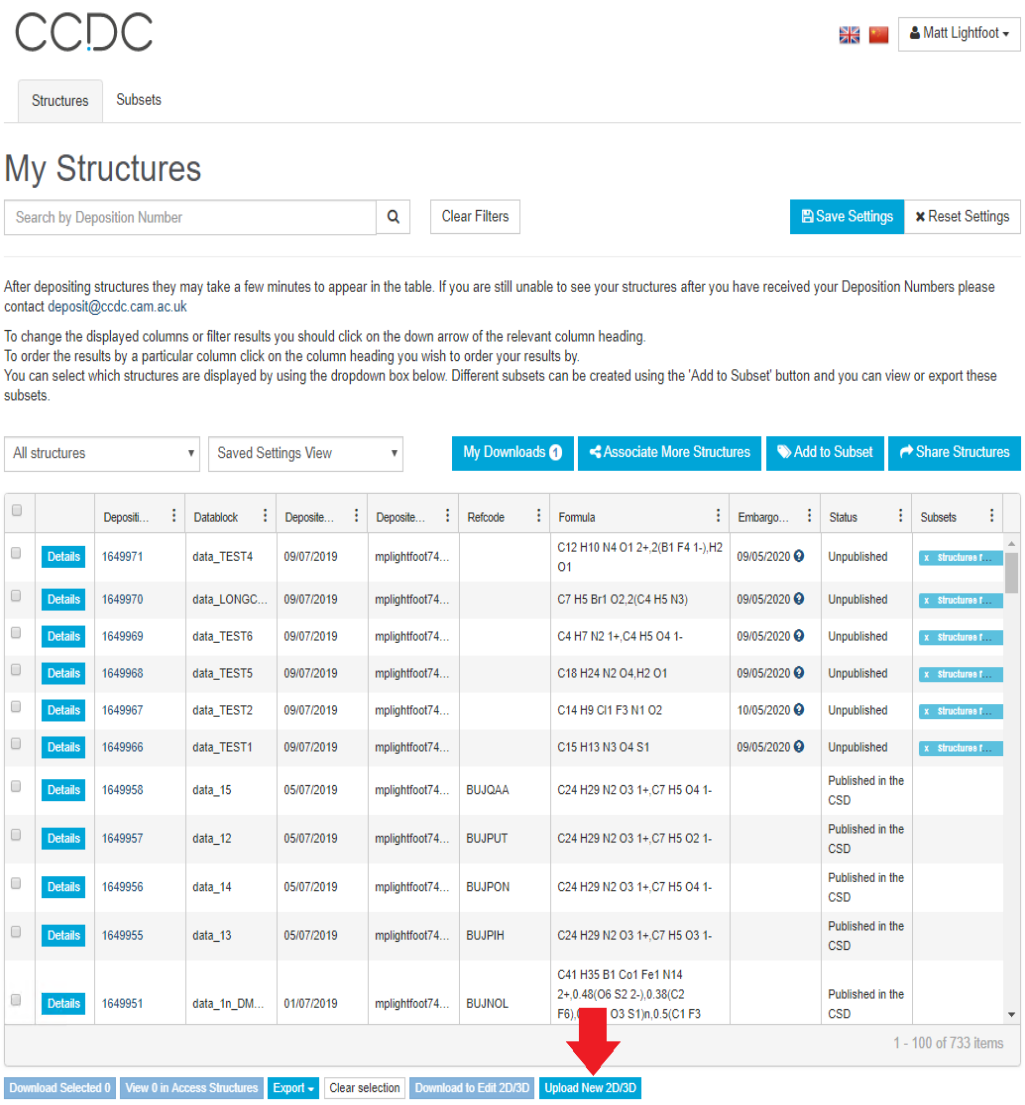


8. The structures will open in the CSD Editor and can be edited. See the 2D/3D Editing in the CSD Editor section for details of how to edit the 2D and 3D in theCSD Editor.

9. Once all the structures have been edited you should save the edits to the database. This can be done by clicking the **Save all structures in session to source database** button. A dialogue will be displayed while the entries are saved and then click **Ok**.

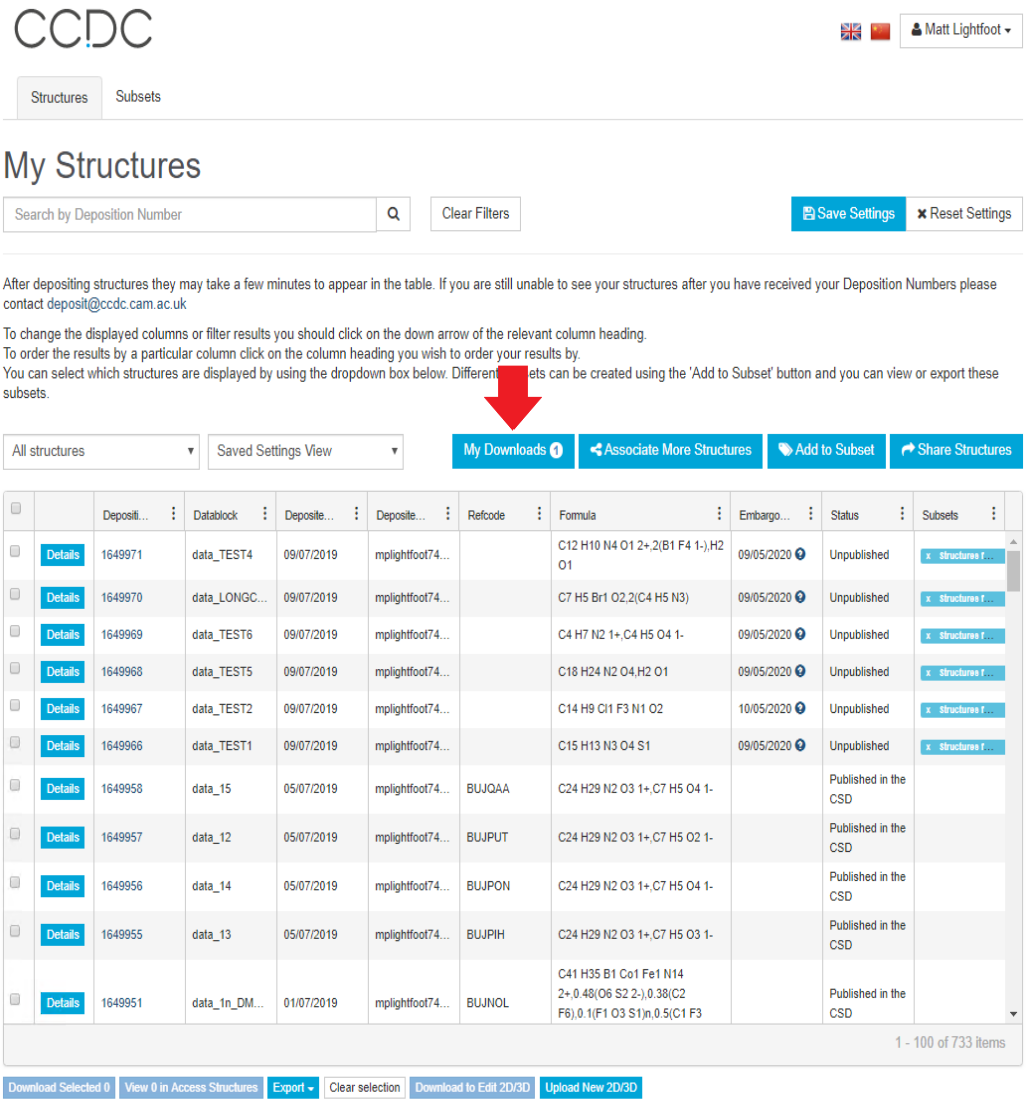


10. The entries will be saved into the same database that you opened in step 7. The next stage is to go back to the **My Structures** view and click the **Upload New 2D/3D** button.

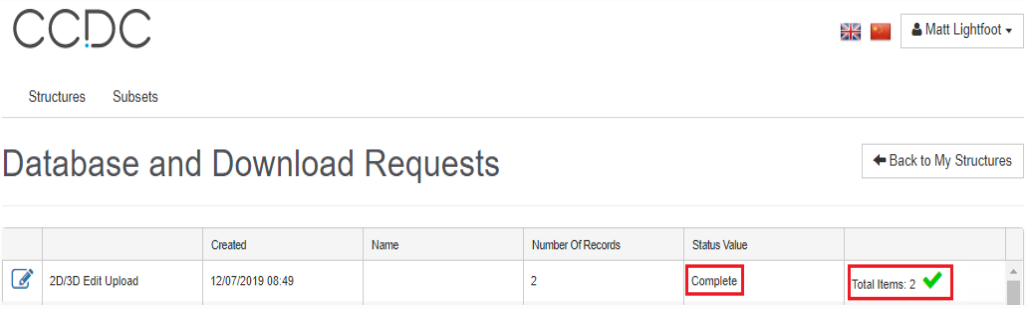


11. A **Upload New 2D/3D** dialogue will appear. Click **Select Files**, locate the same file that you opened in step 7, click **Open** and then click **Confirm**.

12. The files will then be saved into the system. This can take a few minutes and progress can be monitored by clicking the **My Downloads** button.

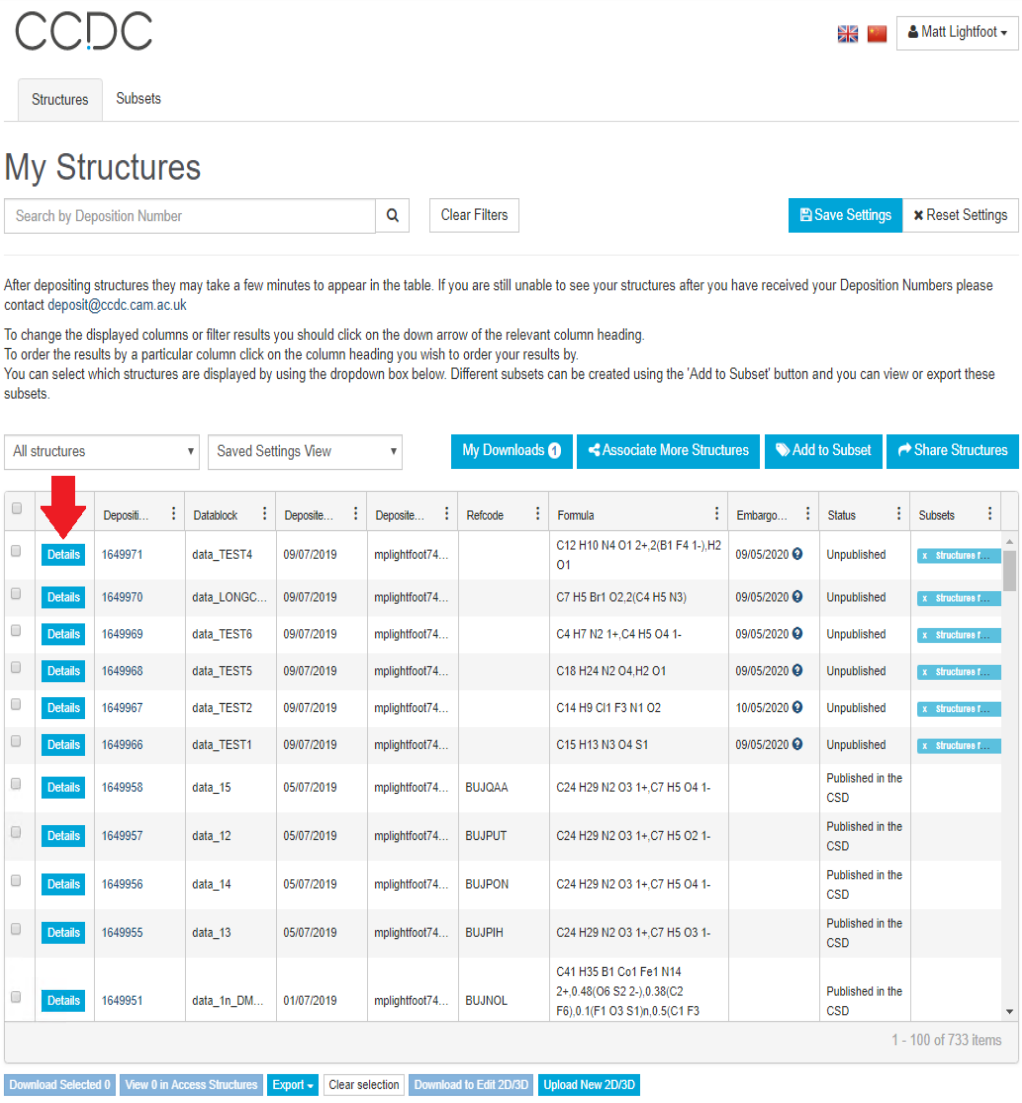


13. When the files have been saved into the system the status will change to complete and there will be tick with a number for the total number of entries that have been saved successfully back into the system.

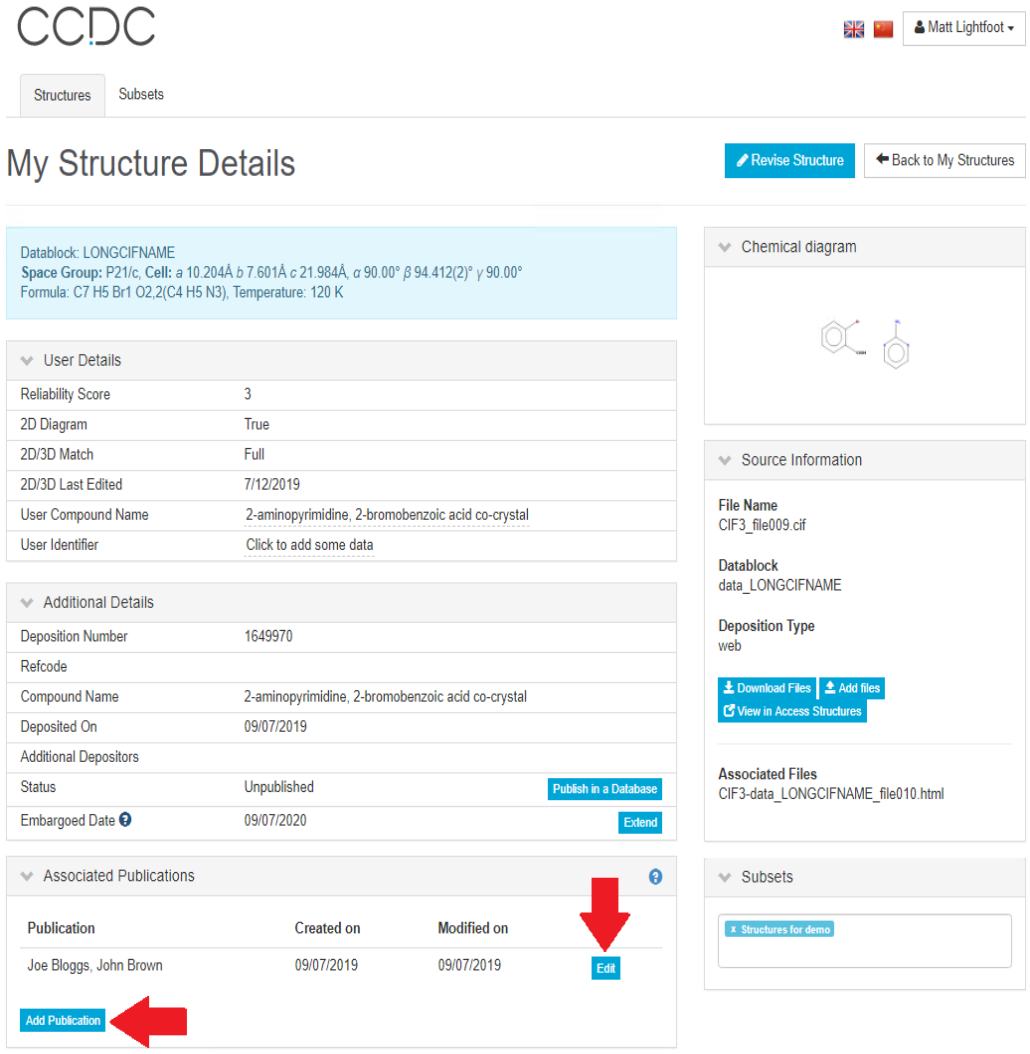


Adding publication details

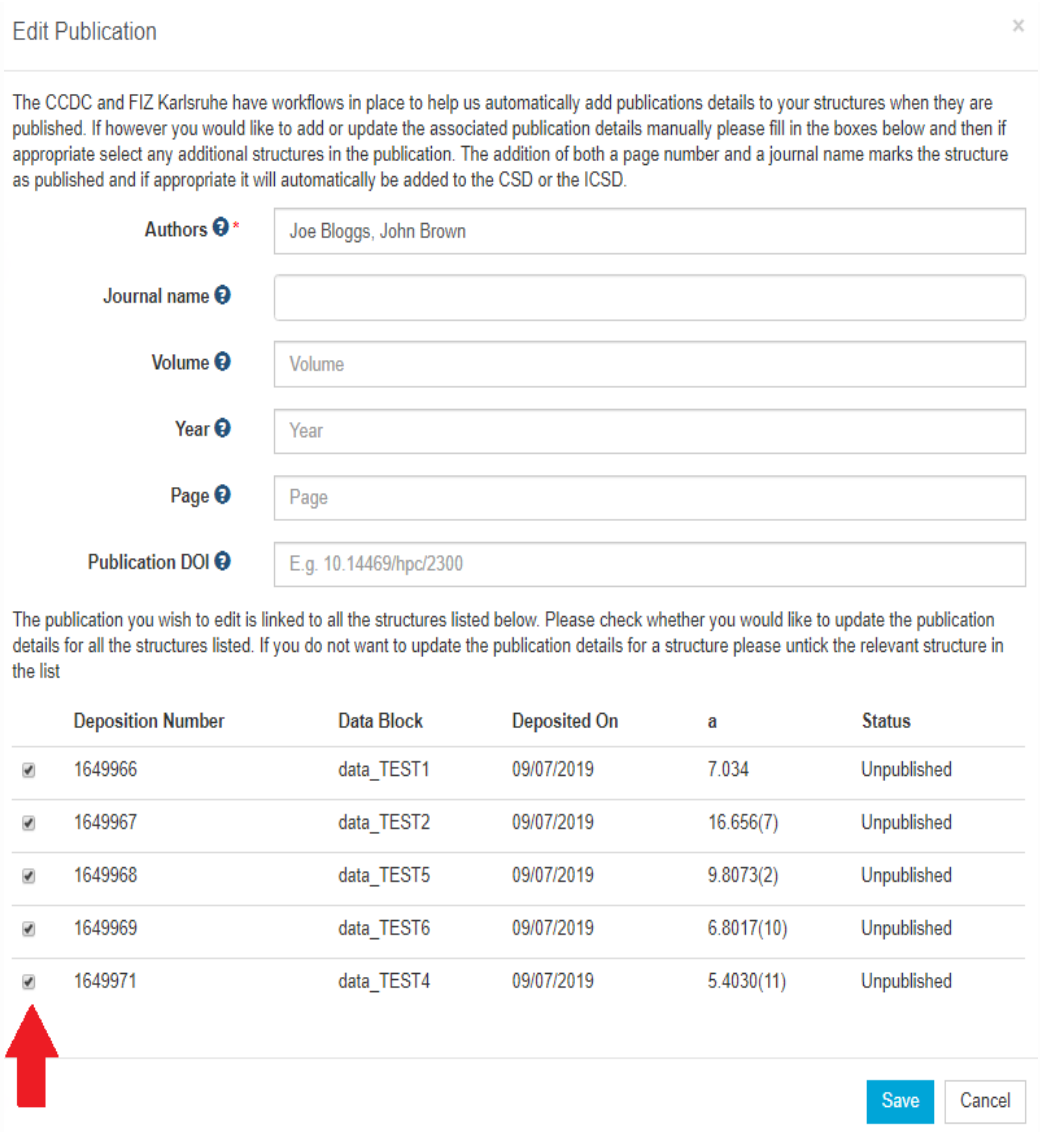
1. You can add publication details for your structures from the **My Structure Details** page. To access the **My Structure Details** page for the structure click on the **Details** button next to the structure that you want to add publication details to.



2. From the **My Structure Details** page you can add a new publication by clicking the **Add Publication** button or you can edit an existing publication by clicking the **Edit** button.



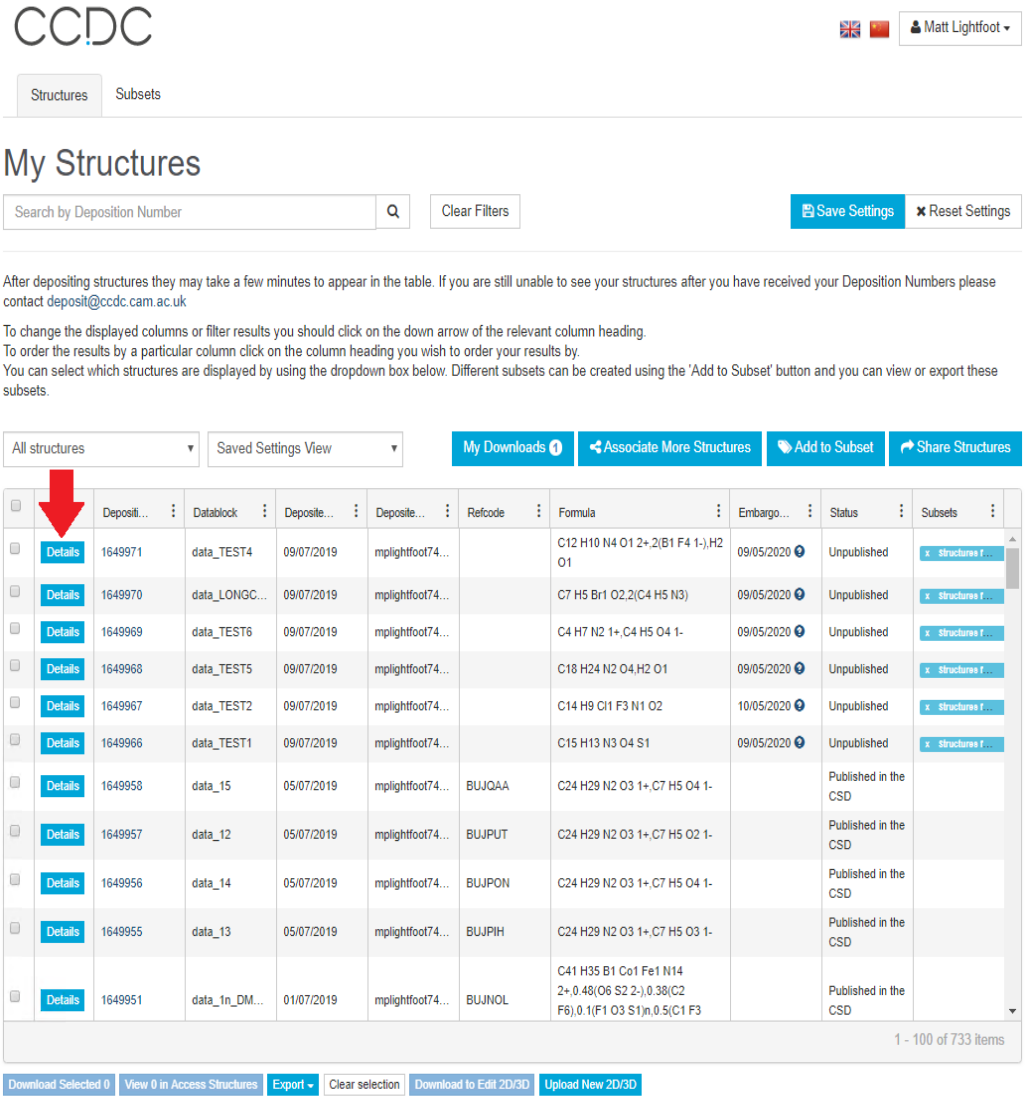
3. This will bring up a **Edit Publication** dialogue where you can add publication details. If you deposited more than one structure during the deposition then a list of Deposition Numbers may be listed at the bottom of the dialogue. You can tick and un-tick the boxes alongside the Deposition Numbers to indicate to which structures you want to update the publication for.



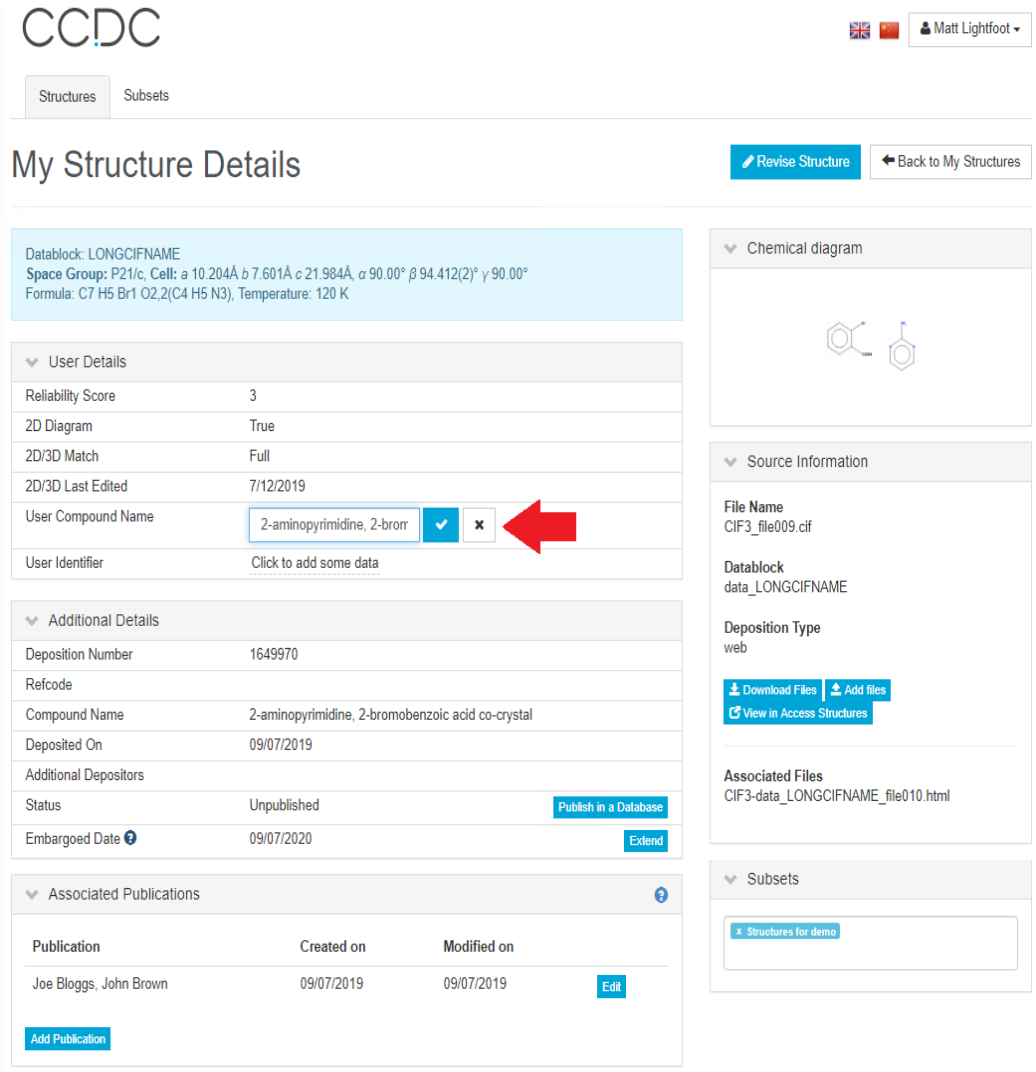
4. Once you have added all the publication details you should click the **Save** button and you should be returned to the **My Structure Details** page.

Adding a compound name

1. You can add a compound name for your structures from the **My Structure Details** page. To access the **My Structure Details** page for the structure, click on the **Details** button next to the structure that you want to add the compound name to.

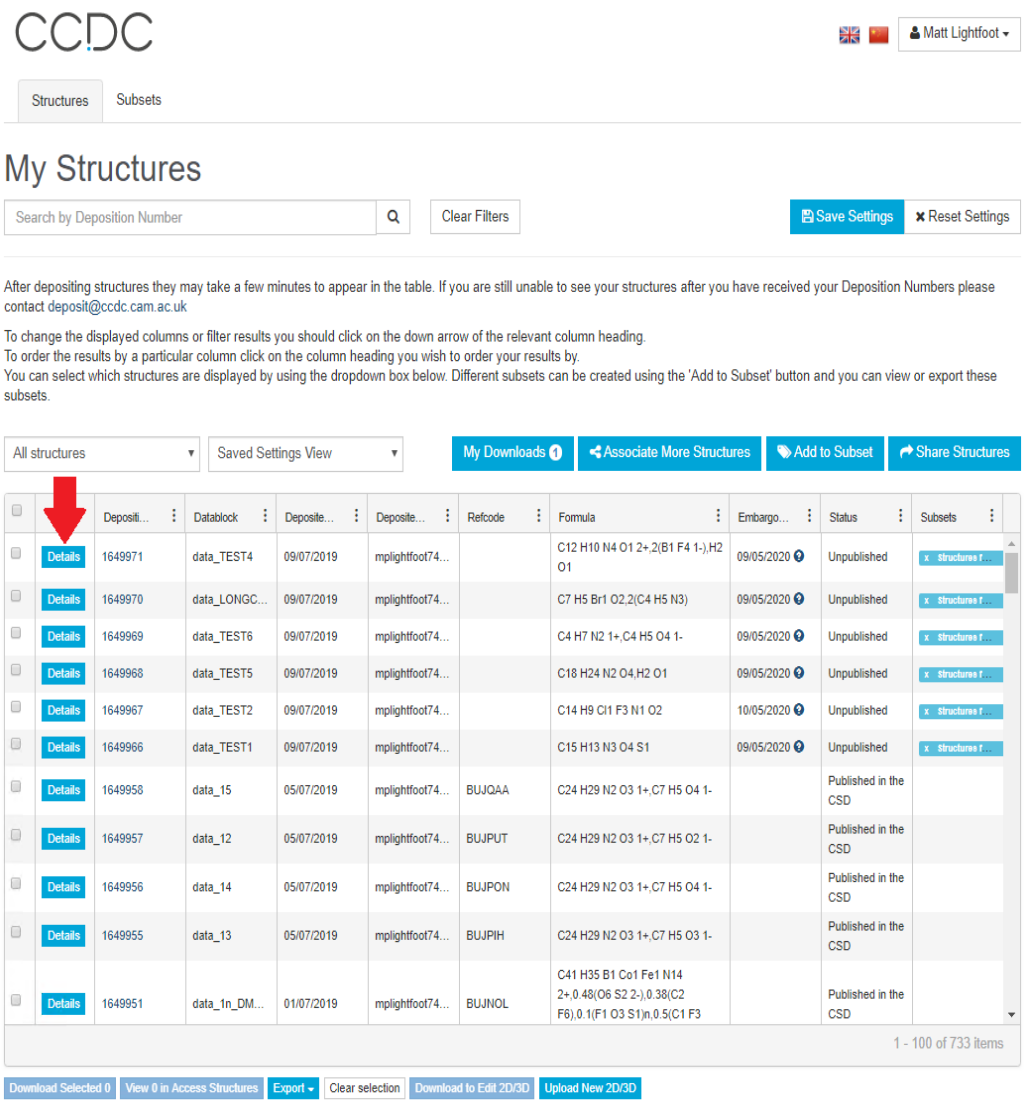


2. To add the compound name you should click the **Click to add some data** text box next to the **User Compound Name** field, type in the compound name and click the tick box to confirm.

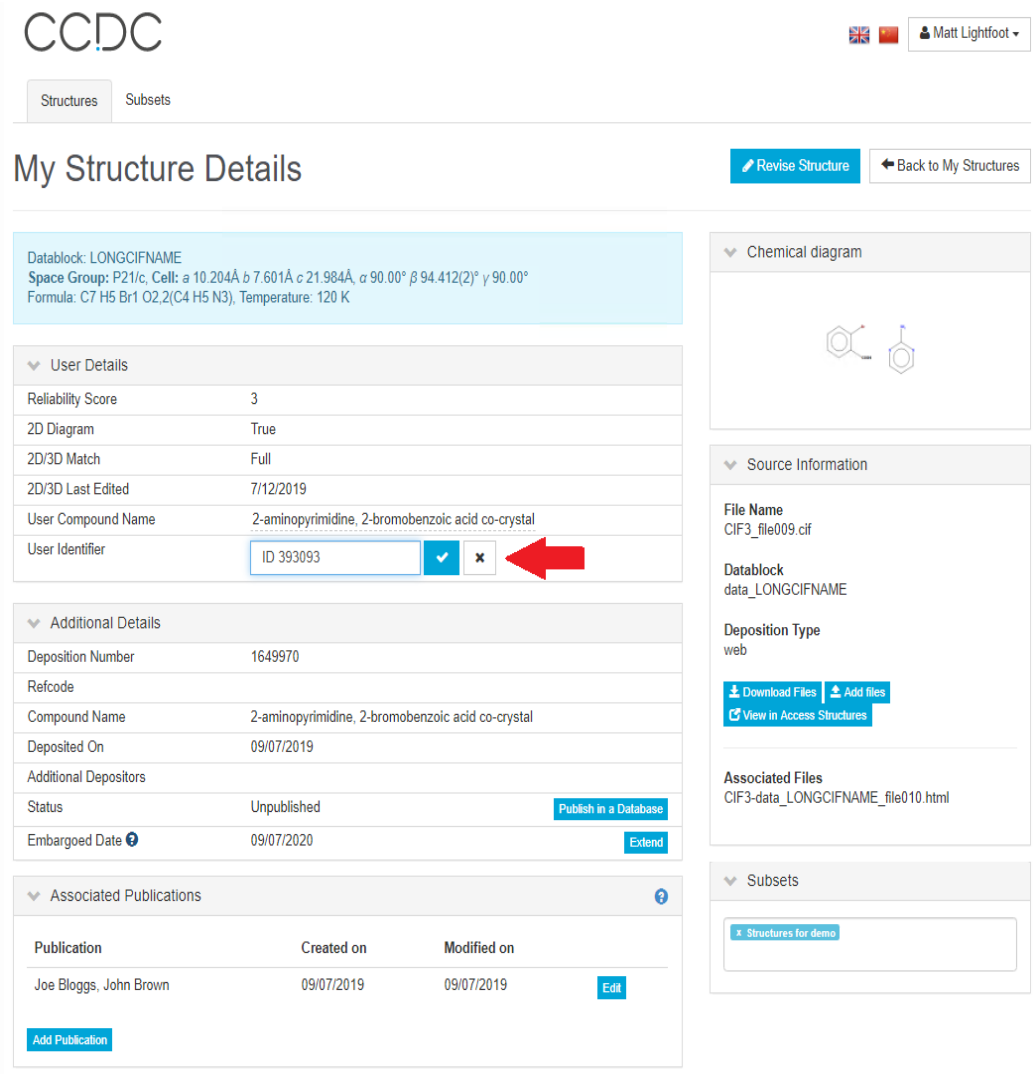


Adding an identifier

1. You can add an identifier for your structures from the **My Structure Details** page. To access the **My Structure Details** page for the structure, click on the **Details** button next to the structure that you want to add the identifier to.



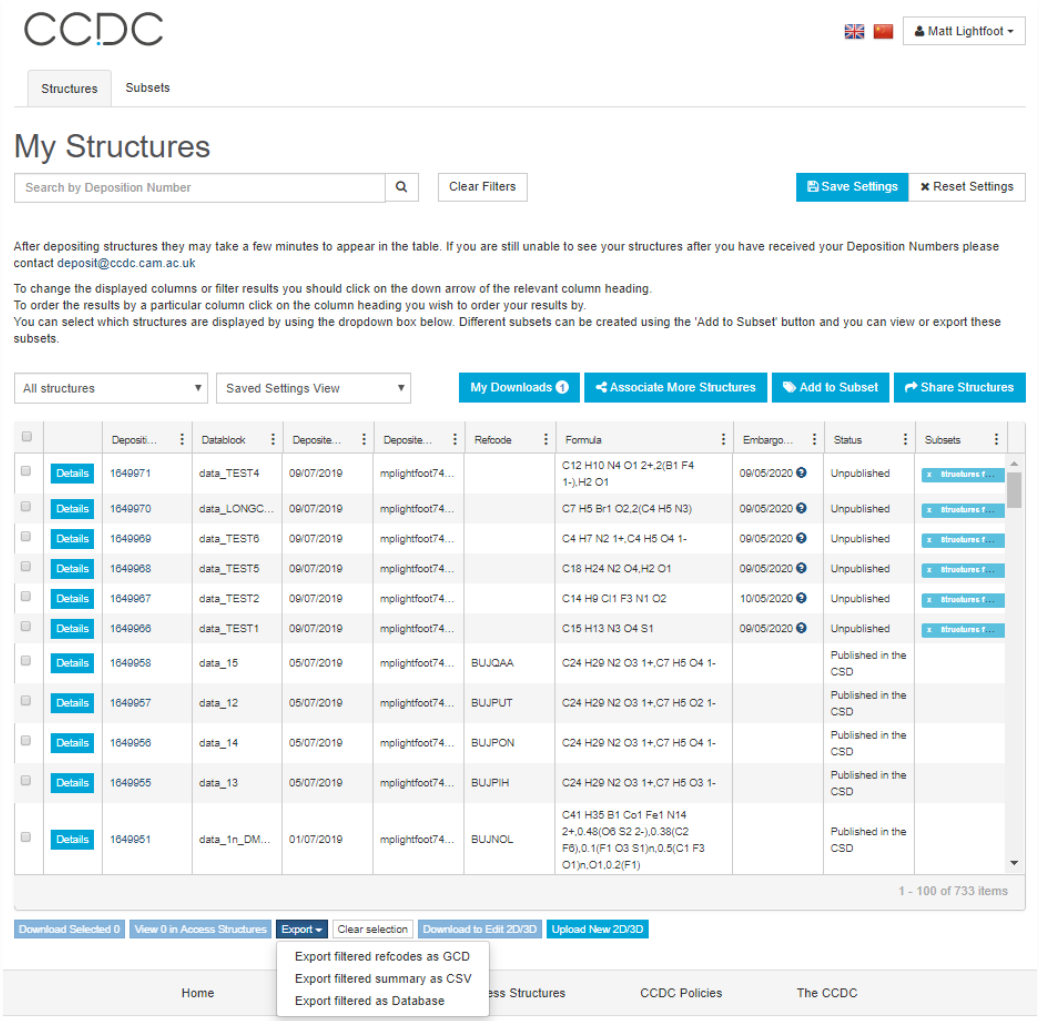
2. To add the identifier you should click the **Click to add some data** text box next to the **User Identifier** field, type in the identifier and click the tick box to confirm.



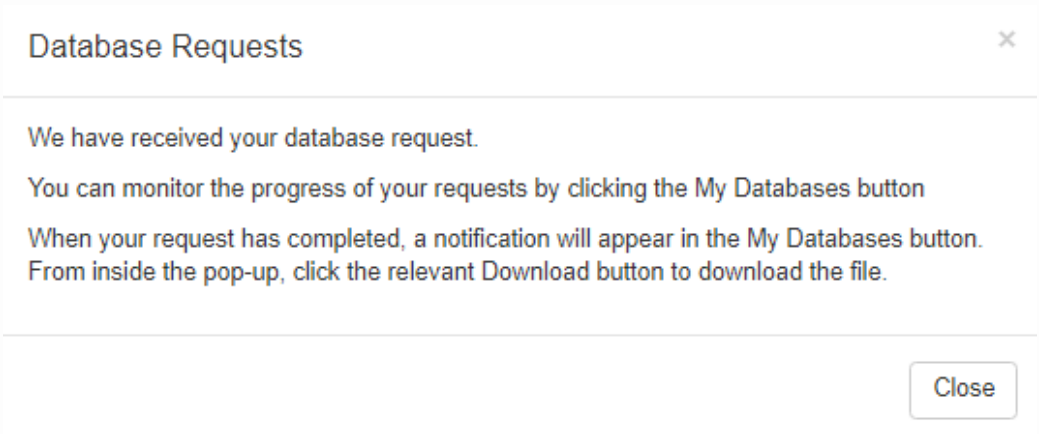
Exporting a database of structures from My Structures to view and search in CSD software

Exporting a database of all structures from the My Structures table

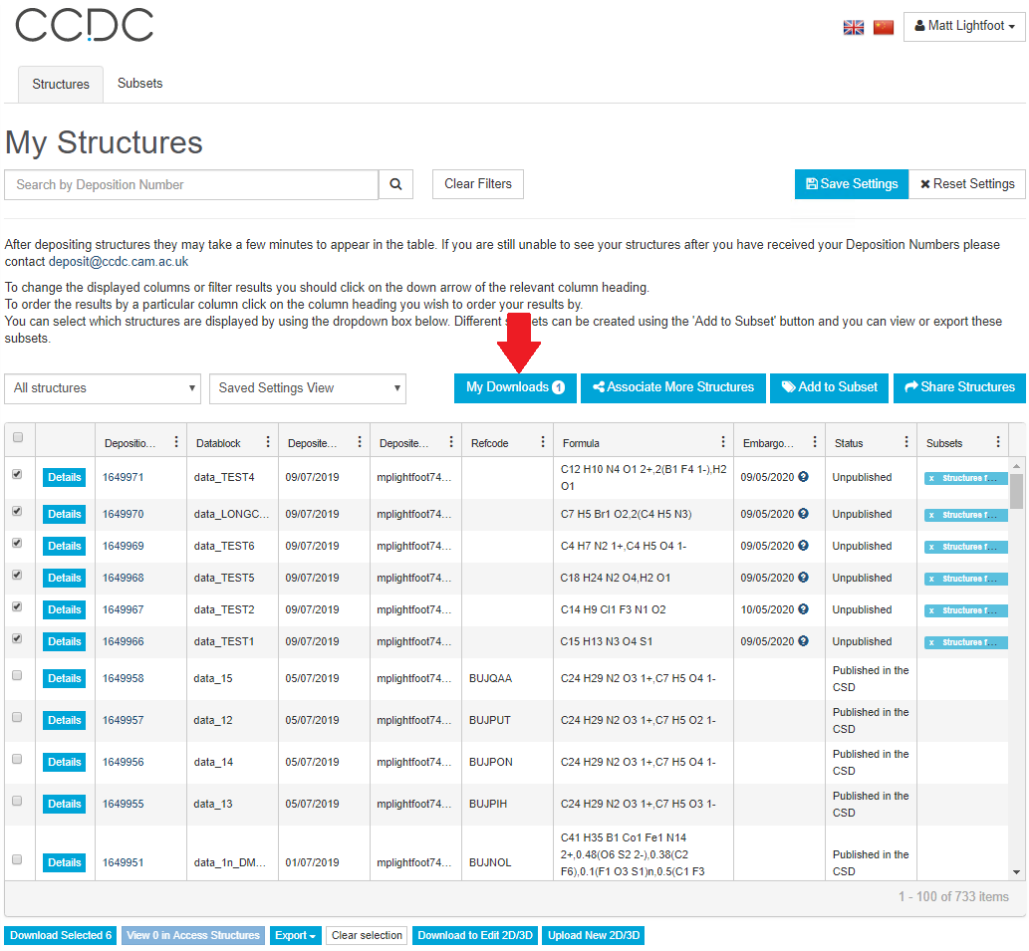
1. Login and go to the My Structures table.
2. Click the **Export** button with no structures selected and select the **Export filtered as a Database** option.



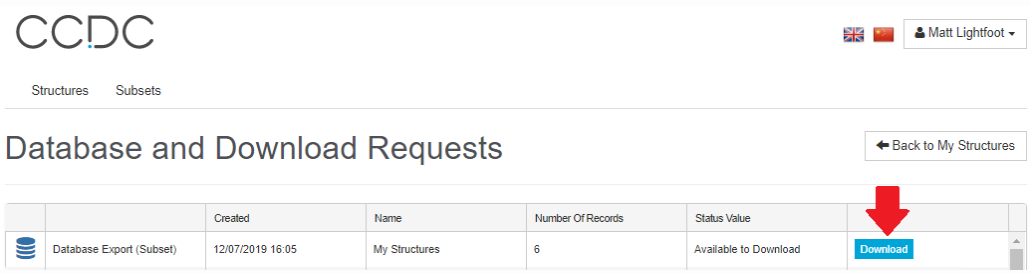
3. A dialogue will appear to say that the download request has been received. Click **Close** to close the dialogue



4. Go back to the My Structures table and click **My Downloads** button



5. The **Database and Download Requests** page will open and the new database export will be displayed at the top of the table. When the database is ready to be downloaded the Status will be **Available to Download** and a **Download** button will appear. Click the **Download** button to download the database (`.csdsql` file format).



Using in-house databases with CSD Portfolio software

Activating your in-house database for use with ConQuest

ConQuest can search in-house databases separately or in addition to the main CSD database. After you create or update an in-house database that you wish to search using ConQuest it must first be activated using the procedure described below.

In order to activate your in-house database you must copy (or soft-link: Linux only) the in-house database file (`*.csdsql`) to the same directory as the CSD V5.42 database files.

On Linux this is typically: `<INSTALLDIR>/CSD_2022/CSD_543`

While on Windows, this is normally: `C:\Program Files\CCDC\CSD_2022\CSD_543`

You must then run the Activate program:

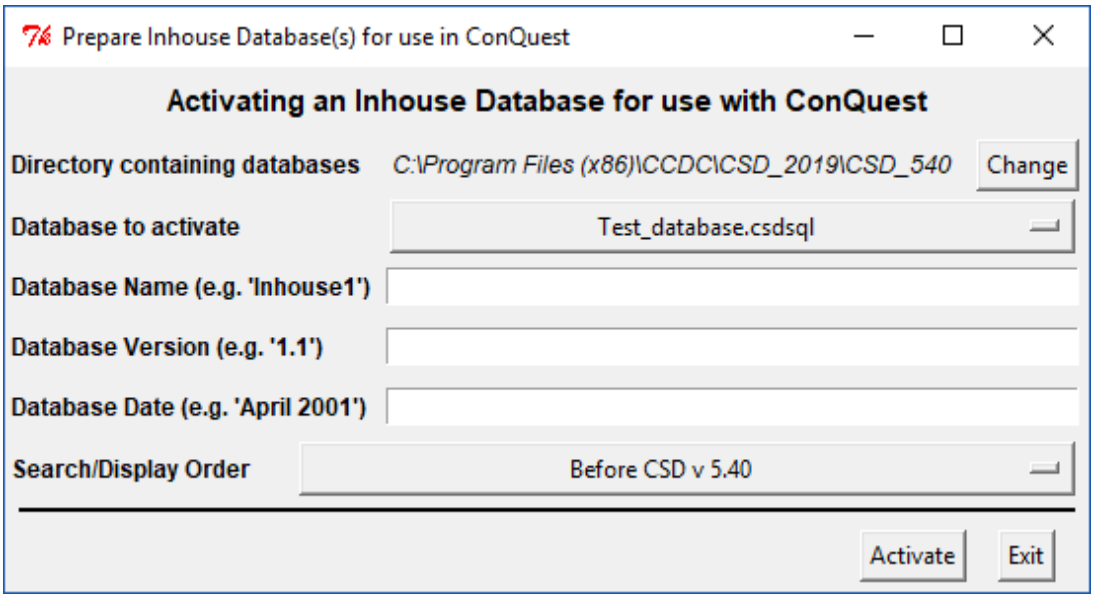
- For Linux, ensure that `<INSTALLDIR>/CSD_2022/bin` is in your PATH and type:

```
activate
```

- For Windows, select **Programs** -> **CCDC** -> **Activate in-house database** from the Windows Start menu.

Note: Windows 10 users will require escalated administrator privileges to activate databases. To do so, right-click on the **Activate Inhouse Databases** menu item and select **Run as Administrator**.

In both cases a pop-up window like the one shown below will be displayed:



- The activation program attempts to find the directory where the database is located by examining your ConQuest defaults file. However, if the correct directory cannot be found then use the **Change** button to locate the required directory.

- All databases in the selected directory which have not been activated will be displayed in the **Database to activate** pull-down menu. Simply select the databases you wish to activate.

- The contents of the **Database Name** dialogue box will be used by ConQuest to identify which databases you wish to search or view. Choose a name relevant to the database contents.

- Enter a version number for the database in the **Database Version** dialogue box. If you have an earlier version of a database, with the same Database Name in the same directory, it is important to make sure that the most recent version has the largest version number so that it is used in preference to the others.

- Enter the date for the database in the **Database Date** dialogue box.

- Use **Search/Display Order** pull-down menu to select the order in which activated databases will be displayed and searched by ConQuest. Taking the above example, if you select **After CSD v5.42,** when both databases are selected for searching in ConQuest the main CSD database will be searched before the in-house database.

- When you are happy with your selections press the **Activate** button; this will create an `.inf` file for the database, which will then be viewable and searchable the next time you start ConQuest.

To close the activate database program press the **Exit** button.

In ConQuest, navigate to **View Databases** > **Available Databases**

This opens an **Available Databases** pane which allows you to add a directory containing your new database, and also manage which databases are searched.

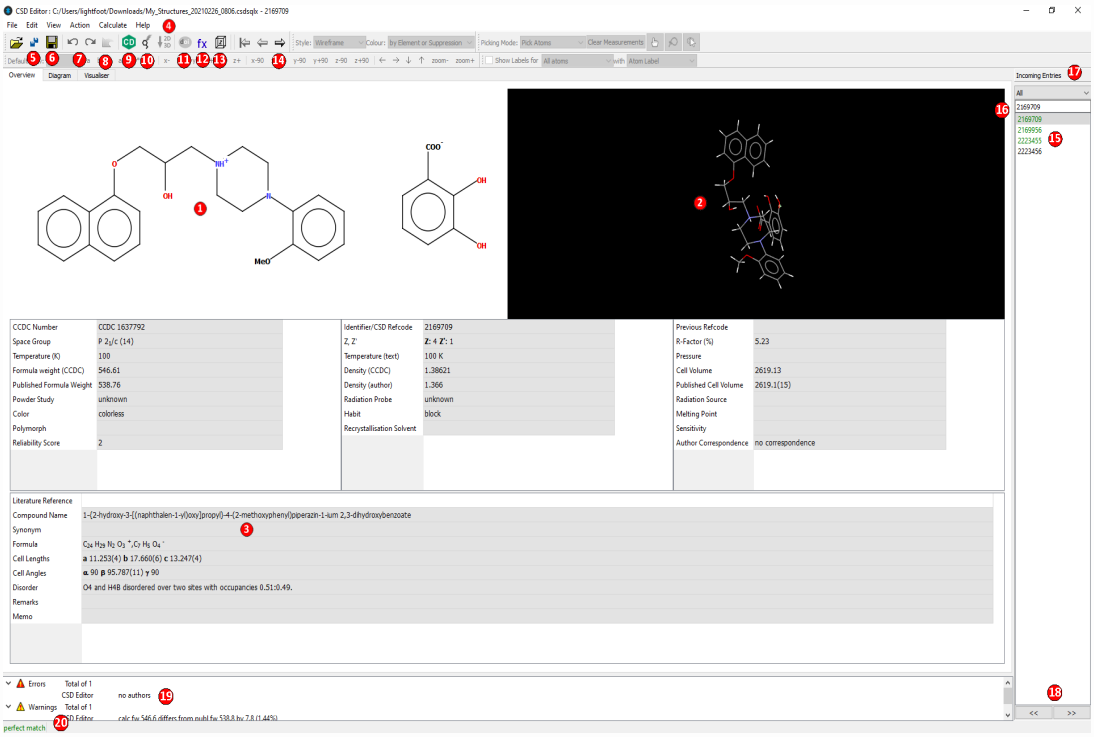
Using your in-house database with Mercury

Mercury will use the current CSDS database format (`.csdsql`) ; from the Mercury **CSD-Core** menu, the **Select Databases** option will allow selection of the appropriate database file.

2D/3D Editing in the CSD Editor

The CSD Editor has three different tabs. The functionality of these tabs will be described over the next few pages.

Overview Tab



1. **2D chemical diagram.**

2. **3D crystal structure.** Generated from the atomic coordinates.

3. **Crystallographic, numeric and textual data items.** It is not possible to edit these data items and the boxes are greyed out to indicate that they are not editable.

4. **Top menu bars.** The menu items **File**, **Edit**, **View**, **Insert**, **Action**, **Calculate** and **Help** are available. These menus contain a number of different options but all of these options can also be accessed through toolbars and buttons on the interface. Note that there are no options available in the **Insert** menu.

5. **Save All button.** Saves all the structures back into the database from which they were downloaded.

6. **Save the Current Entry button.** Saves just the current structure that is displayed back into the database from which it was downloaded.

7. **Undo and redo buttons.** Allows the last command(s) to be undone or redone.

8. **Undo All button.** Allows all the changes since the entry was loaded (or last saved) to be undone. If you move onto a different entry then you can no longer undo the changes made to the previous entry.

9. **ChemDraw Chemical Diagram button.** Enables the 2D chemical diagram to be edited using the ChemDraw program (if this is installed on the computer). The location of the installation of ChemDraw can be stored by clicking on the **Help** menu item and selecting **Session Info**. The path for ChemDraw can then be added to the **External Diagram Editor** field.

10. **Generate Chemical Diagram from current crystal structure button.** Generates a 2D chemical diagram from the 3D crystal structure. Note that the diagram generated each time the button is used may be different.

11. **DOI button.** If a DOI is included as part of the **Literature Reference** field, clicking this button opens the relevant paper in a browser if access to the article is available.

12. **Generate Formula from Chemical Diagram button.** Opens a dialogue which allows the formula to be calculated. If there are multiple molecules in the chemical diagram then the multipliers for each molecule can be defined.

13. **Generate a Packing Summary for the Crystal Structure.** Displays the Cell contents, the Formula unit and the Z and Z' values for the crystal structure.

14. **Arrows to move between structures.** The left hand button moves to the first entry in the list, the central button to the previous entry and the right hand button to the next entry.

15. **List of entries.** The software determines the relevant menu depending on the current entry being viewed. In most cases the display gives a list of all the entries in the current editing session colour coded by matching status. Green indicates that all of the chemical moieties in the 2D diagram match perfectly on to the moieties in the 3D structure. Amber indicates that only some of the chemical moieties in the 2D diagram match moieties in the 3D structure, likely to be due to disordered or unmodeled

molecules in the 3D structure. A purple colour indicates moieties present in the 3D structure have not been represented in the 2D diagram, suggesting the 2D diagram may not represent all moieties modelled from the X-ray data. Red indicates that none of the moieties in the 2D diagram match the moieties in the 3D structure. Black indicates that a match is impossible because of the absence of a 2D diagram.

16. **Current entry identifier.** The identifier for the structure currently displayed.

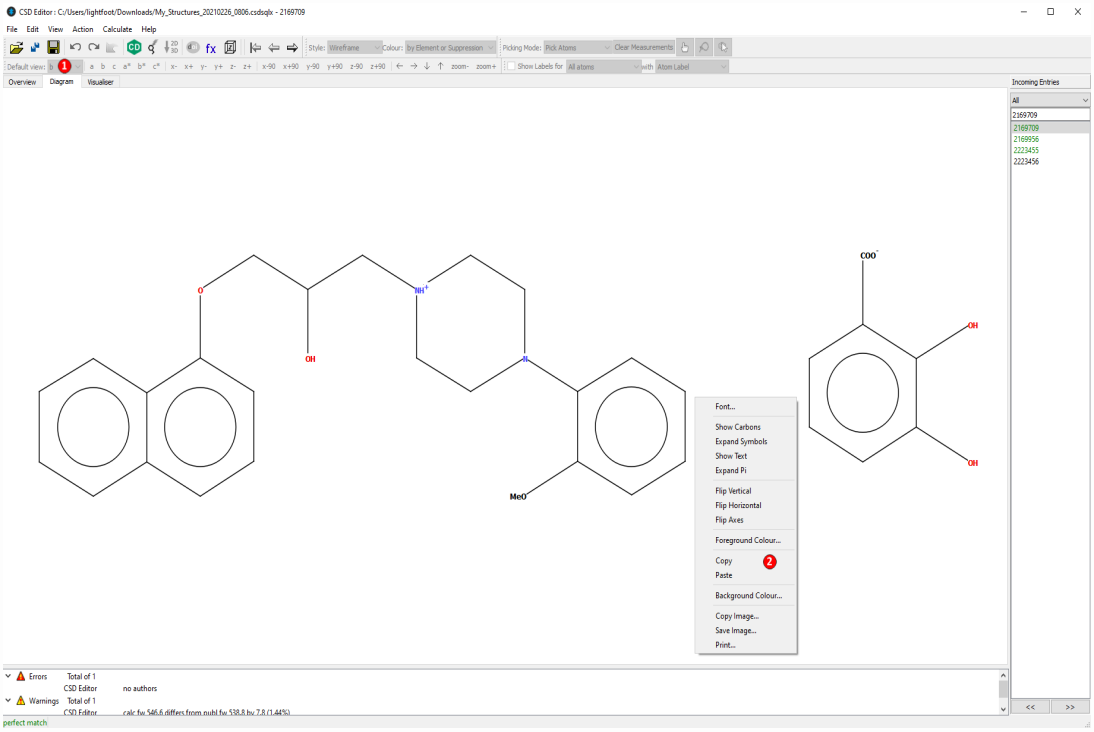
17. **Filter Structure Menu.** A drop-down menu which can be used to filter the list of entries. The filter options allow display of either all the structures in the current editing session, just the Not matched (red) entries or just the Partially matched (amber) entries.

18. **Arrows to move between structures.** Moves between structures in the displayed list.

19. **Details of Errors, Warnings and Remarks.** This section gives a list of the errors, warnings and remarks related to the structure. Some of the messages are from the initial analysis of the structure during conversion, and some are calculated from the current edits to the structure. A list of the common errors and warnings are given in the Appendix.

20. **Matching Status.** Gives details of the matching status of the entry.

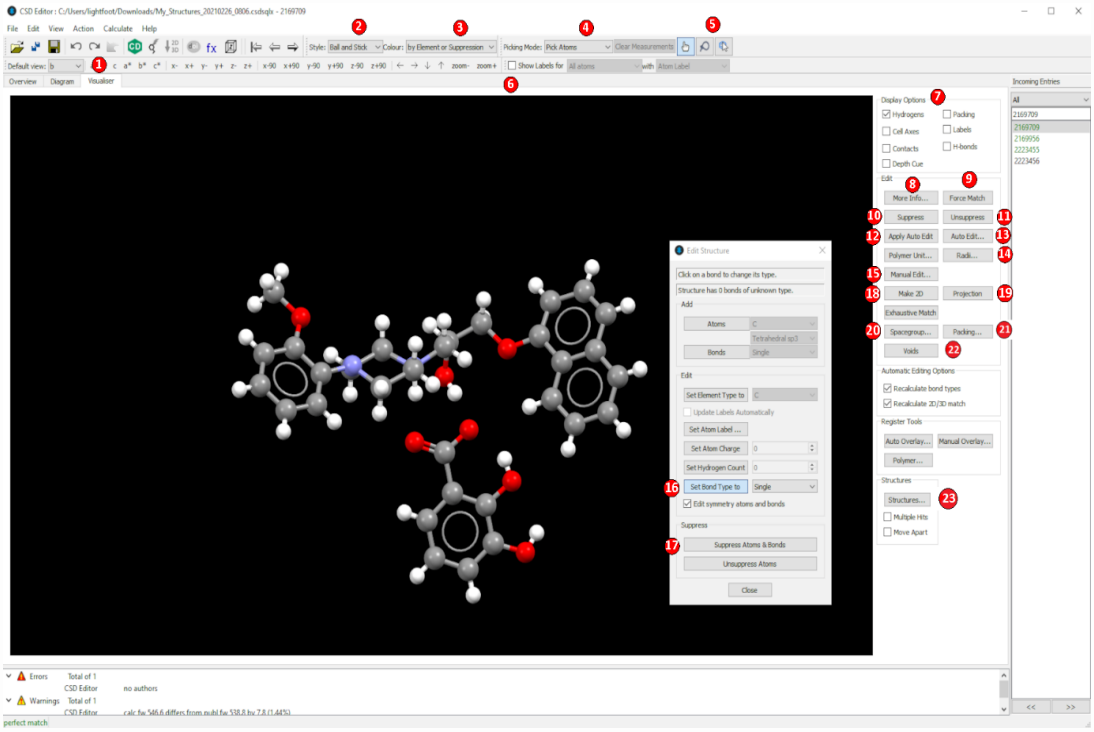
Diagram tab



1. **Diagram tab.**

2. **Right-click menu.** The diagram can be copied and pasted between entries by right-clicking on the diagram and using the **Copy** and **Paste** options. It can also be used to **Print** the diagram.

Visualiser tab



A lot of the functionality is identical to the functionality in Mercury. For a more detailed description of the functionality in the **Visualiser** tab see the Mercury documentation.

1. **Visualiser tab.**

2. **Display Style.** Select the display style for the 3D structure from the options in the drop-down menu.

3. **Colour Mode.** Select the colouring scheme for the atoms and bonds in the 3D structure. A particularly useful function in some cases is the ability to colour the 3D structure by matching status so that it is possible to see which molecules in the structure are matched to the 2D (green) and which are unmatched (red). Another useful function is the **by Element or Suppression** option which indicates which atoms have been suppressed in the 3D structure.

4. **Picking Mode.** Select the picking mode from options in the dropdown box. This defines what happens when you left-click on items in the 3D structure; whether it selects the atoms or measures a distance, angle, etc.

5. **Normal and lasso picking modes.** Click the icons to change the picking mode from the normal picking mode to the lasso picking mode.

6. **Show Labels options.** Click the **Show Labels** check box to show/hide atom labels. Select options from the two drop-down menus to select the type of atom that is labelled and the type of label that is shown. A useful function is the **Show Labels for Siteless Neighbours** option which will display the labels for only atoms which have siteless atoms (e.g. atoms with hydrogens that have no coordinates).

7. **Display Options.** Click the relevant check box to display certain options in the 3D structure.

8. **More Information button.** Opens the **More Information** dialogue. From this dialogue, it is possible to suppress, unsuppress, set the hydrogen count for or delete atom(s) using a mouse click for a single row, Shift+click for a block and Ctrl+click for separated rows. This dialogue is customisable and can show different attributes about the atoms, including label, occupancy and ADP.

9. **Force Match button.** Used in situations where edits have been made to either the 2D diagram or the 3D structure and there is no longer a perfect or partial match between the two. In such a situation, if the chemistry represented in the 2D diagram is close enough to correctly matching the 3D structure, then the bond types/hydrogen atom assignments etc. in the 3D will automatically be edited to achieve as complete a match as possible.

10. **Suppress button.** Used to suppress atoms in the 3D structures, to help represent disordered molecules. Select all the atoms that you want to suppress and then click the Suppress button. The suppressed atoms will be coloured light green and will not bond to any other atoms. See the FAQ '**How should I deal with disordered structures?'** for more information.

11. **Unsuppress button.** Used to unsuppress atoms in the 3D structures. Select all the atoms that you want to unsuppress and then click the Unsuppress button.

12. **Apply Auto Edit button.** Useful if the chemistry of the structure has not been determined correctly (often shown by the presence of unknown bond types in the 3D structure for a severely disordered structure). The ‘Apply Auto Edit’ button is a quick one-click option that uses the default settings suitable for most situations. To manually configure the Auto Edit options the ‘Auto Edit’ button should be used instead.

13. **Auto Edit button.** Useful if the chemistry of the structure has not been determined correctly (often shown by the presence of unknown bond types in the 3D structure for a severely disordered structure). The default settings are suitable for most situations and clicking **Apply** produces another pop-up window to show how many (if any) bonds and atoms have been changed, added or removed and presents a choice to **Accept** or **Revert** the changes.

14. **Radii button.** Used to edit the default bonding limits for pairs of elements in the structure and can be a useful way of removing unwanted bonds from the 3D structure. A tick box is provided to either include or exclude chemically-unlikely bonds. For most common cases it is better for this box to be unchecked.

15. **Manual Edit button.** This opens the dialogue shown in the 3D structure and allows editing of the 3D structure including adding atoms and bonds, changing element types and editing atom and bond properties.

16. **Set Bond Type to button.** Used to change the bond type of bonds in the 3D structure.

17. **Suppress Atoms and Bonds button.** Used to suppress atoms and bonds in the 3D structure (the **Unsuppress atoms** button below will unsuppress atoms). This functionality can be useful if you have disorder that has not been correctly resolved.

18. **Make 2D button.** Generates a 2D chemical diagram from the 3D crystal structure.

19. **Projection button.** This produces a 2D diagram in the same orientation as the currently selected view of the 3D structure. This diagram is generally of lower quality than the diagram produced by the **Make 2D** button but it is much faster.

20. **Spacegroup button.** Allows alternative settings of the space group to be chosen.

21. **Packing button.** Allows various options for packing and slicing the structure.

22. **Voids button.** Calculates the void volume as a percentage of the unit cell volume.

23. **Structures button.** Used when there are two 3D structures in the display to colour the structures differently and to move them apart. This will not be useful in most common situations.

Saving entries in the CSD Editor

The entries that you have selected will be saved in a local temporary database (usually in `C:\Users\USERNAME\csd_editor`). When you edit these structures the edits will be saved in this temporary database every time you move between entries or close the CSD Editor. Since the edits are saved you can close the CSD Editor and reopen it which will reopen the edited structures. When you click **Save All** the edits will be saved back into the My Structures database from which you selected the structures initially. When you have saved the structures back into the database you can upload the edited structures back to My Structures (see Editing 2D/3D step 11).

CSD Editor FAQs

How should I deal with polymeric structures?

The easiest way to deal with polymeric structures is to reduce the relevant bond distance pairs to the metal until the structure is not polymeric. This can be done by going to the **Visualiser** tab, pressing the **Radii** button and reducing the relevant bond distance limits for all bonds which occur to the metal in the structure. Once all the

polymeric bonds have gone the **Make2D** button can be used to generate a new diagram. In some cases it may be necessary to use the **Force Match** button to match the structure.

How should I deal with disordered structures?

If a structure contains disorder then the minor occupancy sites must be suppressed to leave a single representative atomic position that will then be matched against the chemical diagram. Suppressed atoms are not deleted; they simply take no further part in the establishment of the crystallographic connectivity and therefore will not be used in ConQuest 3D searches. In the majority of cases, the initial CIF file conversion will have dealt with any disorder in the structure. If there are atoms in the 3D structure that have not been dealt with correctly then these atoms can be suppressed and unsuppressed manually using either the **Manual Edit** dialogue or the **More Info** dialogue in the **Visualiser** pane. It is advisable to check that in the top menu, colour is set to **by Element** or **Suppression**.

How do I select all atoms in a molecule in the 3D structure?

This can be done by holding the **Shift** key and clicking an atom in the molecule that you want to select.

How do I select a group of atoms in the 3D structure?

This can be done by holding the **Shift+Alt** keys and using the mouse to lasso atoms.

What does the colour coding in the identifier list signify?

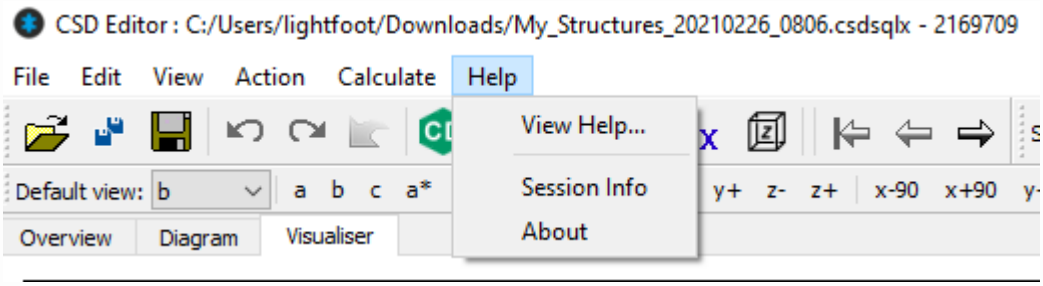
Green indicates that all of the chemical moieties in the 2D diagram match perfectly on to the moieties in the 3D structure. Amber indicates that only some of the chemical moieties in the 2D diagram match moieties in the 3D structure, likely to be due to disordered or unmodeled molecules in the 3D structure. A purple colour indicates moieties present in the 3D structure have not been

represented in the 2D diagram, suggesting the 2D diagram may not represent all moieties modelled from the X-ray data. Red indicates that none of the moieties in the 2D diagram match the moieties in the 3D structure. Black indicates that a match is impossible because of the absence of a 2D diagram.

How can I tell where the CSD Editor is saving edits to my database?

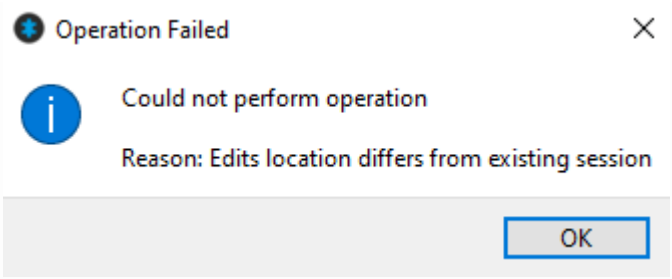
Any additional structures or updates of existing database entries are only added to your existing file once the CSD Editor session has been saved, when the changes are applied to the original source database. CSD Editor can be closed and reopened without uploading database entries; in this case edits made within CSD Editor will be saved but not applied to your source database.

The location of the source database can be found from the **Help** menu under the **Session Info** option. This will record your database location as the **Data Source**, with the **Session File** and **Database File** locations referring to the files updated during the CSD Editor session.



Why do I see an 'Operation Failed' message when trying to open my database in CSD Editor?

When making changes to database entries in CSD Editor the structures are saved as a separate CSD Editor session file. If you attempt to re-open a database as part of a pre-existing session it may cause an error message to occur (see below).



To resolve the error: First close the CSD Editor session, and then locate the folder containing the CSD Editor session files (typically `C:\Users\USERNAME\csd_editor`) and delete the files present. Once these files are removed CSD Editor can be reopened and used as normal.

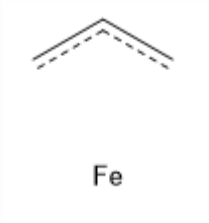
What should I do if I get an 'internal error' warning?

When deleting and adding entries to a database you may very occasionally get an 'internal error' warning message. If you get this message then it is recommended that you close and reopen the CSD Editor.

How do I add a pi-bond to a chemical diagram using ChemDraw?

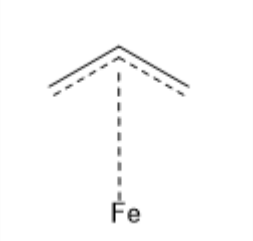
Open ChemDraw and draw the atoms for the structure.

Select the **Multiple bonds** option and change all the pi-bonded bonds to the single and dotted bond (tautomeric bond).



Select all the atoms that are to be pi-bonded to the metal and select **Structure** > **Add Multi-Center Attachment**. A multi-center attachment point will appear in the diagram.

Then select the dotted bond option and draw a bond between the metal atom and the multi-center attachment point.



Close ChemDraw and the diagram in the CSD Editor will have the pi-bonds displayed.

What is the '-journal' file that is sometimes created alongside my database files?

This is a temporary file that appears alongside the database file and is used as part of the normal database transaction rollback mechanism. This file should not be deleted while the database is in use.

CSD Editor errors and warnings

Below is a list of the common errors and warnings that are found in the CSD Editor along with an explanation of each. Note that A, B, C and D will be replaced by the relevant atom(s) or calculated value in the messages given in the CSD Editor.

No formula given - no comparison with connectivity
: The formula may be missing and can be calculated by generating a diagram.

Given formula does not agree with chemical connectivity - Abstracted: A; Calculated: B
: The formula does not agree with the 2D diagram and can be recalculated by using the **Generate Formula from Chemical Diagram** button

formula has unbalanced charges
: The formula does not charge balance. The charges can be edited and the formula recalculated using the **Generate Formula from Chemical Diagram** button.

2D: A x B valency C atoms D'

The 2D diagram contains atoms which have unusual valencies. There may be H atoms missing from C atoms and these can be added to the atoms from the **Visualiser** tab.

Diagram atom A has both aromatic and delocalised bonds

An atom in the 2D diagram has unusual aromatic and delocalised bonds. This can be fixed by manually editing the diagram from the **visualizer** tab and then regenerating the diagram using the **Make2D** button.

B aromatic atoms(s) that are in rings with poor geometry

In the 2D diagram an aromatic ring has unusual geometry. This can be fixed by regenerating the diagram using the **Make2D** button in the **visualizer** tab.

No compound name

The compound name field is empty. Please ignore this.

Compound name: mismatched parentheses A

The compound name does not contain the same number of opening and closing brackets. Please ignore this.

Compound name: letter followed by number

The compound name contains a letter followed immediately by a number. Please ignore this.

Atom A has unusual valency B

In the 3D structure an atom has an unusual valency. This may be ok but can be changed if required by editing the 3D structure in the **Visualiser** tab.

Crystal connectivity not polymeric but formula polymeric

The formula is polymeric but the 3D structure is not. It is possible that the formula should not be polymeric and can be edited by removing the *n* multipliers using the **Generate Formula from Chemical Diagram** button.

Crystal connectivity polymeric but formula not polymeric

The formula is not polymeric but the 3D structure is. It is possible that the formula should be polymeric and can be edited by adding *n* to the multipliers using the **Generate Formula from Chemical Diagram** button.

Crystal connectivity bond: A B C short

A bond in the 3D structure is short. This may be due to unresolved disorder.

Crystal connectivity: long bonds may have been added manually

This is a warning that the 3D structure contains bonds which are longer than the default limits in the CSD Editor. These may

have been added manually and so there is no change required.

Crystal structure: A % voids

This is a warning that the structure contains void space. This may sometimes be due to missing or unmodelled solvent molecules.

Dcalc is too small, no density check

Please ignore this.

Dalc differs from Dx by >2%, try adjusting Z value

Please ignore this.

No R factor for entry category=3

Please ignore this.

Formula: estimated vol A calc vol B differs by C %; check Z

The cell volume is estimated from the molecular formula using average effective atomic volumes derived by D. Hoffman, but based on the '17Å per non-H atom' idea and is compared with the volume calculated from the cell parameters. If there is a difference then the structure may have an incorrect Z value or may contain void space.

Calc fw A differs from publ fw B by C (D %)

The calculated formula weight differs from the formula weight given in the CIF. This may be due to an incorrect formula which can be recalculated using the **Generate Formula from Chemical Diagram** button.

Element A in formula but not in compound name

The calculated formula contains an element that is not given in the compound name. Please ignore this.

Element A in compound name but not in formula

The compound name contains an element that is not given in the calculated formula. Please ignore this.

Compound name: poly or catena needed for polymeric formula

The formula is polymeric but the compound name does not contain ‘catena’ or ‘poly’. Please ignore this.

Chem & Crystal connectivities not matched

None of the chemical moieties in the 2D diagram match with any of the moieties in the 3D structure. This may be fixed by editing the 3D structure or the 2D diagram. Using the **Force Match** button is a way of adding the chemistry in the 2D diagram to the 3D structure.

Crystal fully matches Chem connectivities, but not vice-versa

Some of the chemical moieties in the 2D diagram do not match with some of the moieties in the 3D structure. This may be fixed by editing the 3D structure or the 2D diagram. Using the **Force Match** button is a way of adding the chemistry in the 2D diagram to the 3D structure.

Chem fully matches Crystal connectivities, but not vice-versa

Some of the chemical moieties present in the 3D structure are not represented in the 2D diagram. Using the **Edit > Create Chemical Diagram** option will represent all 3D moieties in the 2D diagram; tools such as the **Auto Edit** function from the **Visualiser** pane may be required to consistently represent the chemistry shown in the 3D structure.

Chem & Crystal matching impossible

It is not possible to match the moieties in the 3D structure with the moieties in the 2D structure. This is probably due to a missing 2D diagram.

Published bond: A B given but not found in calc

A bond given in the CIF does not correspond to a bond given in the calculated 3D structure. This may indicate that there is a bond missing in the 3D structure or that the published bond list contains an incorrect bond. The published bond list can be edited by clicking on **More Info** in the **Visualiser** tab and then clicking on **Published Bond**.

Published bond: A B short

A bond given in the CIF is shorter than the default limits in the CSD Editor. This may indicate that there is a problem with the position of an atom in the 3D structure or that the published bond list is incorrect. The published bond list can be edited by clicking on **More Info** in the **Visualiser** tab and then clicking on **Published Bond**.

Published bond: A B long

A bond given in the CIF is longer than the default limits in the CSD Editor. This may indicate that there is a problem with the position of an atom in the 3D structure or that the published bond list is incorrect. The published bond list can be edited by clicking on **More Info** in the **Visualiser** tab and then clicking on **Published Bond**.

Spacegroup does not agree with symmetry operators

This is a message that is added when an entry is created and indicates that the space group given in the CIF does not agree

with the list of symmetry operators given in the CIF. The list of symmetry operators can be viewed by clicking on More Info in the visualiser tab and then clicking on Symmetry.

No Z value

The Z value is missing from the entry. Please ignore this.