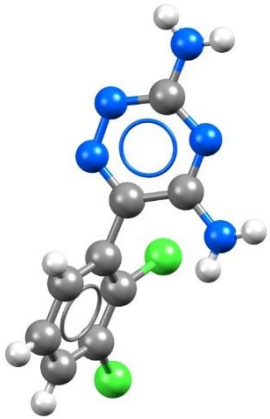
Structure Deposition Workshop

Version 1.0 – January 2019



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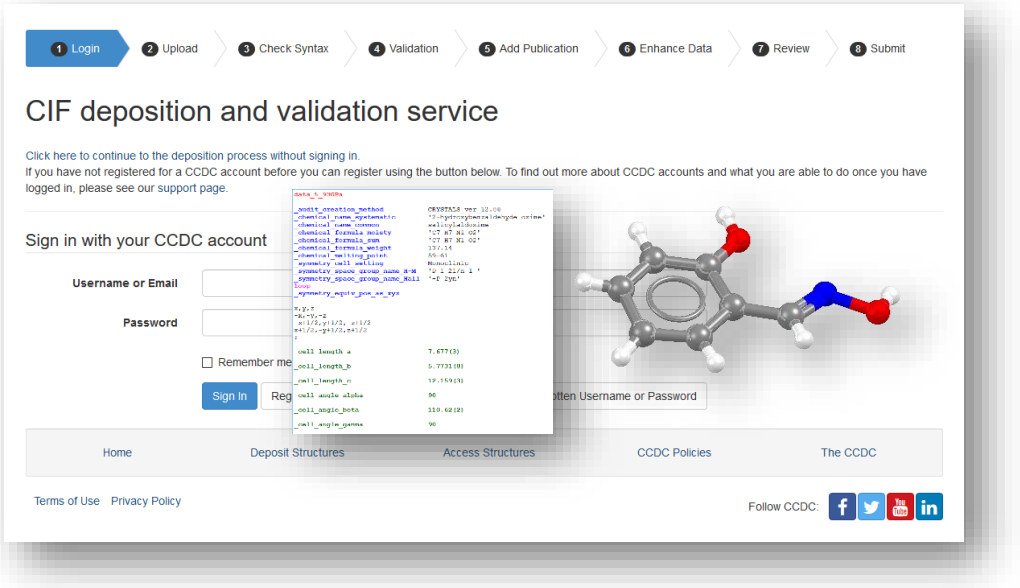
Example 1. Depositing CIF files

In the following example, you will learn how to register for a free account for the CCDC website. This will allow you to deposit data more easily, access and share your data using the MyStructures service. You will then look at depositing crystal data with the CCDC in the CIF file format. To do this, you will use the joint CCDC and FIZ Karlsruhe web deposition service.



Obtaining example CIF files

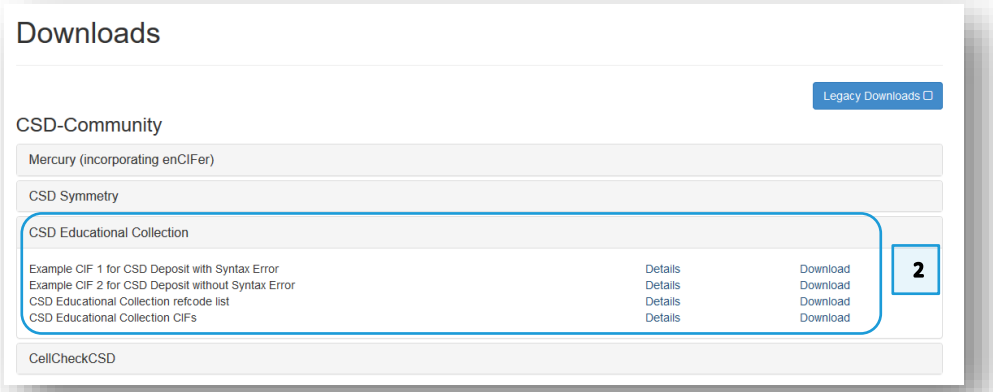
In this example, you will use two example CIF files; one with correct syntax, and one where there are some syntax errors which need to be corrected during the deposition process. These files can be obtained from the CCDC website.

1. Open a web browser and navigate to https://www.ccdc.cam.ac.uk/support-and-resources/downloads/

2. Under *CSD-Community*, click on **CSD Educational Collection** and click **Download** beside *Example CIF 1 for CSD Deposit with Syntax Error*.

3. Click **Agree & Download** and save the “example_1.cif” file.

4. Repeat steps 2 and 3 for *Example CIF 2 for CSD Deposit without Syntax Error* to download the “example_2.cif” file. Remember the location where you save these files.



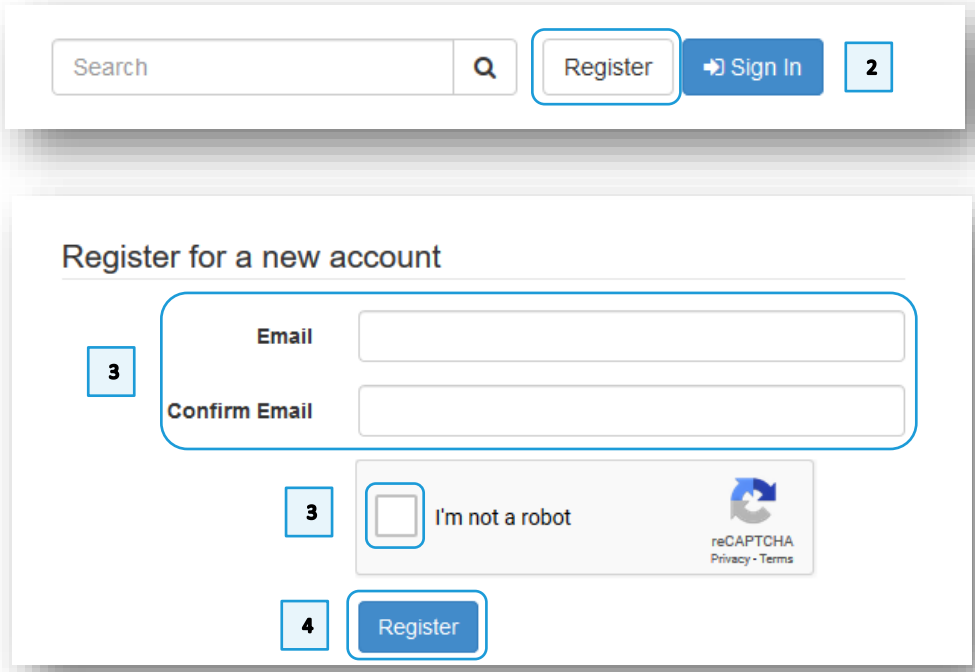
Registering for a CCDC account

1. Open a web browser and navigate to https://www.ccdc.cam.ac.uk/deposit.

2. We recommend creating a CCDC account, which makes depositing structures easier and allows you to access and share your data through our MyStructures service. If you would like to create an account, click on **Register** at the top right of the page. Alternatively, if you would prefer not to create an account, you can click the link to continue the deposition process without signing in and proceed to the section of the workshop 'Personal details and CIF upload'.

3. Enter your email address in the boxes and click the reCAPTCHA to indicate you are not a robot. On this page you may also view our privacy policy before setting up an account.

4. Click **Register** in the blue box at the bottom of the page.



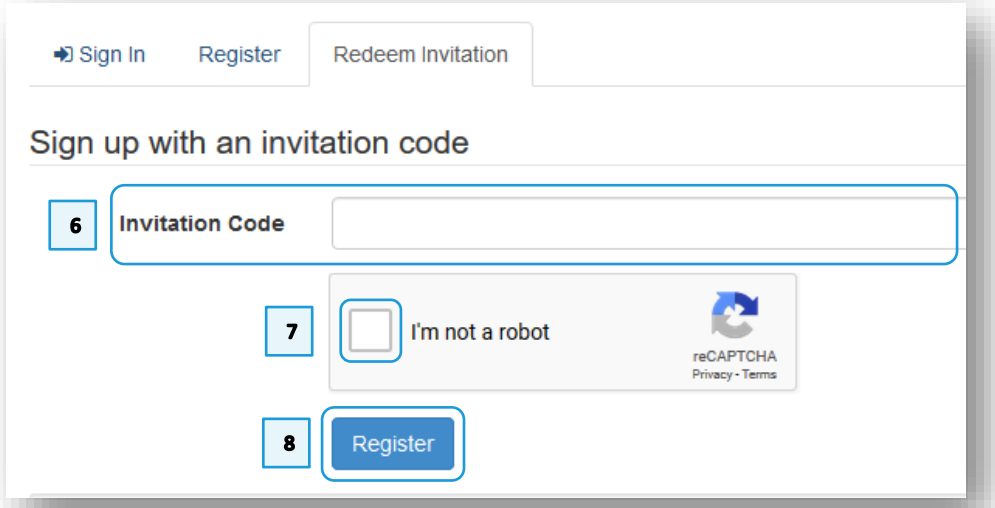
Redeeming an invitation

5. Check your inbox for an email containing your invitation code.

6. Click on the **Redeem invitation** tab and enter the invitation code you received via email.

7. Tick the reCAPTCHA box to indicate you are still not a robot.

8. Click **Register**.

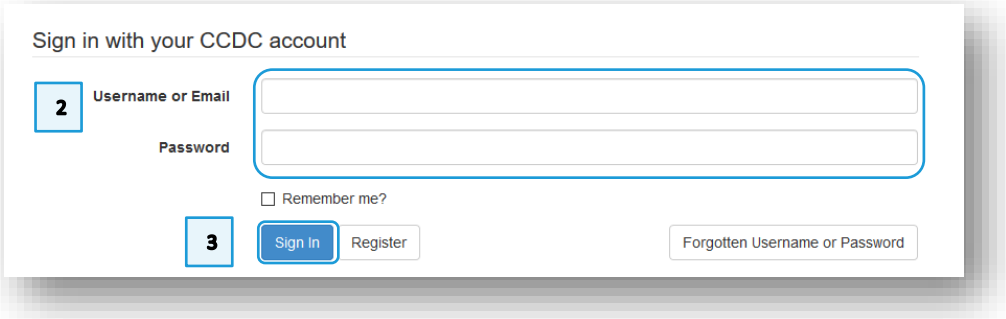


Signing in with your CCDC account

1. Go to the web deposition service at https://www.ccdc.cam.ac.uk/deposit

2. Fill in your *Username* or *Email*, and your *Password*.

3. Click on **Sign In**.



Personal details and CIF upload

4. The details you entered when setting up a CCDC account should appear automatically in the appropriate fields. If you did not sign in with a CCDC account, you will need to enter your details manually; the fields marked with '*' are mandatory.

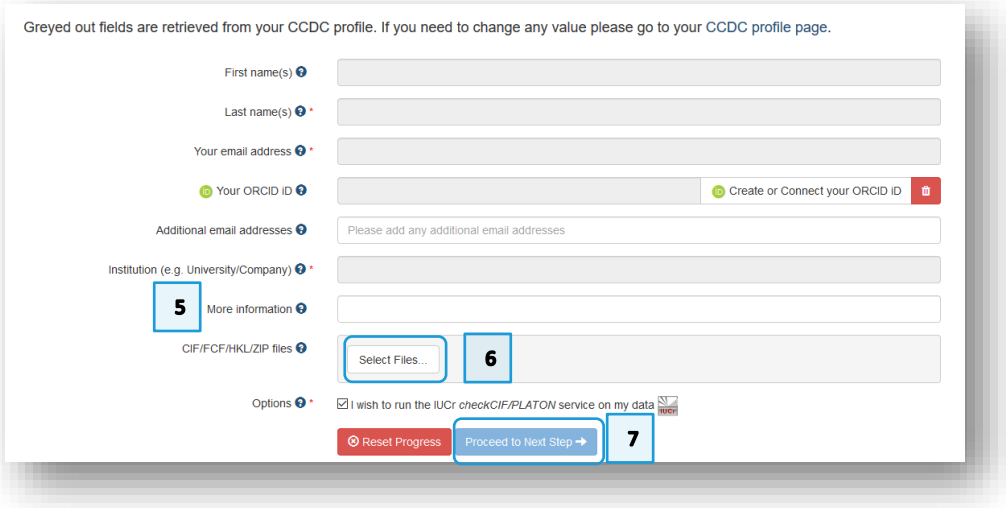
5. In the *More Information* box, type "This is a test".

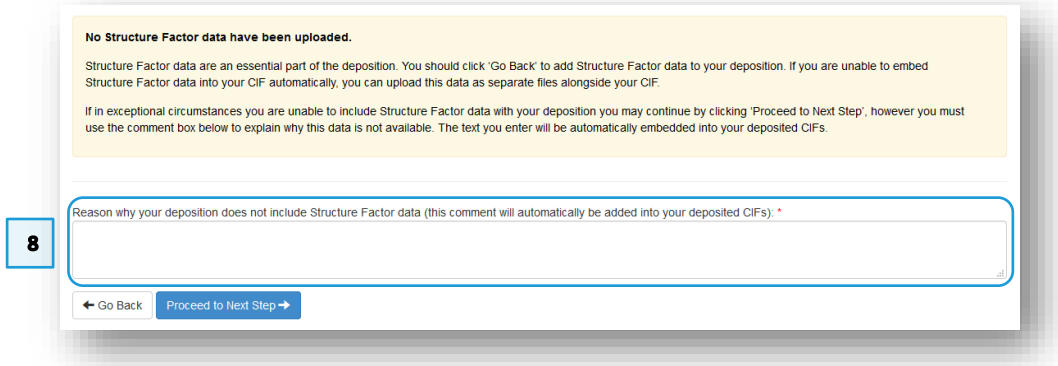
6. To add a CIF file to be uploaded, click on **Select Files…** and select "example_1.cif" and click **Open**. If the file is not in this folder, navigate to the appropriate folder.

7. In order to run the IUCr checkCIF program on your CIF file to check for syntax and other errors, ensure the box is ticked for the option "I wish to run the IUCr checkCIF/PLATON service on my data".

8. Click **Proceed to Next Step**.

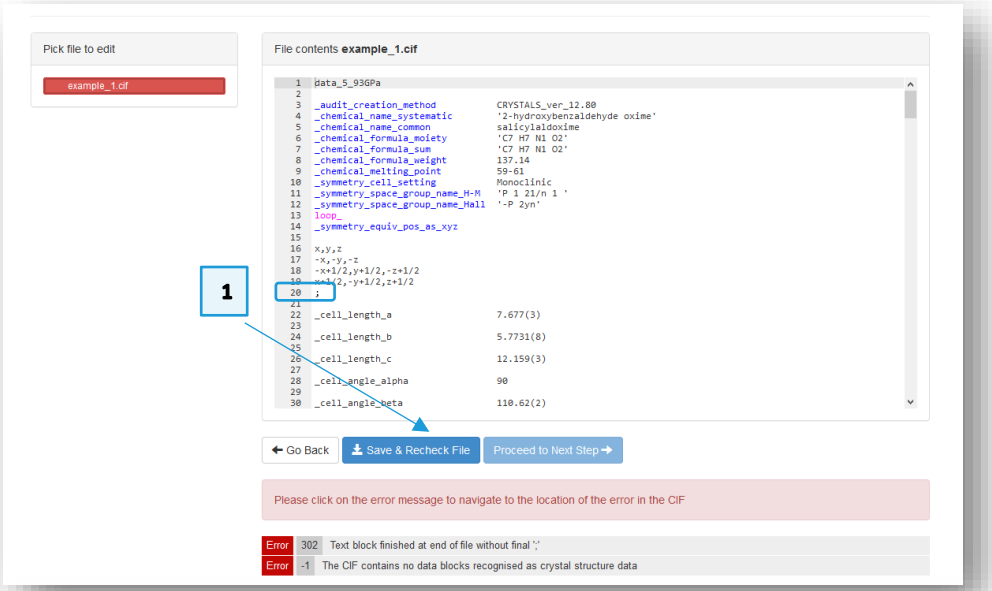
9. A warning message should appear to advise you that *No Structure Factor data have been uploaded*. It is important to include structure factor data in the deposition if available. In this example, however, there are no structure factors included; in the text box enter "Not available" and click **Proceed to Next Step**. The reason provided for the absence of structure factors will be included in the deposited CIF.





Syntax checking

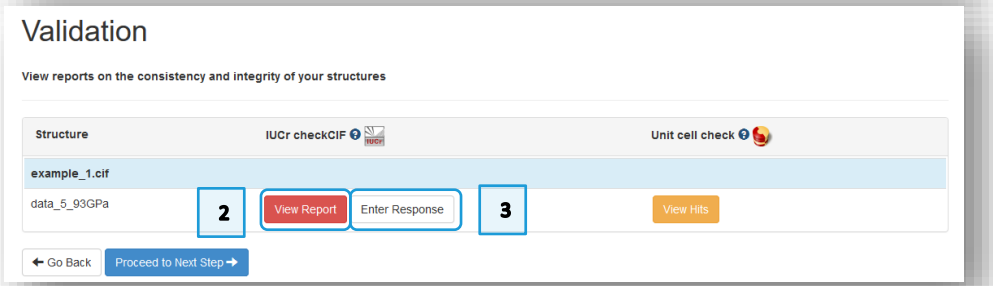
1. You will see a warning in red at the top of the page indicating there are syntax errors with your CIF file which need to be corrected before CheckCIF can be run. Descriptions of the errors are shown at the bottom of the page. Here you can see there is an extra semi-colon in the file. The CIF file display is colour-coded. You will notice that the colour coding changes for the unit cell values. Directly above this section, on line 20, there is a semi-colon that is out of place. Delete the semicolon on line 20 and click **Save & Recheck File**. Once you delete the semi-colon, you see the colour-coding re-appears (green). This should result in no syntax errors in the file and you can click **Proceed to Next Step**.



Validation and CheckCIF reports

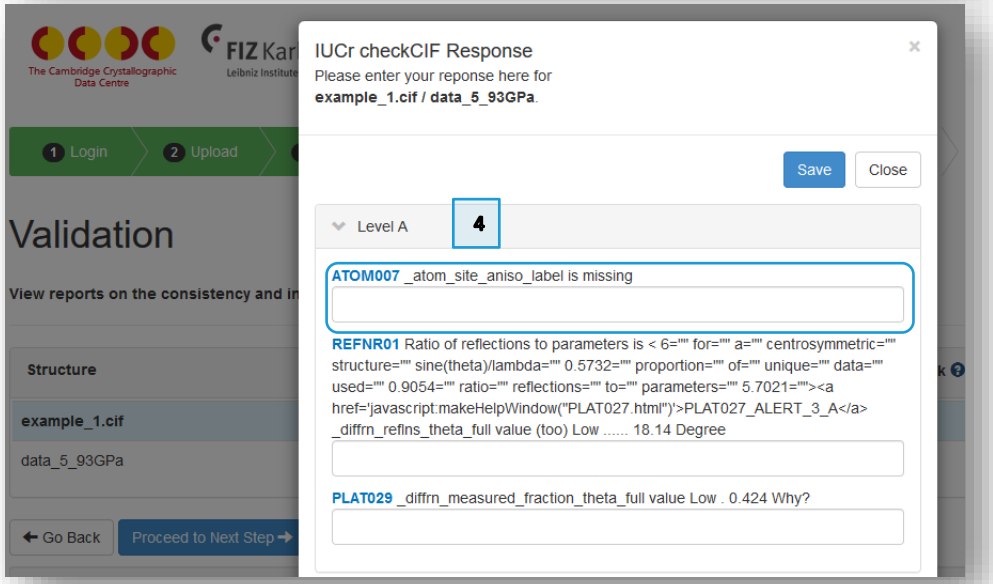
2. The IUCr checkCIF/PLATON service should run and you should be able to click **View Report** to see a report on the consistency and integrity of the structure.

3. Any responses you may wish to provide to the Level A, B or C alerts found by the checkCIF report can be provided by clicking **Enter Response on the main page**. These responses will be added to the deposited CIF and may also be downloaded along with the checkCIF report at the end of the deposition process. The alert titles are hyperlinked to the IUCr website and will give explanations about the nature of the error and possible solutions.



4. For this example, we will address the first of the A-level alerts. In practice you should first try to resolve the alerts by fixing the underlying problems with the structure refinement and upload a revised CIF file. If it is not possible to fix the issues, then enter a response to be included in the deposited CIF. For the purposes of this workshop, for the level A alert "ATOM007 _atom_site_aniso_label is missing", enter the response "This is a test" and click **Save**.

5. Click **Proceed to Next Step**.



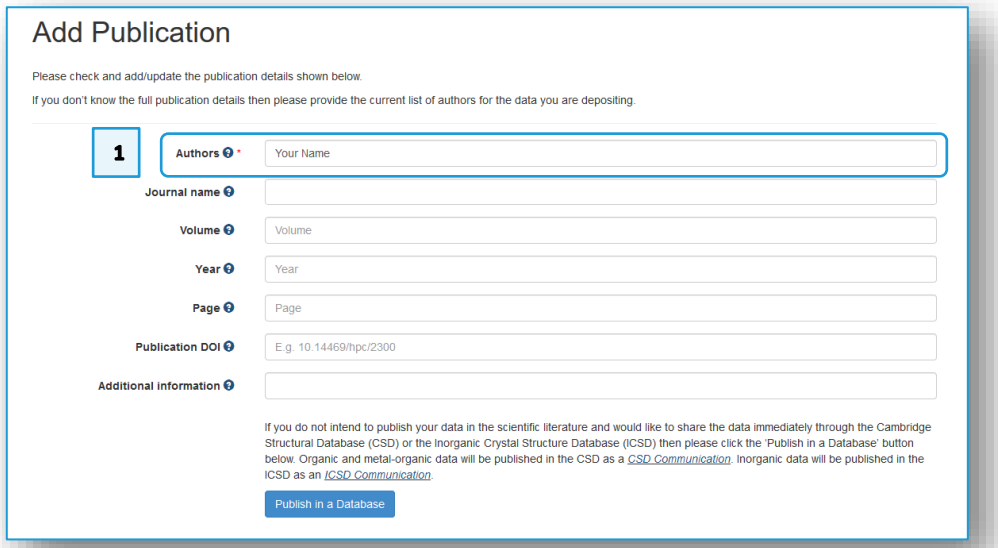
Adding publication details

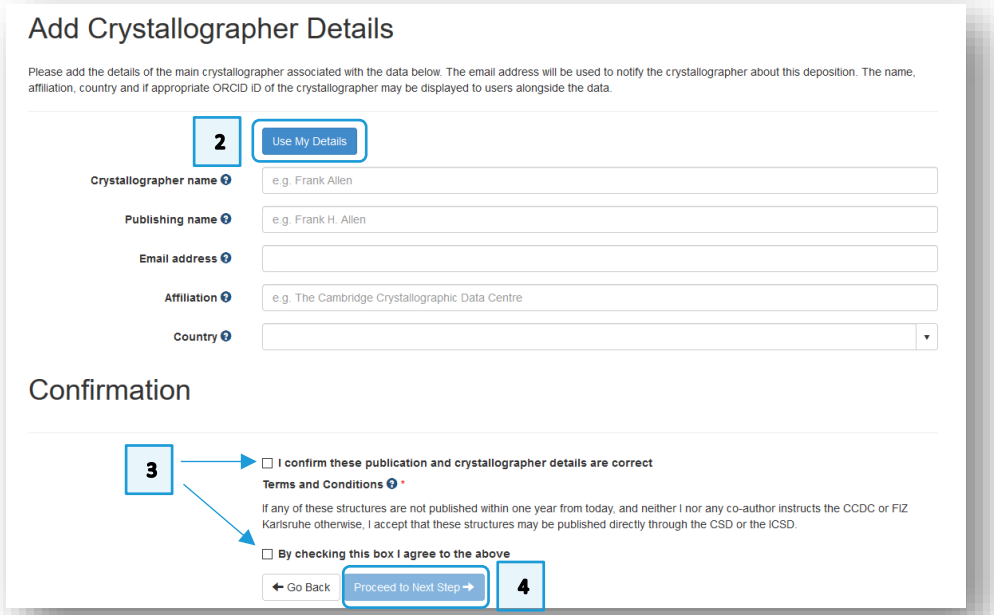
1. Your name should be automatically entered in the *Authors* field. Further publication details can also be entered on this page; namely *Journal name*, *volume*, *year*, *page* and *DOI* if applicable, as well as any *additional information* you may wish to include. For this example, change the *Authors* field to "P.A.Wood, R.S.Forgan, D.Henderson, S.Parsons, E.Pidcock, P.A.Tasker, J.E.Warren" and enter "Acta Crystallographica, Section B: Structural Science" in the *Journal name* field.

2. The crystallographer's details can also be entered in the *Add Crystallographer Details* section. If the crystallographer is not included in the list of authors for a publication, their details can be included here as a way for their contribution to be recognised when the data are available in the database. If you are the crystallographer, click the **Use My Details** button to automatically fill in the details from your profile.

3. Tick the two boxes in the *Confirmation* section to confirm the details are correct and that you accept the Terms and Conditions.

4. Click **Proceed to Next Step**.





Enhancing your data

The Enhance Data page allows you to preview how the structure(s) to be deposited will look as a 2D chemical diagram and as viewed in 3D, as well as add extra information to the CIF file prior to deposition. The data fields on the right of the page can be edited and enhanced, the changes saved, and the modifications to the CIF can be seen in the pane on the left.

1. From the *Crystallisation method* drop-down menu, select “Re-crystallisation from solvent”.

2. Click **Save Changes**.

3. Click **Proceed to Next Step**.

Reviewing and submitting your data

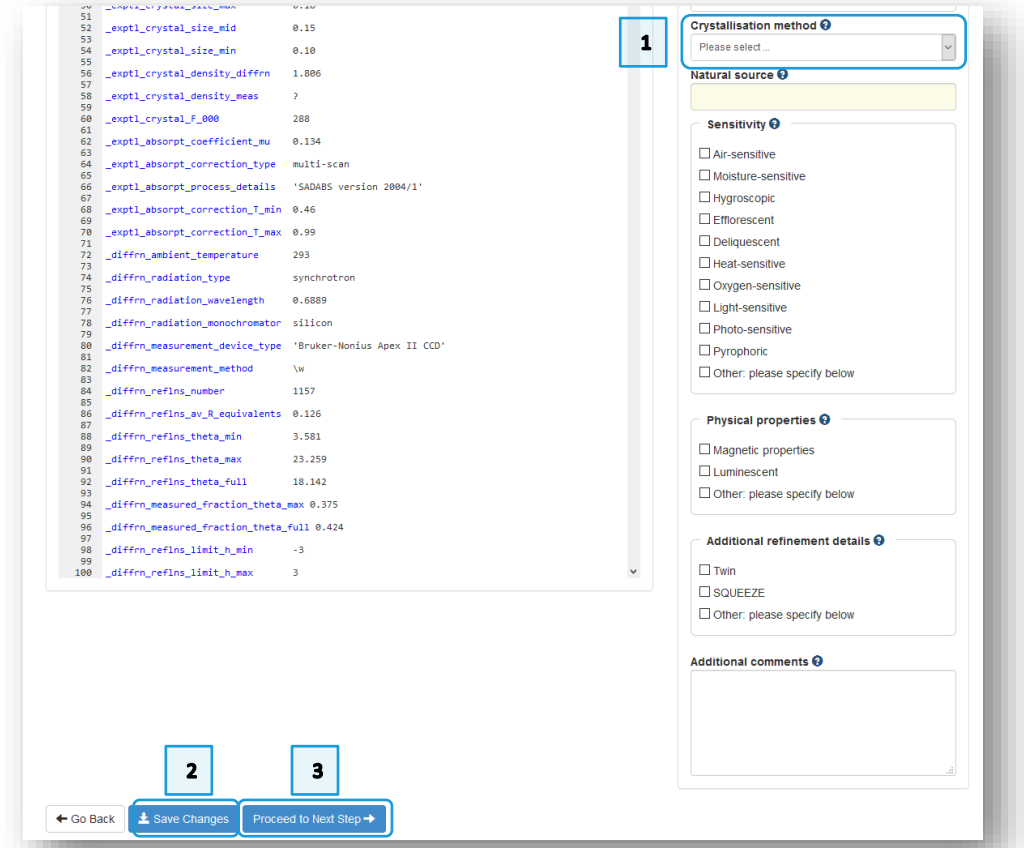
A final check on the data before deposition…

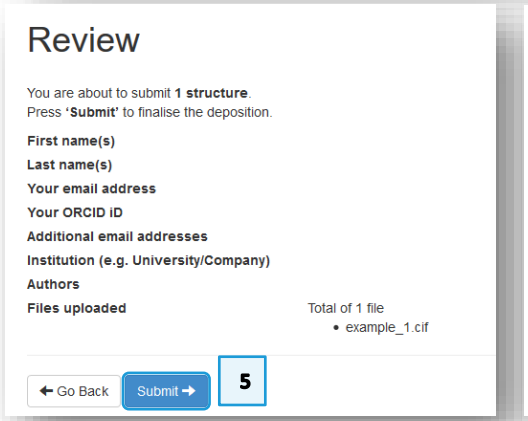
4. Check the details on the Review page, where you can click **Go Back** if you want to make any changes.

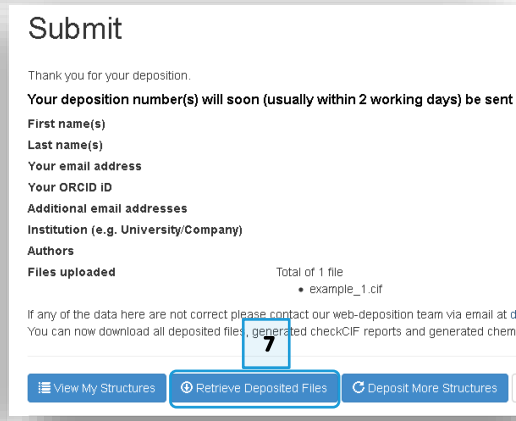
5. Click **Submit**.

6. A message should appear to confirm your file has been deposited and you will receive deposition numbers by email. The buttons at the bottom of the page then allow you to either start the process again to deposit more CIF files, view your structures in the *My Structures* section of your profile, or download a copy of the data as deposited.

7. Click **Retrieve Deposited Files**; this will allow you to download a zip file containing the deposited CIF, a html-format checkCIF report generated during the deposition process, and the automatically generated 2D diagram as a .png and .mol file.







Conclusion

In conclusion, you have learned how to deposit a CIF file using our online deposition service, correcting CIF syntax, generating a checkCIF report and enhancing the data in the deposited CIF file in the process.

Further exercises

- Click on **Deposit More Structures**. Repeat the exercise using example_1.cif up until you reach the *Validation* page. Click **View Hits** to examine the results of the Unit cell check. The results should include the example structure itself, SALOXM09, as well as a structure from the ICSD.

- Repeat the worked example, but instead deposit example_2.cif.