

CCDC

Structure Deposition Workshop (DEP-001)

Mar 2023

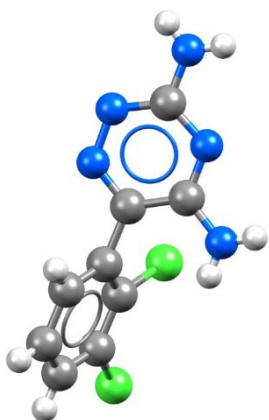


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Introduction

Structure deposition to the CCDC can be conducted through our CIF deposition and validation service. The web services enable you to submit CIF and associated structure factor files to the joint CCDC and FIZ Karlsruhe deposition service. During the deposition process, you can correct syntax errors, check the integrity and novelty of your data, and add metadata. You can also generate checkCIF reports and 2D chemical diagrams that can be downloaded at the end of the deposition process.

Learning Outcomes

This tutorial will guide you through the use of the CIF deposition and validation process. At the end of this tutorial, you will be able to:

- Deposit CIFs.
- Generate validation and checkCIF reports.
- Enhance your crystallographic data.

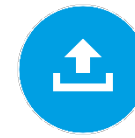
It will take approximately **25 minutes** to complete deposition of the first example file. If you decide to complete the further exercises, the total workshop time will be approximately **40 minutes**. The words in *Blue Italic* in the text are reported in the [Glossary](#) at the end of this handout.

Pre-required Skills

There are no pre-required skills for this workshop.

Materials

In this workshop, 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 our website. You will need a CCDC account to download the files. The instructions to create an account and to download the materials are part of the workshop.



CCDC

FIZ Karlsruhe

Leibniz Institute for Information Infrastructure

Register

Sign In

1 Login

2 Upload

3 Check Syntax

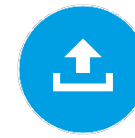
4 Validation

5 Add Publication

6 Enhance Data

7 Review

8 Submit



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 and to 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.

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 need to create an account, click on **Register** at the top right of the page. Alternatively, if you already have an account, you can click the link to continue the deposition process and proceed to the section of the workshop 'Obtaining example CIF files'.
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.
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**.

Obtaining example CIF files

9. Open a web browser and navigate to <https://www.ccdc.cam.ac.uk/support-and-resources/downloads/>
10. A CCDC account is required for downloading the example files. On the downloads page, click on **Sign In**. Enter your login details and click Sign In to return to the Downloads page.
11. Under *CSD-Community (Free Software)*, click on **CSD Educational Collection** and click **Download** beside *Example CIF 1 for CSD Deposit with Syntax Error*.
12. Click **Agree & Download** to accept the agreement displayed and save the "example_1.cif" file.
13. Repeat **Steps 11** and **12** 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.

The screenshot shows the 'Redeem Invitation' tab selected. Below the navigation bar, the heading 'Sign up with an invitation code' is displayed. A form contains an 'Invitation Code' input field (labeled 6), a reCAPTCHA box with the text 'I'm not a robot' (labeled 7), and a 'Register' button (labeled 8).

The screenshot shows the CCDC website header with navigation links. The 'Sign In' button is highlighted (labeled 10). Below the header, the heading 'Sign in with your CCDC account' is shown. A form contains 'Username or Email' and 'Password' input fields (labeled 10), a 'Remember me?' checkbox, and 'Sign In' and 'Register' buttons. A 'Forgotten Username or Password' link is also present.

The screenshot shows the 'CSD-Community (Free Software)' page. A table lists various collections. The 'CSD Educational Collection' is highlighted (labeled 11). The table has columns for the collection name and 'Details' and 'Download' links.

Collection Name	Details	Download
Example CIF 1 for CSD Deposit with Syntax Error	Details	Download
Example CIF 2 for CSD Deposit without Syntax Error	Details	Download
CSD Educational Collection refcode list	Details	Download
CSD Educational Collection CIFs	Details	Download
CellCheckCSD		
CSD MOF Collection		
Mercury (incorporating enCIFer)		

Personal details and CIF upload

1. Go to the web deposition service at <https://www.ccdc.cam.ac.uk/deposit>
2. You should still be logged in but if you are not, click Sign in, fill in your Username or Email and Password and click on **Sign In**.
3. The details you entered when setting up a CCDC account should appear automatically in the appropriate fields. The fields marked with “*” are mandatory. You can also link your [ORCID iD](#) here if you have one. Hover your mouse on the “?” icon for more information on each field.
4. In the *More Information* section, you can enter any information here but for this workshop, type “This is a test”.
5. 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.
6. 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”.
7. Click **Proceed to Next Step**.
8. 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 (read [here](#) why). The CCDC accepts structure factor data in *.fcf* or *.hkl* format. In this example, however, there are no structure factors included. In the text box enter “Not available – This is a test” and click **Proceed to Next Step**. The reason provided for the absence of structure factors will be included in the deposited CIF.

1 Login 2 Upload 3 Check Syntax 4 Validation 5 Add Publication 6 Enhance Data 7 Review 8 Submit

Greyed out fields are retrieved from your CCDC profile. If you need to change any value please go to your CCDC profile page.

First name(s) ? Test

Last name(s) ? Account

Your email address ?

3 Your ORCID ID ? Create or Connect your ORCID ID

Additional email addresses ? Please add any additional email addresses

Institution (e.g. University/Company) ? CCDC

4 More information ? This is a test

CIF/HKL/RES/FCF/Word/ZIP files ? 5 Select Files...

Options ? ☒ I wish to run the IUCr checkCIF/PLATON service on my data

Reset Progress Proceed to Next Step 7

No Structure Factor data have been uploaded.

Structure Factor data are an essential part of the deposition. You should click 'Go Back' to add Structure Factor data to your deposition. If you are unable to embed Structure Factor data into your CIF automatically, you can upload this data as separate files alongside your CIF.

If in exceptional circumstances you are unable to include Structure Factor data with your deposition you may continue by clicking 'Proceed to Next Step', however you must use the comment box below to explain why this data is not available. The text you enter will be automatically embedded into your deposited CIFs.

8 Reason why your deposition does not include Structure Factor data (this comment will automatically be added into your deposited CIFs): *

Not available

Go Back Proceed to Next Step

Syntax checking

The CIF format has a specific structure, or syntax, that needs to be followed to allow the file to be read by crystallographic programs. This stage in the deposition process checks the CIFs for any potential errors.

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. In this case there is an extra semi-colon in the file. This is indicated by the error **'Text block finished at end of file without final ';'.** Semi colons are used in CIFs to enclose longer data responses that span multiple lines in the CIF. The CIF file display is colour-coded, which can help you find the location of the error.
2. Near the top of the CIF 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 reappears (blue). This should result in no syntax errors in the file and you can click **Proceed to Next Step**.

The screenshot displays the 'Check Syntax' step of a deposition process. At the top, a progress bar shows steps 1 through 8: Login, Upload, Check Syntax (highlighted), Validation, Add Publication, Enhance Data, Review, and Submit. Below the progress bar, the title 'Check Syntax' is followed by a blue box containing the number '1'. A red banner contains the following text: 'The files highlighted in red in the left-hand column contain errors that need fixing before proceeding. Please click on any red file names in the left-hand column, make the appropriate edits and then click the 'Save & Recheck File' button before proceeding to the next step. For more information on how to fix errors please see our [correcting CIFs](#) page.'

Below the banner, there is a section titled 'Pick file to edit' with a red-bordered box. To the right, a window titled 'File contents example_1.cif' displays the content of a CIF file. The file content is color-coded: blue for general data, red for unit cell parameters, and green for symmetry information. Line 20 is highlighted in red and contains a semi-colon (;). A blue box with the number '2' and an arrow points to this semi-colon. Below the file content, there are three buttons: 'Go Back', 'Save & Recheck File' (highlighted), and 'Proceed to Next Step'.

At the bottom, a red banner contains the text: 'Please click on the error message to navigate to the location of the error in the CIF'. Below this, a table lists the errors:

Error	302	'Text block finished at end of file without final ';'.
Error	-1	The CIF contains no data blocks recognised as crystal structure data

Validation and CheckCIF reports

IUCr checkCIF/PLATON is a service which allows CIF files to be checked for problems. The responses are reported with a Level A, B, C or G (from most serious to least) and a type depending on what kind of alert it is. You can find more information on correcting CIFs [here](#) and other resources linked from the page.

1. 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.
2. 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.
3. 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**.
4. Click **Proceed to Next Step**.

1 Login 2 Upload 3 Check Syntax 4 Validation 5 Add Publication 6 Enhance Data 7 Review 8 Submit

Validation

View reports on the consistency and integrity of your structures

Structure	IUCr checkCIF	Unit cell check
example_1.cif		
data_5_93GPa	1 View Report Enter Response 2	View Hits

Go Back Proceed to Next Step

CCDC FIZ Karlsruhe Leibniz Institute for Crystallography

Validation

View reports on the consistency and integrity of your structures

Structure

example_1.cif

data_5_93GPa

Go Back Proceed to Next Step

IUCr checkCIF Response

Please enter your response here for example_1.cif / data_5_93GPa.

Save Close

Level A

ATOM007 _atom_site_aniso_label is missing

This is a test

PLAT027 _diffn_reflns_theta_full value (too) Low 18.14 Degree

PLAT029 _diffn_measured_fraction_theta_full value Low . 0.424 Why?

Level B

Level C

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.

The author's names should be added in the same order as on the publication. Each name should be separated by a comma and space, without any additional characters or salutation. You can use initials (no spacing between them) or expand the first name; if you are using initials, then you do not need spaces between them.

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 [1983-2012]" in the *Journal name* field.

2. The crystallographer's details are required and should 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. For this example, click the Use My Details button. If nothing is filled in, click Use Different Details and enter your information.
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**.

1 Add Publication

Please check and add/update the publication details shown below.

If you don't know the full publication details then please provide the current list of authors for the data you are depositing.

Authors * Test Account

Journal name

Volume Volume

Year Year

Page Page

Publication DOI E.g. 10.14469/hpc/2300

Additional information

If you do not intend to publish your data in the scientific literature and would like to share the data immediately through the Cambridge Structural Database (CSD) or the Inorganic Crystal Structure Database (ICSD) then please click the 'Publish in a Database' button below. Organic and metal-organic data will be published in the CSD as a *CSD Communication*. Inorganic data will be published in the ICSD as an *ICSD Communication*.

Publish in a Database

Add Crystallographer Details

Please add the details of the main crystallographer associated with the data below. The email address will be used to notify the crystallographer about this deposition. The name, affiliation, country and if appropriate ORCID ID of the crystallographer may be displayed to users alongside the data.

2 Use My Details

Crystallographer name e.g. Frank Allen

Publishing name e.g. Frank H. Allen

Email address

Affiliation e.g. The Cambridge Crystallographic Data Centre

Country

Confirmation

3

Terms and Conditions

By depositing this data you certify that your contribution is your original work; that all authors concur with and are aware of the submission; and that all workers involved in the study are listed as authors and given proper credit.

If any of these structures are not published within one year from today, and neither I nor any co-author instructs the CCDC or FIZ Karlsruhe otherwise, I accept that these structures may be published directly through the CSD or the ICSD.

☐ I confirm these publication and crystallographer details are correct *

☐ By checking this box I agree to the above *

Go Back Proceed to Next Step **4**

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. Other information can be added to the structure, such as a DOI link to deposited raw diffraction data files. These are the files measured during experimental data collection. The CCDC does not currently store [raw data](#) files. However, if you have deposited your raw data files with another repository and have a DOI link for this then you can associate this DOI link with the relevant files you have deposited with CCDC. You can do this during the deposition process by adding the DOI at the 'Enhance Data' stage of the process, found under 'Associated DOIs'. We will leave this blank for this workshop.
2. From the *Crystallisation method* drop-down menu, select "Re-crystallisation from solvent".
3. Click **Save Changes**.
4. Click **Proceed to Next Step**.

data_5_93GPa

```
1 data_5_93GPa
2 # start Validation Reply Form
3 _vrf_ATOM007_5_93GPa
4 ;
5 PROBLEM: _atom_site_aniso_label is missing
6 RESPONSE: This is a test
```

1 Associated DOIs

Raw data DOI ?

2 Crystallisation method ?

Please select ...

Please select ...

Re-crystallisation from solvent

Sublimation

Vapour deposition

From the Melt

Other: please specify below

☐ Air-sensitive

☐ Moisture-sensitive

☐ Hygroscopic

☐ Efflorescent

☐ Deliquescent

☐ Heat-sensitive

```
50 _cell_measurement_theta_max 21
51
52 _cell_measurement_temperature 293
53
54 _exptl_crystal_description block
55
56 _exptl_crystal_colour colourless
57
58 _exptl_crystal_size_max 0.18
59
60 _exptl_crystal_size_mid 0.15
61
62 _exptl_crystal_size_min 0.10
63
64 _exptl_crystal_density_diffn 1.806
65
66 _exptl_crystal_density_meas ?
67
68 _exptl_crystal_f_000 288
69
70 _exptl_absorpt_coefficient_mu 0.134
71
```

120 _diffn_standards_interval_count ?
121
122 _diffn_standards_interval_time ?
123
124 _diffn_standards_decay_% ?
125
126 _reflns_number_total 296

3 4

Go Back Save Changes Proceed to Next Step →

Additional refinement details ?

☐ Twin

☐ SQUEEZE

☐ Other: please specify below

Additional comments ?

Reviewing and submitting your data

A final check on the data before deposition

1. Check the details on the Review page, where you can click **Go Back** if you want to make any changes.
2. Click **Submit**.
3. 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.
4. 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.

How to cite your own data in a publication

To reference your data in the corresponding publication, you should do so by reporting the [CCDC number](#) (the 6 or 7-digit number that would be assigned to the structure by CCDC after deposition).

Conclusion

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

Review

You are about to submit **1 structure**.
Press **Submit** to finalise the deposition.

First name(s) Test
Last name(s) Account
Your email address
Your ORCID ID
Additional email addresses
Institution (e.g. University/Company) CCDC
Authors P.A.Wood, R.S.Forgan, D.Henderson, S.Parsons, E.Pidcock, P.A.Tasker, J.E.Warren
Files uploaded Total of 1 file
• example_1.cif

Go Back Submit

Submit

Thank you for your deposition.

Your deposition number(s) will soon (usually within 2 working days) be sent to

First name(s) Test
Last name(s) Account
Your email address
Your ORCID ID
Additional email addresses
Institution (e.g. University/Company) CCDC
Authors P.A.Wood, R.S.Forgan, D.Henderson, S.Parsons, E.Pidcock, P.A.Tasker, J.E.Warren
Files uploaded Total of 1 file
• example_1.cif

If any of the data here are not correct please contact our web-deposition team via email at deposit@ccdc.cam.ac.uk
You can now download all deposited files, generated checkCIF reports and generated chemical diagrams by clicking the Retrieve Deposited Files button below.

View My Structures Retrieve Deposited Files Deposit More Structures Return to CCDC Homepage

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.

Summary

This workshop introduced the process of depositing your structure to the CSD. You should now be familiar with:

- Depositing CIF files.
- Generating validation and checkCIF reports.
- Enhancing your crystallographic data.

Next Steps

Other CSD-Community self-guided workshops can be found [here](https://www.ccdc.cam.ac.uk/community/training-and-learning/workshop-materials/csd-community-workshops/) (<https://www.ccdc.cam.ac.uk/community/training-and-learning/workshop-materials/csd-community-workshops/>), including an introduction to *CSD Communications* and how to publish them (available in English and Chinese).

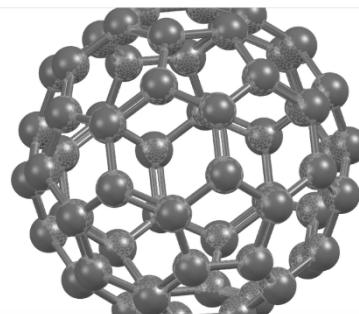
For more information, visit our website:

<https://www.ccdc.cam.ac.uk/community/access-deposit-structures/deposit-a-structure/>.

Feedback

We hope this workshop improved your understanding of the Deposition process and you found it useful for your work. As we aim to continuously improve our training materials, we would love to get your feedback. Click on [this link](#) to a survey, it will take less than 5 minutes to complete. The feedback is anonymous. You will be asked to insert the workshop code, which for this self-guided workshop is DEP-001. Thank you!

CSD-Community Workshops



These self-guided workshops are tutorials intended to guide you through the use of various tools included with the free version of Mercury as well as our online Access and Deposition services.

Tell us what you think!

We hope you found these workshops helpful. As we aim to continuously improve our training materials, we would like to hear your feedback. You can do so by [filling out this survey](#). When asked, insert the workshop code that you find in the workshop description in this page. It will only take 5 minutes and your feedback is anonymous. Thank you!

Structure Visualizations



This is a self-guided workshop demonstrating the use of Mercury to create quality graphics of your structures.

Prerequisites: None, but see note below

Workshop code: MER-001

Note: This handout is also part of the CSDU module Visualization 101 – Visualizing structural chemistry data with Mercury. Visit the module webpage for more demos, tricks and tips! Upon completion of the module, you can also earn a completion certificate.

[Download material](#)

Measuring and Calculating Objects in Mercury



This is a self-guided workshop on how to measure distances, angles and torsions and how to calculate centroids and planes in Mercury.

Prerequisites: Basic Mercury knowledge (see MER-001 or try the CSDU module Visualization 101 – Visualizing structural chemistry data with Mercury)

Workshop code: MER-005

[Download material](#)

Access Structures



This is a self-guided workshop demonstrating the use of our free online Access Structures services for conducting searches, viewing results in the 3D viewer, exploring links to other databases and downloading structures.

Prerequisites: None

Workshop code: WCSD-001

[Download material](#)

CCDC number

checkCIF

CIF

DOI

ORCID iD

Raw data

Raw data refers to the data collected during a crystallographic experiment by measuring the diffraction pattern of a crystal using a diffractometer. They may also be called diffraction images.

Structure factors

Structure factors are created from experimental crystallographic data during the structural solution process. The information can be used to describe the distribution of electron density in the structure. Currently there are two types of information that CCDC accepts as 'structure factor' information, these are the structure factors themselves (often found in a .fcf file) and the reflection intensities (.hkl). They can also be appended to the CIF file, as is the default in many crystallographic programs. See more on our website at <https://www.ccdc.cam.ac.uk/Community/depositastructure/cif-deposition-guidelines/structure-factor/>.

