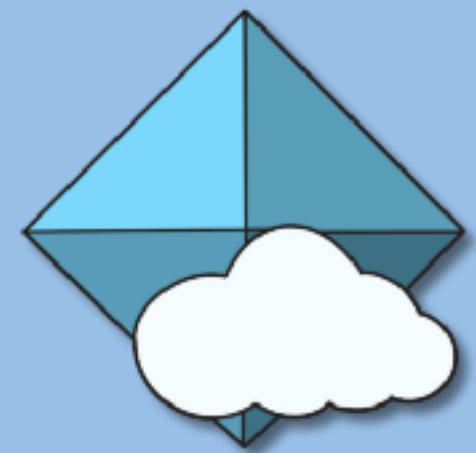




cloud ccp4 ac uk

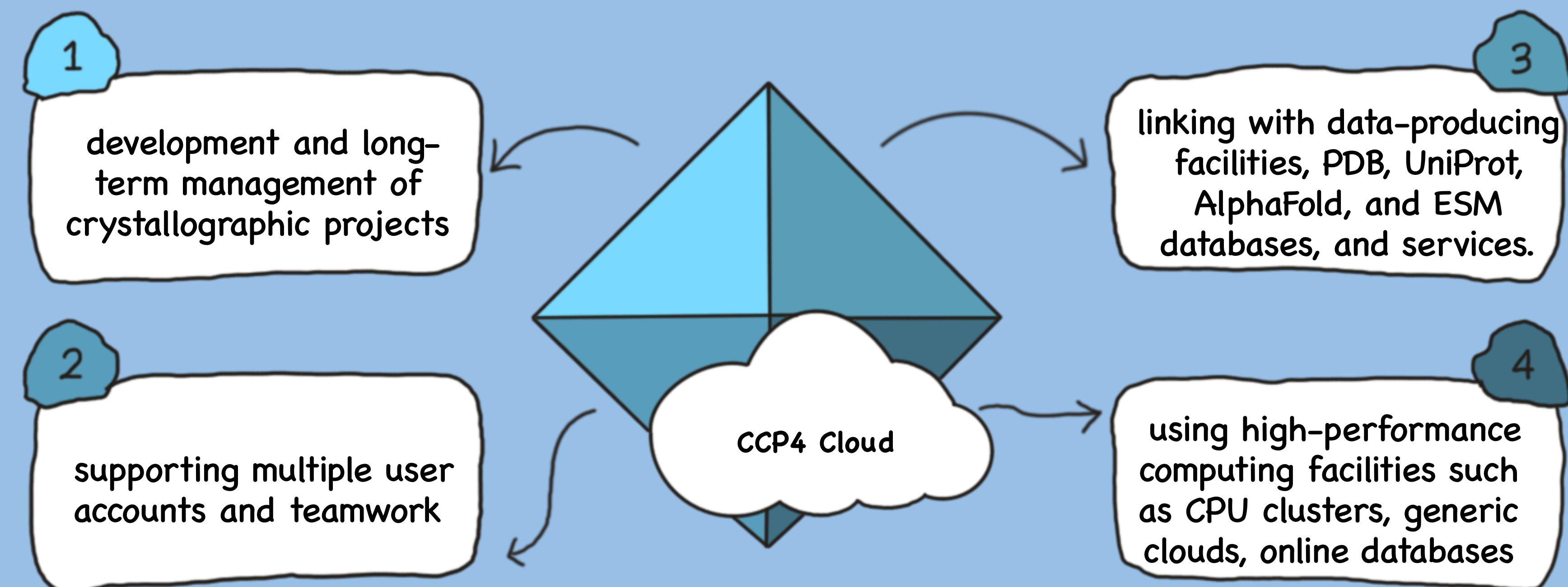


# CCP4 Cloud

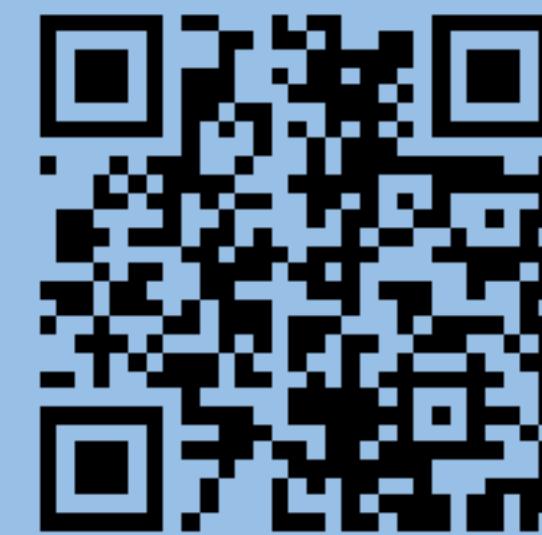
**Maria Fando**

[maria.fando@stfc.ac.uk](mailto:maria.fando@stfc.ac.uk)

## What is Cloud?



# Roadmap



## Data import

- Import local files
- Import Sequence(s) by Copy-Paste
- Import from PDB/AFDB
- Import data from Cloud
- Import & Replace
- Continue projects started elsewhere

ASU

01

02

03

04

04

06

07

08

09

## Image processing

- Auto-processing with Xia-2
- Image processing with DIALS/DUI
- Image processing with XDS GUI
- Image processing with iMosflm
- Data Reduction with Aimless

## EP

- Auto-EP with Crank-2
- Heavy-Atom Substructure with SHELX
- EP with Phaser

## Model Building

- Buccaneer
- CCP4Build
- Arp/wArp
- Modelcraft
- Nautilus
- Coot

## Ligands

- Prepare ligand structures with AceDrg
- Auto-fit ligands with Coot
- Auto-fit waters with Coot

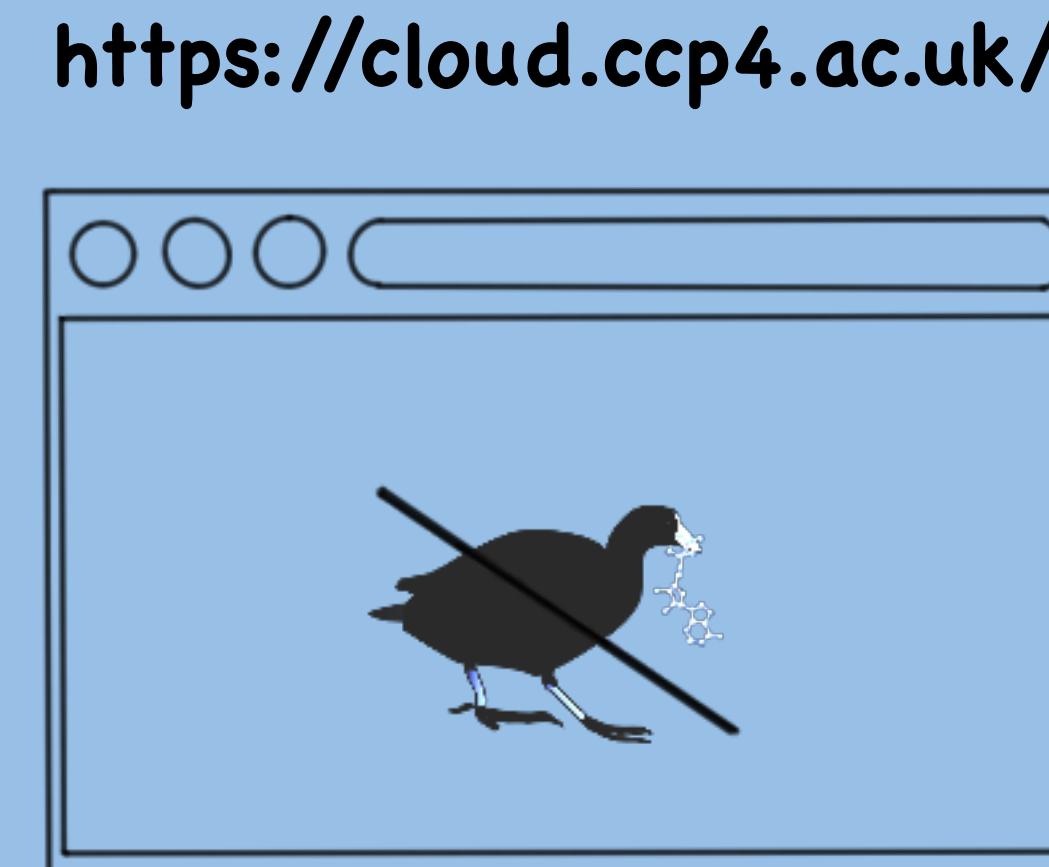
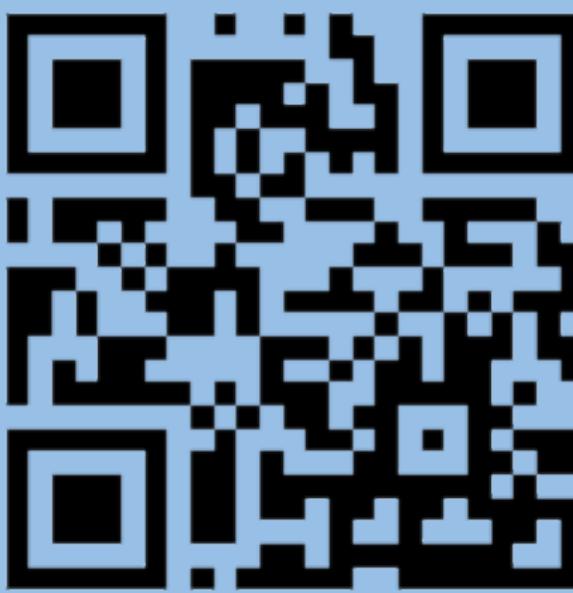
## Refinement

- Refmac
- Dimple
- Buster
- Lorestr
- Comb
- Pairef
- PDB-REDO

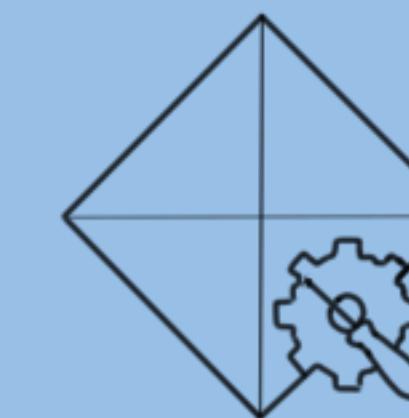
## Validation and deposition

- Zanuda
- Validation of carbohydrate structures with Privateer
- PISA
- Deposition

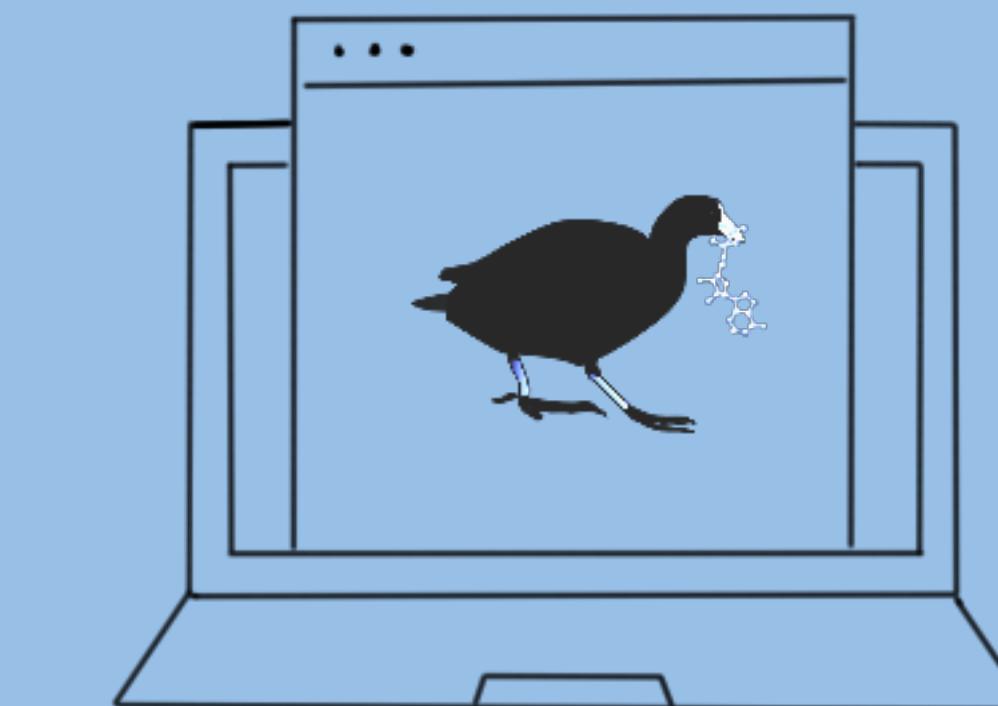
## Operation modes



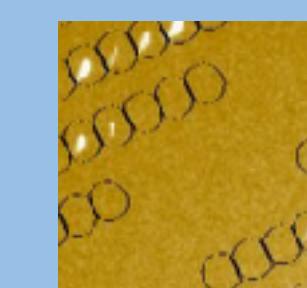
<https://cloud ccp4.ac.uk/>



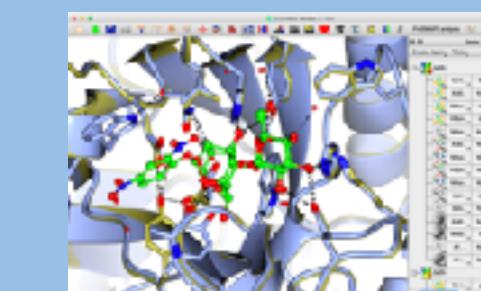
CCP4 Software Suite



DIALS  
DIALS GUI  
(DUI)

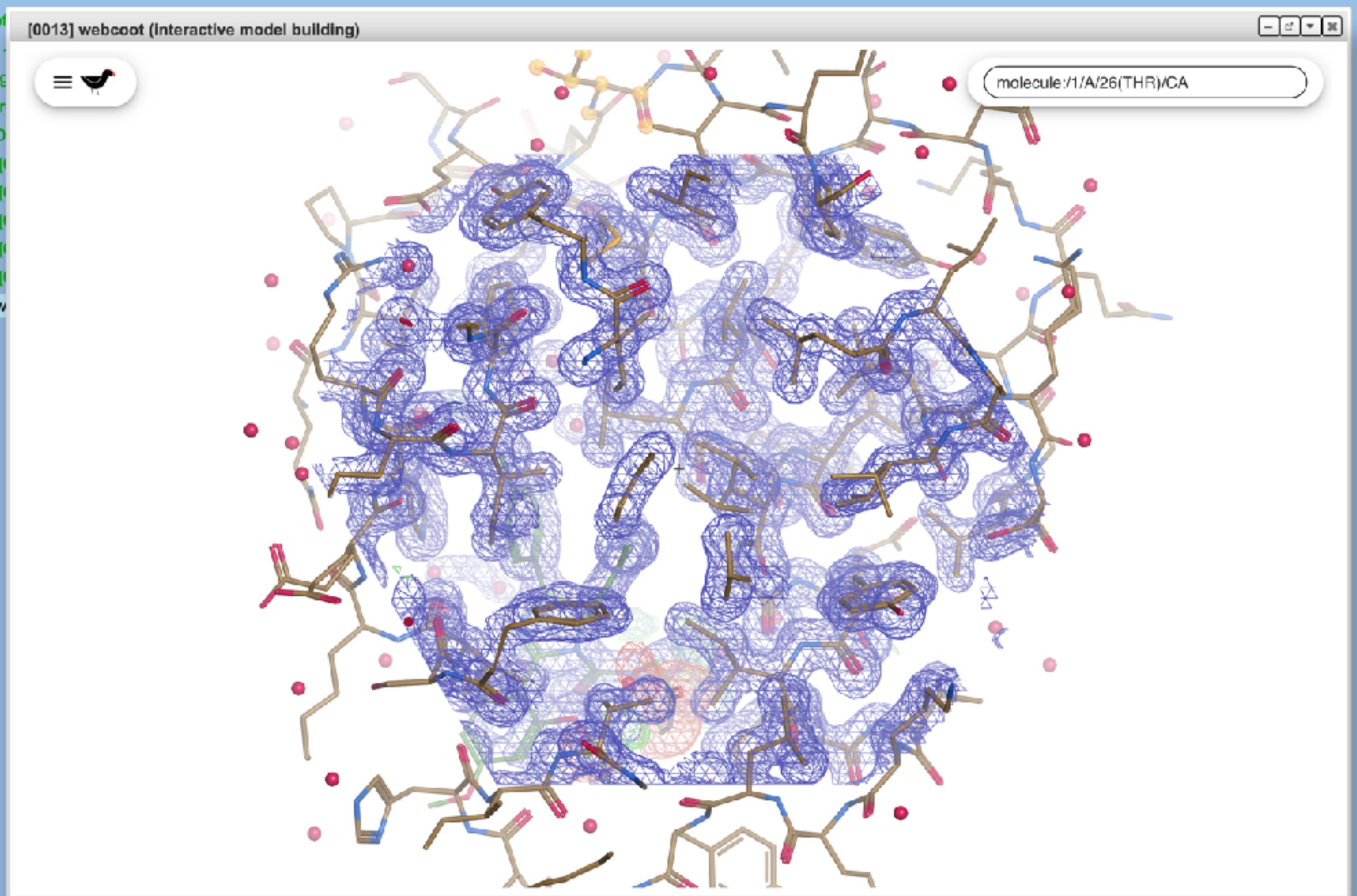


XDS GUI



CCP4 mg

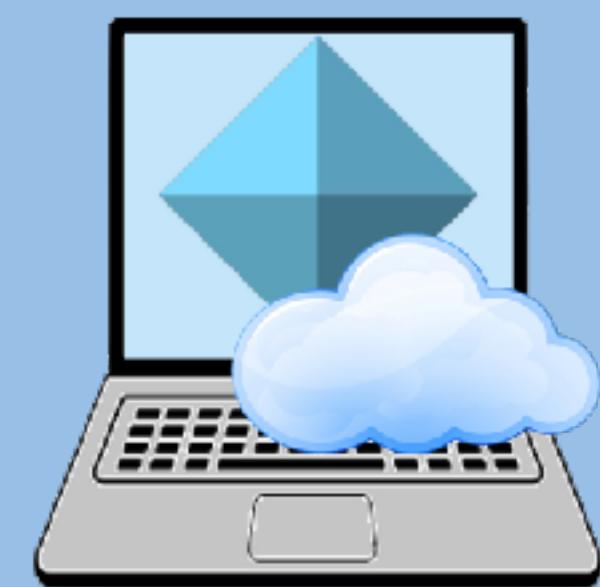
(devel):[dpIWFTest]  
DPL auto-DPL:[0001] Dimple Ref  
D auto-DPL:[0002] dimple  
auto-DPL:[0003] fit lig  
auto-DPL:[0004] r  
auto-DPL:[0005] r  
auto-DPL:[0006] r  
auto-DPL:[0007] r  
auto-DPL:[0008] r  
auto-DPL:[0009] r  
auto-DPL:[0010] r  
auto-DPL:[0011] r  
auto-DPL:[0012] r  
auto-DPL:[0013] r  
[0013] w



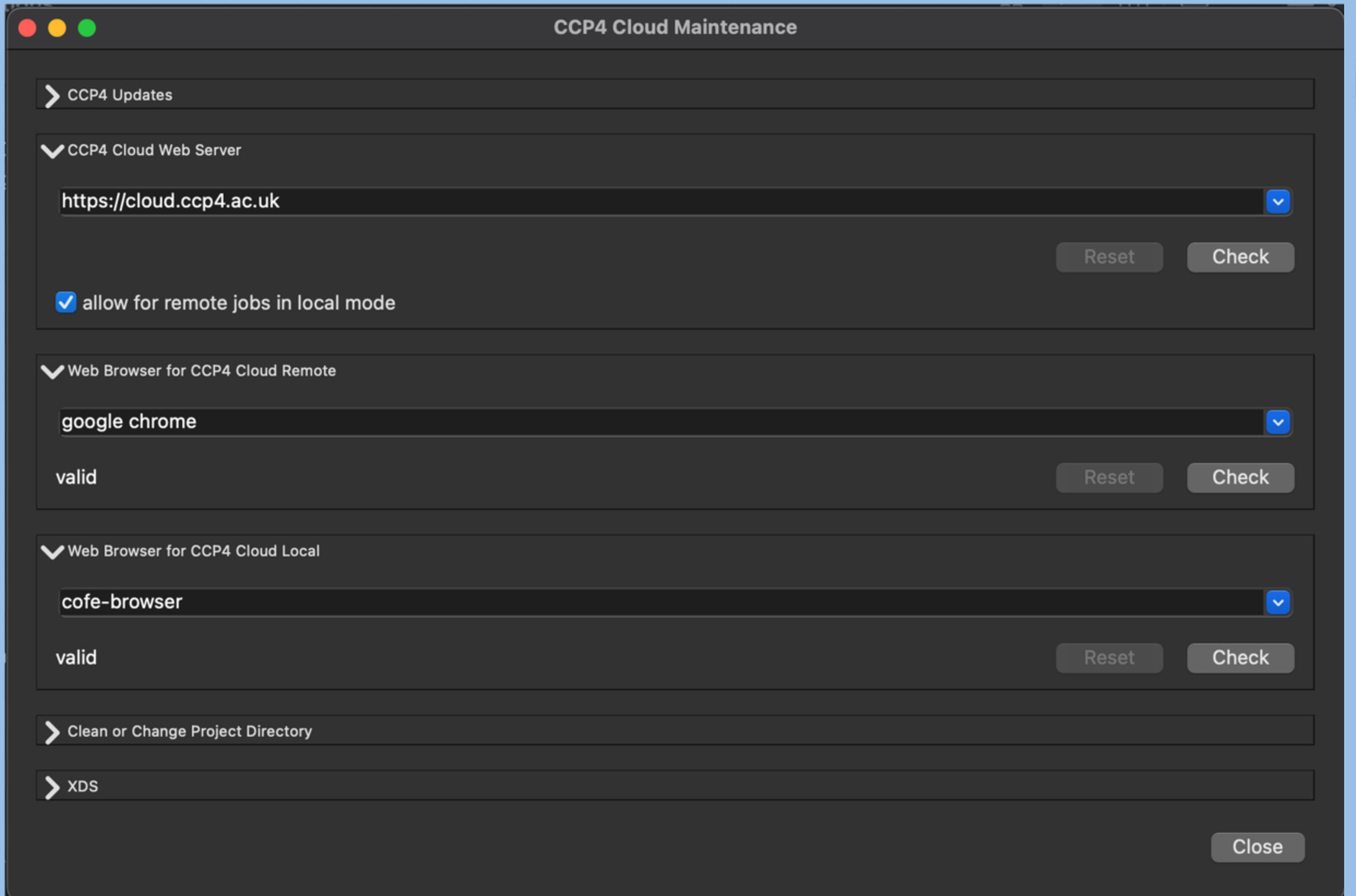
Web COOT



Installation



```
$ ccp4cloud-config
```



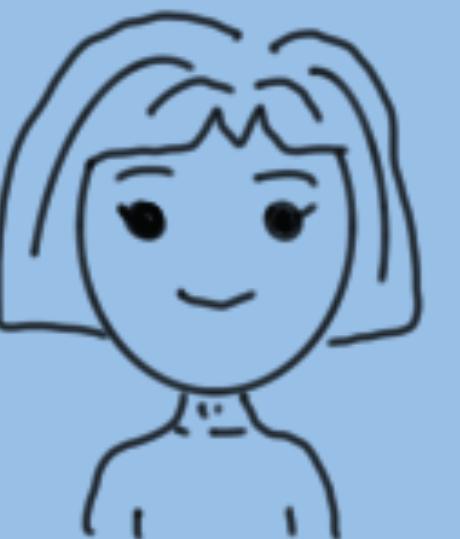
## Configuration utilities



CCP4 Cloud Configuration

```
$ ccp4cloud-local
```

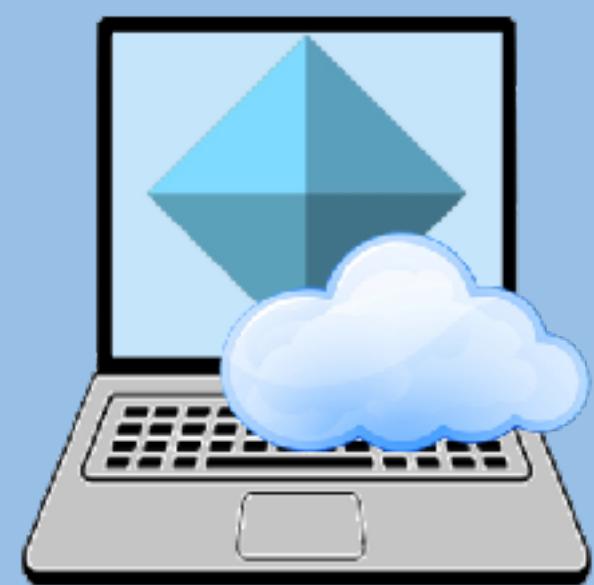
Local mode



User



User's machine



CCP 4 Cloud Local

\$ ccp4cloud-local



**Collaborative Computational Project No.4**  
Science and Technology Facilities Council UK  
Rutherford Appleton Laboratory  
Didcot, Oxon OX1 0FA, United Kingdom  
<https://www ccp4.ac.uk>

## CCP4 Cloud

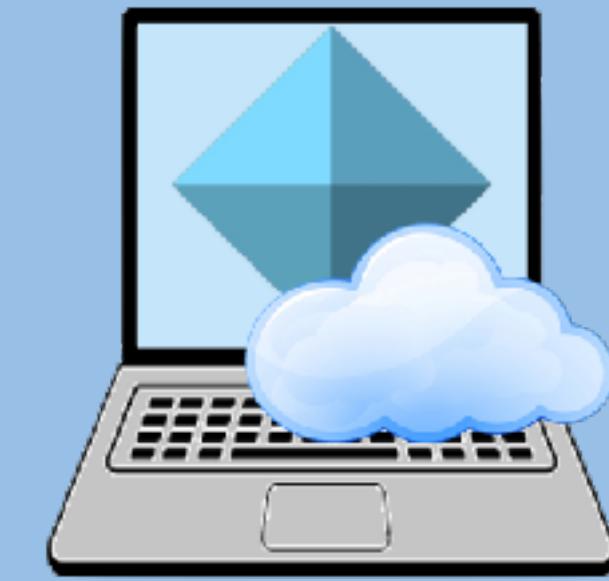
### Local Setup

- Projects and data stored on your machine:  
`/Users/maria/ccp4cloud_data/desktop/cofe-projects`
- Projects and data **not** synced with CCP4 Cloud server(s)  
(use project export/import for manual syncing)
- Jobs run on your machine  
(except for cases involving third-party web services and jobs designated for remote execution)
- Remote job execution server:  
<https://cloud ccp4.ac.uk>
- You have 112GB free disk space & 10 cores @ 2.4 GHz

[!\[\]\(b16059d7582cfbd44776b82254580985\_img.jpg\) Go to your projects](#)

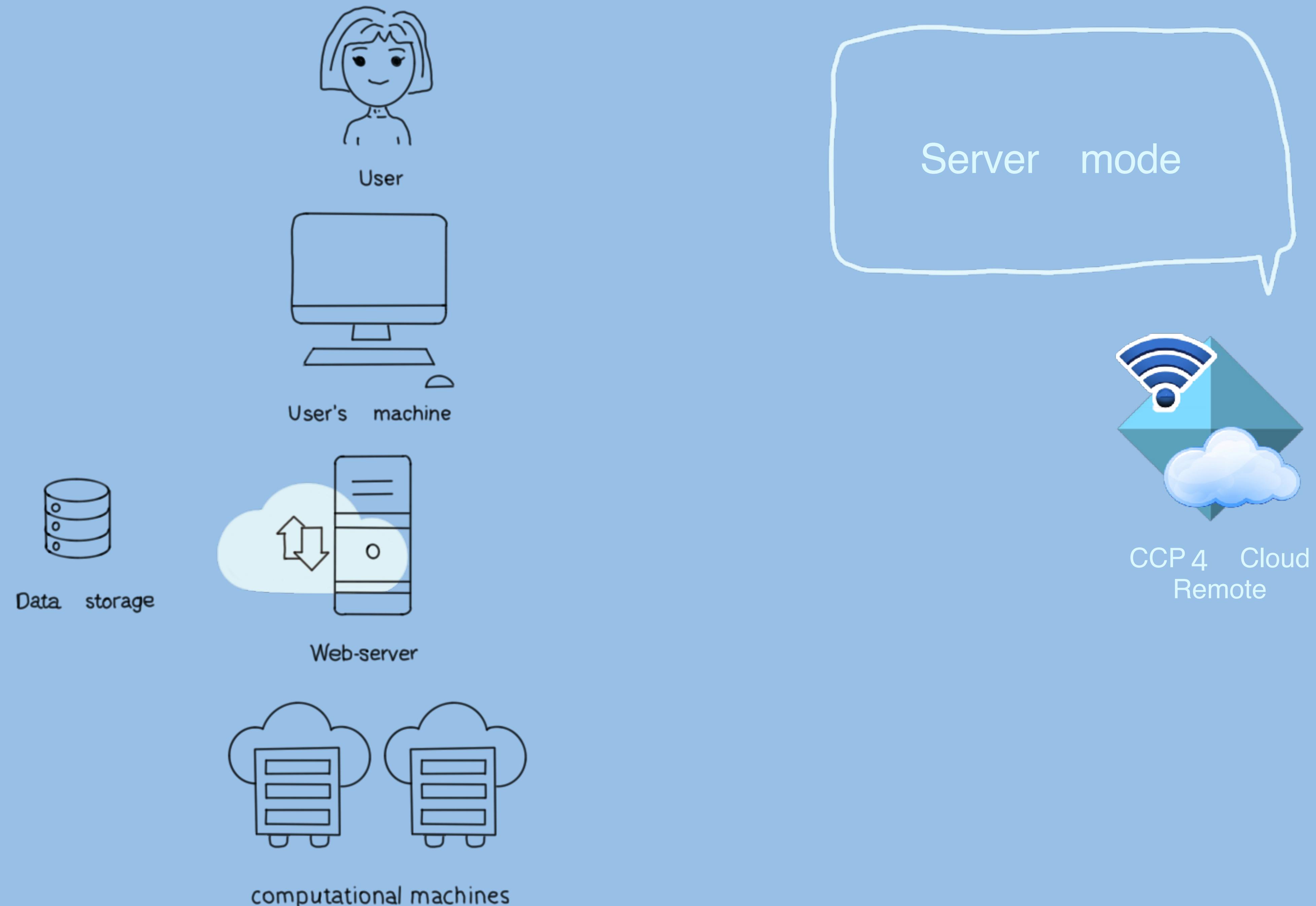
💡 Are you using the Task Dock yet? Read [here](#) about it.

Local mode



CCP4 Cloud  
Local

```
$ ccp4cloud-remote
```



# CCP4 Cloud

@ CCP4-Harwell

LOGIN

PASSWORD

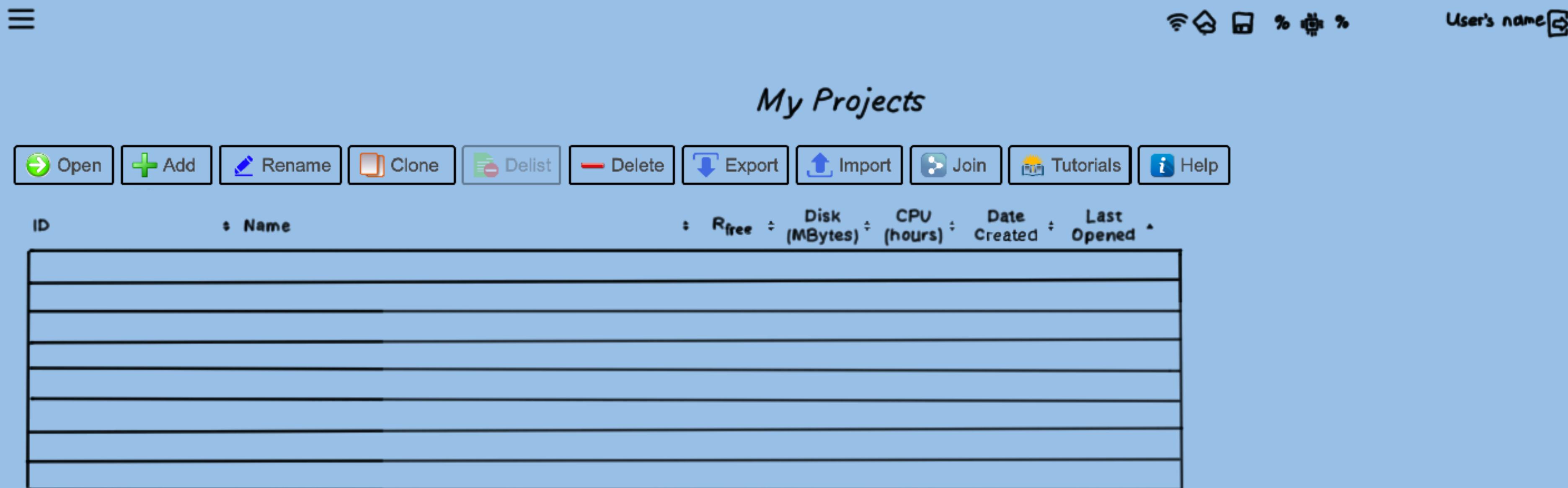
**Login**

Login page

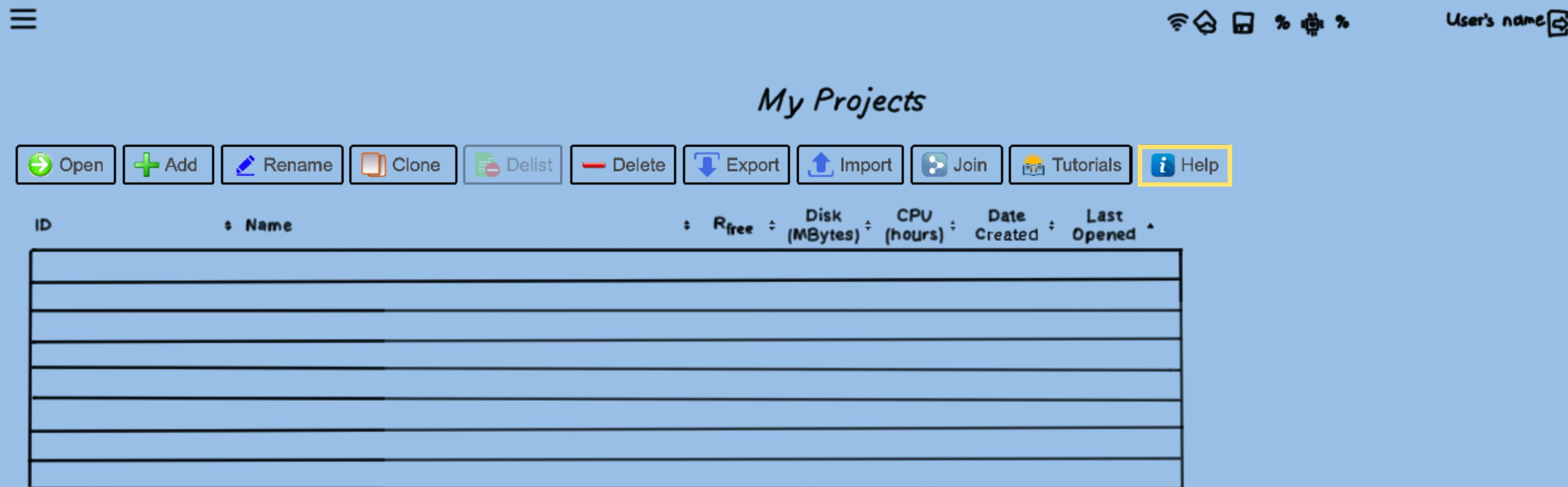


Did you know that you can save a click by login straight into your last Project? See [how](#).

# Projects page



# Projects page



# User Guide

Help

1. CCP4 Cloud interface documentation
2. Structure solution with CCP4 Cloud
3. Starting CCP4 Cloud projects from the command line
4. Cloud Run facility in CCP4i interface
5. CCP4 Cloud Archive
6. CCP4 Cloud education capabilities
7. Questions and Answers
8. Troubleshooting
9. CCP4 Cloud Version Log



All projects

Open Add Rename Clone Delist Delete Export Import Join Tutorials Help

ID	Name	R <sub>free</sub>	Disk (MBytes)	CPU (hours)	Date Created	Last Opened
7MRQ	demo	0.3626	70	1.9221	2022-08-21	2023-08-10
7NAZ	demo	0.4866	170	39.9619	2022-08-21	2023-05-04
(tutorials):A1.2.3	Auto-MR with Balbes	0.2018	27.4	0.2079	2022-12-09	2023-08-10
(tutorials):A1.3.1	MR without sequence using Simbad	0.282	20.2	0.2318	2022-12-09	2023-05-25
Auto_MR	wf	0.3301	431.6	8.2346	2023-04-27	2023-08-10
CCP4-HC3.M9M4-rev1	Demo_2: Revision #1	0.2345	44.2	0.9743	2023-01-03	2023-08-10
(tutorials):D01-clone	Simple Auto-MR with MoRDa (cloned)	0.2036	160.1	1.5182	2022-06-13	2023-02-22
Demo	MR	0.2075	3061.1	95.2955	2023-04-27	2023-05-10
Demo_0	demo	0.2872	1966.9	8.0392	2023-01-06	2023-05-11
Demo_1	demo	0.4768	251.5	5.9498	2023-01-03	2023-05-09
Hg	demo	0.3497	152.9	0.7069	2022-08-21	2023-02-23
(tutorials):MCCS-2023	MR tutorial	0.4762	570.5	34.4695	2023-05-03	2023-05-15
MCCS_2023_2	Automated Molecular Replacement with Workflow and Standart modes	0.33	271.6	5.2126	2023-05-11	2023-08-10
MCCS_WebCoot	WebCoot tutorial		4.3	0.0005	2023-05-11	2023-05-11
MCCS_WebCooler	Moorhen Tutorial 1: Fix up the Cyclin-Dependent Kinase		4.3	0.0006	2023-05-11	2023-05-11
Struktura_auto	demo struktura #\\$	0.244	178.1	0.6577	2023-05-30	2023-06-09
Struktura_standart	demo	0.3763	166.9	1.0187	2023-05-30	2023-06-09
(tutorials):T1_001	Data processing and SAD phasing		0	0	2021-11-10	2023-05-30
T2_002	The multi-domain Molecular Replacement	0.2079	219.6	7.3081	2022-09-16	2023-05-17
(tutorials):T2_003	Structure prediction for Molecular Replacement		1.7	0.0007	2022-09-22	2023-05-11
(tutorials):T2_004	Protein-ligand structure determination by Molecular Replacement	0.2386	447.9	12.9488	2023-05-22	2023-05-26
(tutorials):T2_005	MR with predicted model	0.4762	194.7	33.1263	2023-05-03	2023-05-30
(tutorials):T3_004	Beta-Lactamase Experimental Phasing		357	2.944	2021-11-18	2023-05-25
demo	demo		0	0	2023-02-22	2023-07-11
demo_bytes	demo	0.2165	97.9	2.3106	2023-01-06	2023-07-11
gamma	demo	0.2601	270.2	0.7013	2022-08-21	2023-05-10
gamma_demo	developed project	0.2218	477.8	1.7964	2022-08-19	2023-08-10
(tutorials):ligand	Protein-ligand structure determination by Molecular Replacement	0.2313	637.7	24.2626	2023-05-22	2023-05-26
(asca2022):mdm2	MDM2	0.3061	204.4	1.584	2022-11-03	2023-08-07
mcm2_ligand	ligand		22.1	0.0008	2023-05-17	2023-05-25
[bwithd]:mpro-x0692	SARS CoV-2 main protease with bound ligand MR	0.3144	702.8	5.321	2021-07-29	2023-08-07
[rmk65]:mr-tutorial1	Solve structure by MR	0.232	197.3	6.1643	2023-05-25	2023-05-26
simple_MR	Demo	0.2607	891.3	19.7324	2023-04-27	2023-05-10

Powered by CCP4 v8.0.013 CCP4 on-line IRIS

CCP4 Cloud v.1.7.014 [29.06.2023]

Projects folders and lists





# My Account

 CCP4-Harwell

User name:

E-mail:

Login name:

Password:

Retype password:

CloudRun Id:

Licence agreement:

Feedback agreement:

Software authorisations:  [manage](#)



Save changes



Delete my account

## Preferences\*

On login, go to:

Initial size (% of browser window):

width height

Job dialogs:

Viewers:

Use project name as default file prefix

Remember Task List state

Guide through data import

Send end-of-job notifications

for jobs taking longer than  hours

\* Save changes for Preferences to take an effect

Account page



# My Account

 CCP4-Harwell

User name:

E-mail:

Login name:

Password:

Retype password:

CloudRun Id:

Licence agreement:

Feedback agreement:

Software authorisations:  [manage](#)



Save changes



Delete my account

## Preferences \*

On login, go to:

- "All Projects" list ▾
- "All Projects" list
- "My Projects" folder
- last used project folder
- last opened project

Initial size (% of browser window):

width      height

Job dialogs:

Viewers:

Use project name as default file prefix

Remember Task List state

Guide through data import

Send end-of-job notifications

for jobs taking longer than  hours

\* Save changes for Preferences to take an effect

Account page

# Projects folders and lists

Online Help

CCP4 Cloud 1.7 documentation

CCP4 Cloud 1.7 documentation 1. CCP4 Cloud interface documentation 1.5. Tips and Tricks

CCP4 Cloud 1.7 documentation

1. CCP4 Cloud interface documentation

1.1. My Projects

1.2. Project Management

1.3. Task List

1.4. Job Dialog

1.5. Tips and Tricks

1.5.1. Coot Task Recovery

1.5.2. Task Dock

1.5.3. Using Remarks

1.5.4. Project Sharing

1.5.5. Login in Project or List of Projects

1.5.6. Working modes of CCP4 Cloud

1.5.7. Hot Task Launchers

1.5.8. End of Job Notifications

1.5.9. File name customisation

1.5.10. Using AlphaFold2 and Rosetta models

1.5.11. Work with diffraction images within CCP4 Cloud

1.5.12. Project folders

1.5.13. CCP4 Cloud Archive

2. Structure solution with CCP4 Cloud

3. Starting CCP4 Cloud projects from the command line

## 1.5.12. Project folders

Project in CCP4 Cloud can be organised in folders.

In order to display Project folders available click on the name of the folder you are currently in (1) or look for the Menu icon: in the top-left corner of the page and then press the Change project folder button in drop-down menu (2).

By doing so the Project folders menu appears:





# My Account

 CCP4-Harwell

User name:

E-mail:

Login name:

Password:

Retype password:

CloudRun Id:

Licence agreement:

Feedback agreement:

Software authorisations:  [manage](#)



Save changes



Delete my account

## Preferences\*

On login, go to:

Initial size (% of browser window):

width height

Job dialogs:

Viewers:

Use project name as default file prefix

Remember Task List state

Guide through data import

Send end-of-job notifications

for jobs taking longer than  hours

\* Save changes for Preferences to take an effect

Account page



# My Account

CCP4-Harwell

User name:

E-mail:

Login name:

Password:

Retype password:

CloudRun Id:

Licence agreement:

Feedback agreement:

Software authorisations:



Save changes



Delete my account

## Preferences\*

On login, go to:

Initial size (% of browser window):

width height

Job dialogs:

Viewers:

Use project name as default file prefix

Remember Task List state

Guide through data import

Send end-of-job notifications

for jobs taking longer than  hours

\* Save changes for Preferences to take an effect

Account page

The screenshot shows the 'My Account' page for CCP4-Harwell. At the top, there is a navigation bar with icons for search, user profile, and account settings. The main title 'My Account' is displayed above a CCP4-Harwell logo. Below the title, there are several input fields for account information:

- User name: Maria Fando
- E-mail: maria.fando@slfc.ac.uk
- Login name: Fando
- Password: [redacted]
- Retype password: confirm password
- CloudRun Id: woGn-qxde-1y5i-p26 | [renew](#)

Below these fields are checkboxes for agreements:

- Licence agreement: academic
- Feedback agreement: accepted (1)
- Software authorisations: manage

At the bottom of the page are two buttons: 'Save changes' and 'Delete my account'. A large blue speech bubble on the right side of the screen contains the text 'Account page'.

**Preferences\***

On login, go to: "All Projects" list

Initial size (% of browser window):  
width: 125 height: 85  
Job dialogs: 125 85  
Viewers: 140 97

Use project name as default file prefix  
 Guide through data import  
 Send end-of-job notifications  
for jobs taking longer than 24 hours

\* Save changes for Preferences to take an effect

Powered by CCP4 v.8.0.013 | CCP4 on-line | HK Iris | CCP4 Cloud v.1.7.014 [29.08.2023]

Tutorials



User's name

## My Projects

Open Add Rename Clone Move Delete Export Import Join Tutorials Help

Cloud File Browser

ID

Date Created : Last Opened

Tutorials

- .. (↑ upper directory)
- 1. From images
- 2. Molecular replacement
- 3. Experimental phasing
- 4. Refinement
- 5. Other
- Data
- Demo projects

Powered by CCP4

CCP4 Cloud v

Open Select Close

Tutorials



User's name

## My Projects

Open Add Rename Clone Move Delete Export Import Join Tutorials Help

ID




Date Created : Last Opened \*


Powered by CCP4

CCP4 Cloud v

Open Select Close

**CCP4 Cloud 1.7 documentation**

1. CCP4 Cloud interface documentation

2. Structure solution with CCP4 Cloud

    2.1. Work with CCP4 Cloud

    2.2. AlphaFold and RoseTTAFold models in CCP4 Cloud

    2.3. Automatic workflows

**2.4. CCP4 Cloud Atlas**

        2.4.1. Molecular Replacement with known sequence and structural homolog(s)

        2.4.2. Molecular Replacement with known sequence and unknown structural homolog(s)

        2.4.3. Molecular Replacement with unknown sequence

        2.4.4. Experimental Phasing with known sequence

        2.4.5. Automatic Experimental Phasing with known sequence

        2.4.6. Experimental Phasing with unknown sequence

        2.4.7. Molecular Replacement in electron density and hybrid approaches

        2.4.8. Various structure solution techniques

3. Starting CCP4 Cloud projects from the command line

4. Cloud Run facility in CCP4 interface

5. CCP4 Cloud Archive

6. CCP4 Cloud education capabilities

7. Questions and Answers

8. Troubleshooting

9. CCP4 Cloud API

## 2.4. CCP4 Cloud Atlas

This atlas presents different ways of solving structures in CCP4 Cloud depending on available data. Only schematic structure solution projects are shown, which only demonstrate general scenarios.

For solving a structure, you need at least experimental observations (reflections) either merged or unmerged. Unmerged reflections must be scaled and merged with Aimless task before use in other programs.

**Note**

Further actions will vary

**Note**

Atlas projects are available from the *Tutorials* directory

**"Contents"**

2.4. CCP4 Cloud Atlas

    2.4.1. Molecular Replacement with known sequence and structural homolog(s)

    2.4.2. Molecular Replacement with known sequence and unknown structural homolog(s)

    2.4.3. Molecular Replacement with unknown sequence

    2.4.4. Experimental Phasing with known sequence

    2.4.5. Automatic Experimental Phasing with known sequence

    2.4.6. Experimental Phasing with unknown sequence

    2.4.7. Molecular Replacement in electron density and hybrid approaches

    2.4.8. Various structure solution techniques

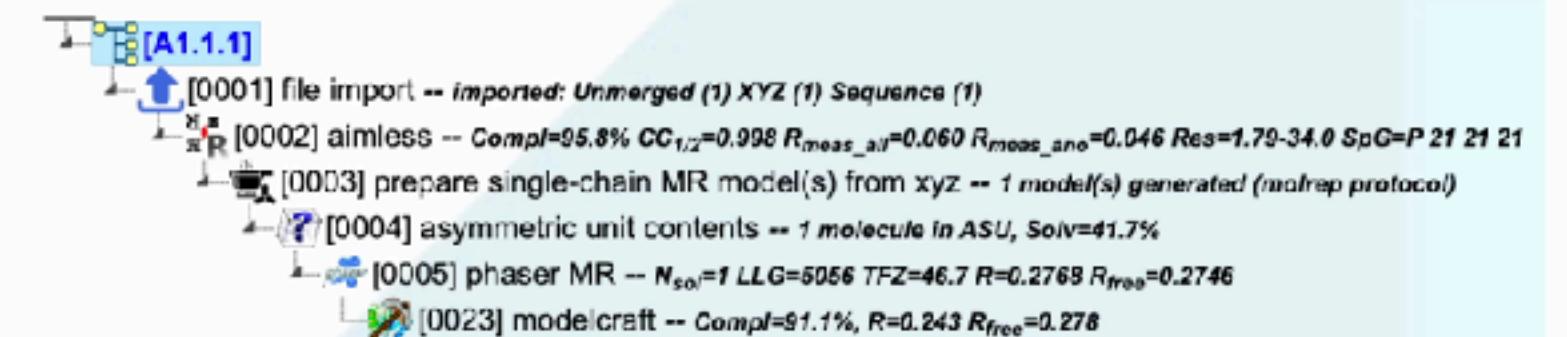
# CCP4 Cloud Atlas



### 2.4.1. Molecular Replacement with known sequence and structural homolog(s)

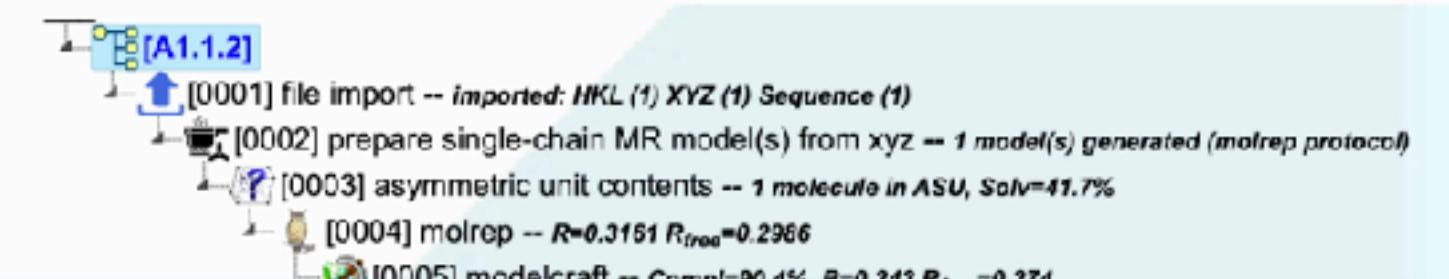
#### A1.1.1 Single-chain model, solution with Phaser

Starts from importing unmerged MTZ, sequence and PDB files, finishes with phased and rebuilt model.



#### A1.1.2 Single-chain model, solution with Molrep

Starts from importing merged MTZ, sequence and PDB files, finishes with phased and rebuilt model.



Create a project

Add New Project

ID	Name
e.g., project-1	Put a descriptive title here

**Project plan**

Manual mode

No project plan will be used; develop your project manually by using suitable tasks.

Alternatively, choose a predefined plan to automatically develop your project. You can switch to manual mode from any plan

Add Project Cancel

Create a project

Add New Project

ID Name

e.g., project-1 Put a descriptive title here

Project plan

Manual mode

Manual mode

- Plan 1. Molecular Replacement using AlphaFold model
- Plan 2. Molecular Replacement using structure databases
- Plan 3. Molecular Replacement using a known model
- Plan 4. Automatic Experimental Phasing
- Plan 5. Import already solved structure for completion

Add Project Cancel



Create a project

Add New Project

ID Name

e.g., project-1 Put a descriptive title here

**Project plan**

Plan 1. Molecular Replacement using AlphaFold model

**Data needed:**

- reflection data (merged or unmerged; .mtz, .hkl, .sca)
- sequence (.fasta, .pir, .seq)
- (optional) ligand description (.cif, .lib)

**Plan description:** Structure template prediction, pruning and slicing; ASU estimate; Molecular Replacement; ligand fitting (if provided); refinement and water modelling

Add Project Cancel

Create a project

**Add New Project**

<b>ID</b> <i>e.g., project-1</i>	<b>Name</b> <i>Put a descriptive title here</i>
-------------------------------------	--

**Project plan**

Plan 2. Molecular Replacement using structure databases

**Data needed:**

- reflection data (merged or unmerged; .mtz, .hkl, .sca)
- sequence (.fasta, .pir, .seq)
- (optional) ligand description (.cif, .lib)

**Plan description:** Finding structure template in the PDB, AFDB and ESM data banks; ASU estimate; Molecular Replacement; ligand fitting (if provided); refinement and water modelling

**Add Project** **Cancel**



Create a project

Add New Project

ID	Name
e.g., project-1	Put a descriptive title here

**Project plan**

Plan 3. Molecular Replacement using a known model

**Data needed:**

- reflection data (merged or unmerged; .mtz, .hkl, .sca)
- structure model (.pdb, .cif, .mmcif)
- (optional) sequence (.fasta, .pir, .seq)
- (optional) ligand description (.cif, .lib)

**Plan description:** Model preparation; ASU estimate; Molecular Replacement; ligand fitting (if provided); refinement and water modelling

Add Project Cancel

Create a project

**Add New Project**

**ID** *e.g., project-1*

**Name** *Put a descriptive title here*

**Project plan**

Plan 4. Automatic Experimental Phasing

**Data needed:**

- reflection data with anomalous signal (merged or unmerged; .mtz, .hkl, .sca)
- sequence (.fasta, .pir, .seq)
- (optional) ligand description (.cif, .lib)

**Plan description:** ASU estimate; automatic Experimental Phasing; ligand fitting (if provided); refinement and water modelling

**Add Project** **Cancel**

**Add**

Create a project

**Add New Project**

**ID** *e.g., project-1*    **Name** *Put a descriptive title here*

**Project plan**

Plan 5. Import already solved structure for completion

**Data needed:**

- reflection data (merged .mtz)
- phases (merged .mtz; optional if model is given)
- structure model (.pdb, .cif, .mmcif; optional if phases are given)
- (optional) sequence (.fasta, .pir, .seq)
- (optional) ligand description (.cif, .lib)

**Plan description:** Import data and set up project for further refinement, model building, water finding, ligand fitting, and PDB deposition

**Add Project** **Cancel**

# Create a project

The screenshot shows a web-based interface for managing projects in CCP4 Cloud. The title bar reads "CCP4 Cloud" and the address bar shows "cloud ccp4.ac.uk". The main content area is titled "My Projects/demo". A toolbar at the top includes buttons for Open, Add, Rename, Clone, Move, Delete, Export, Import, Join, Tutorials, and Help. Below the toolbar is a table header with columns: ##, ID, Name, R<sub>free</sub>, Disk (MBytes), CPU (hours), Date Created, and Last ↑ Opened. A message below the header states: "There are no projects in folder 'My Projects/demo'." It provides instructions for creating a new project using the "Add" button, importing from CCP4 Cloud using the "Import" button, joining a shared project using the "Join" button, or loading tutorial/demo projects using the "Tutorials" button. A large green "Add" button is located on the right side of the page.

CCP4 Cloud

cloud ccp4.ac.uk

☰ My Projects/demo

Open Add Rename Clone Move Delete Export Import Join Tutorials Help

##	ID	Name	R <sub>free</sub>	Disk (MBytes)	CPU (hours)	Date Created	Last ↑ Opened
----	----	------	-------------------	---------------	-------------	--------------	---------------

There are no projects in folder "My Projects/demo".

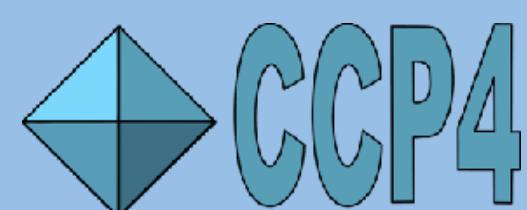
Use "Add" button to create a new Project;  
"Import" button for importing a project exported from CCP4 Cloud;  
"Join" button for joining project shared with you by another user;  
or "Tutorials" button for loading tutorial/demo projects;  
or click on page title or folder icon in it to change the folder.

Add

Powered by CCP4 v.9.0.006

CCP4 Research Complex at Harwell iris alc

CCP4 Cloud v.1.8.005 [29.01.2025]



## Task List

Suggested tasks

All tasks

Workflows

A-Z

### Automatic Workflows

Each workflow will run a series of tasks, see details [here](#).

#### Workflows for starting a Project



##### Molecular Replacement with MrBump or MoRDa

-- data import, ASU definition, automatic MR, refinement, ligand fitting and PDB validation report



##### Molecular Replacement with AlphaFold Model

-- data import, ASU definition, automatic MR, refinement, ligand fitting and PDB validation report



##### Simple Molecular Replacement with Search Model

-- data import, ASU definition, phaser MR, refinement, ligand fitting and PDB validation report



##### Dimple Molecular Replacement

-- data import, ASU definition, Dimple MR, refinement, ligand fitting and PDB validation report



##### Automated Experimental Phasing with Crank-2

-- data import, ASU definition, automatic EP, refinement, ligand fitting and PDB validation report



Add

#### Workflows for using within a Project



##### Dimple Refinement and Ligand Fitting

-- Dimple pipeline, ligand fitting, refinement and PDB validation report



##### Automated Refinement and Ligand Fitting

-- refinement, ligand fitting and PDB deposition, starting from a phased structure

### My Workflows



##### [demo] My Workflow Title

-- my workflow description



##### [mr\_with\_morda] My Workflow Title

-- my workflow description



Add workflow



Help

Close

Create a project

# Custom Workflows



Screenshot of the CCP4 Cloud interface showing the 'Task List' window. The window has tabs for 'Suggested tasks', 'All tasks', 'Workflows' (which is selected), and 'A-Z'. The main content area is titled 'Automatic Workflows' and lists several pre-defined workflows:

- Workflows for starting a Project**
  - Automatic Molecular Replacement with MrBump or MoRDa
    - data import, ASU definition, automatic MR refinement, ligand fitting and PDB deposition
  - Molecular Replacement with AlphaFold Model
    - data import, ASU definition, automatic MR refinement, ligand fitting and PDB deposition
  - Simple Molecular Replacement with Search Model
    - data import, ASU definition, phaser MR, refinement, ligand fitting and PDB deposition
  - Dimple Molecular Replacement
    - data import, ASU definition, Dimple MR, refinement, ligand fitting and PDB deposition
  - Automated Experimental Phasing with Crank-2
    - data import, ASU definition, automatic EP, refinement, ligand fitting and PDB deposition
- Workflows for using within a Project**
  - Dimple Refinement and Ligand Fitting
    - Dimple pipeline, ligand fitting, refinement and PDB validation report
  - Automated refinement and ligand fitting
    - refinement, ligand fitting and PDB deposition, starting from a phased structure

**My Workflows**  
None defined  
[Add workflow](#)

**Workflow scripts library**

These scripts exemplify common structure solution workflows (or project development scenarios). They can be used as templates or starting points for further customization. The library is **read-only**.

**workflow\_scripts**

- Auto-MR from sequence, ligand fitting and refinement.wscript
- Dimple MR with high homology model, ligand fitting and refinement.wscript
- Phaser EP and model building.wscript
- Phaser MR with given model, ligand fitting and refinement.wscript

**Open****Select****Close**

**Workflow Creator**

Workflow ID:

Workflow script (see [reference](#) for details; opens in new window)

```

12 #
13 # Workflow header and input
14
15 # General workflow descriptors
16 NAME Auto-MR workflow
17 ONAME amr_wfLow
18 TITLE Auto-MR Workflow with ligand fitting
19 DESC MrBump followed by water/ligand fitting and refinement
20 ICON Gold # added automatically
21 KEYWORDS auto MR workflow ligand # for using in A-Z keyword search
22
23 ALLOW_UPLOAD # create file upload widgets if started from project root
24
25 # List all data required, "!" specifies mandatory items
26 !DATA HKL UNMERGED TYPES anomalous
27 !DATA SEQ TYPES protein dna rna
28 DATA LIGAND
29
30 # List all parameters required, "!" specifies mandatory items
31 PAR_REAL resHigh
32   LABEL High resolution cut-off (Å)
33   TOOLTIP High resolution cut-off, angstrom
34   DEFAULT 1.5
35   RANGE 0.1 5.0
36
37 PAR_CHECK reqValReport
38   LABEL Request PDB Validation Report
39   TOOLTIP Check if deposition files should be prepared and PDB validation report obtained
40   DEFAULT Unchecked
41
42 # Workflow itself
43
44 PRINT_VAR reso_high
45
46 ESCALE AND MERGE
47   IFDATA unmerged
48   DATA ds0 unmerged
49   PARAMETER RESO_HIGH resHigh
50   RUN Aimless
51
52 # If unmerged file was not provided, cut resolution of merged dataset
53 @CHANGERESO
54   IF NOTDATA unmerged
55   IF reso_high < resHigh
56     PROPERTY HKL res_high resHigh
57   RUN ChangeReso
58
59 @DEFINE_ASU
60   RUN ASUDef
61
62 @MOLECULAR REPLACEMENT
63   RUN MrBump
64
65 @REBUILD

```

Library   Add task   Insert task    Save    Cancel

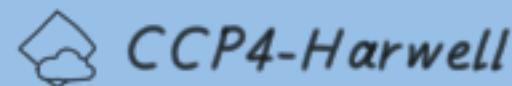
**Custom Workflows**

Bash ▾

```
$ cloudrun -t auto-af2 > auto-af2.com
$ cat auto-af2.com
# CloudRun template command file for auto-af2 task.
#
# The task uploads files specified, creates CCP4 Cloud Project (if it
# does not exist already) and starts the "Auto-AFMR" workflow (this
# requires an AlphaFold (or OpenFold or ColabFold) to be installed
# in CCP4 Cloud).
#
# Notes: a) hash indicates a comment b) line order is insignificant
#        c) CloudRun tasks are added at Project's root.
#
URL      https://ccp4cloud.server    # mandatory
#
# User authentication: either in-line specification
#
USER      user_login                # mandatory
CLOUDRUN_ID aaaa-bbbb-cccc-dddd    # mandatory, found in "My Account"
#
# or reading user_login and aaaa-bbbb-cccc-dddd (in that order)
# from a file:
# AUTH_FILE /path/to/auth.dat       # mandatory
#
PROJECT   project_id                # mandatory
TITLE     Optional Project Title    # used only if project is created
TASK      auto-af2                  # mandatory
TASK_NAME Optional Task Name       # if not given, default name is used
#
HKL       /path/to/hkl.mtz          # reflection data
SEQ_PROTEIN /path/to/file.[seq|fasta|pir] # protein sequence
#
# Either SMILES or LIG_CODE should be used for optional ligand description,
# but not both.
#
SMILES   smiles-string  # ligand smiles string, not enquoted
LIG_CODE ATP           # 3-letter ligand code, e.g., ATP
$
```

CloudRun utility

## My Account



User name:	<input type="text"/>
E-mail:	<input type="text"/>
Login name:	<input type="text"/>
Password:	<input type="text"/>
Retype password:	<input type="text"/>
CloudRun Id:	<input type="text"/> <a href="#">renew</a>
Licence agreement:	<input type="checkbox"/>
Feedback agreement:	<input type="checkbox"/>
Software authorisations:	<a href="#">manage</a>

---



Online Help

CCP4 Cloud 1.7 documentation

Search

## 3. Starting CCP4 Cloud projects from the command line

CCP4 Cloud projects can be initiated and executed from the command line, which may be useful in many scenarios. For example, data collection session at a synchrotron beamline may include sending reflection data, sequence, optional structural homolog and ligand descriptions, automatically to the specified CCP4 Cloud account and starting a suitable structure solution workflow in it. Or, large series of structure solution projects can be initiated by custom script to save time for manipulations with CCP4 Cloud's graphical interface.

**Note**

Functionality, described in this article, requires local CCP4 setup version 8.0.003 or higher.

### 3.1. CloudRun utility

CloudRun utility, included in CCP4 Software Suite, can create projects, upload data and start automatic structure solution workflow in a single run as shown below (CCP4 8.0.003+ environment is assumed on Linux/Mac OSX, use CCP4 Console on Windows):

```
$ cloudrun -c command_file
```

where `command_file` is a text file with instructions given as keyword-value pairs (described below). An alternative syntax may also be used:

```
$ cloudrun -i <<eof
keyword value
.....
eof
```

Back Forward Return Detach Close

CloudRun utility



**CCP4Interface 8.0.011 running on SCLT264MAC Project: MDM2**

Program List	Job ID	Time	Status	Program
Buccaneer - autobuild/refine	12	18:42:11	FINISHED	refmac5
Buccaneer - fast build only	11	18:39:01	FINISHED	refmac5
Carl	10	18:36:16	FINISHED	buccaneer_pi
CCP4 Cloud Workflows	9	18:28:58	FINISHED	refmac5
CCP4 Molecular Graphics	8	18:26:40	FINISHED	refmac5
CCP4i DBviewer	7	18:24:01	FINISHED	refmac5
Chainsaw	6	18:21:52	FINISHED	molrep
Chooch	5	18:20:00	FINISHED	import
Contact	4	18:18:54	FAILED	import
Coordconv	3	18:17:56	FINISHED	reindex
Coot - Model Building	2	18:13:48	FINISHED	molrep
	1	18:11:23	FINISHED	aimless

**Directories&ProjectDir**

- View Any File
- View Files from Job
- Search/Sort Database..
- Graphical View of Project
- Delete/Archive Files..
- Kill Job
- ReRun Job..
- Edit Job Data
- Preferences

*CCP4 is up to date*

**Cloud Run**

Job title: CCP4 Cloud Workflow

Run: Hop on CCP4 Cloud on this machine

in project: MDM2

HKL in	MDM2	Browse	View
XYZ in	MDM2	Browse	View
SEQ in	MDM2	Browse	View
LIB in	MDM2	Browse	View

Continue your work in CCP4 Cloud or export results

Start / Show

Close

From CCP4i to CCP4 Cloud

CCP4Interface 8.0.011 running on SCLT264MAC Project: MDM2

Program List

12	18:42:11	FINISHED	refmac5	
11	18:39:01	FINISHED	refmac5	
10	18:36:16	FINISHED	buccaneer_pi	
9	18:28:58	FINISHED	refmac5	
8	18:26:40	FINISHED	refmac5	
7	18:24:01	FINISHED	refmac5	
6	18:21:52	FINISHED	molrep	
5	18:20:00	FINISHED	import	
4	18:18:54	FAILED	import	
3	18:17:56	FINISHED	reindex	
2	18:13:48	FINISHED	molrep	
1	18:11:23	FINISHED	aimless	

Directories&ProjectD

- View Any File
- View Files from Job
- Search/Sort Database..
- Graphical View of Project
- Delete/Archive Files..
- Kill Job
- ReRun Job..
- Edit Job Data
- Preferences

CCP4 is up to date

Cloud Run

Job title CCP4 Cloud Workflow

Run Hop on CCP4 Cloud on CCP4 Cloud server in project MDM2

HKL in MDM2 XYZ in MDM2 SEQ in MDM2 LIB in MDM2

Continue your work in CCP4 Cloud or export results

Authentication

URL <https://cloud ccp4.ac.uk> Login CloudRun Id To paste: Ctrl-V Save any changes to Cloud Run configuration on successful submission

Start / Show Close

# My Account



User name: Maria Fando

E-mail: maria.fando@stfc.ac.uk

Login name: fando

Password:

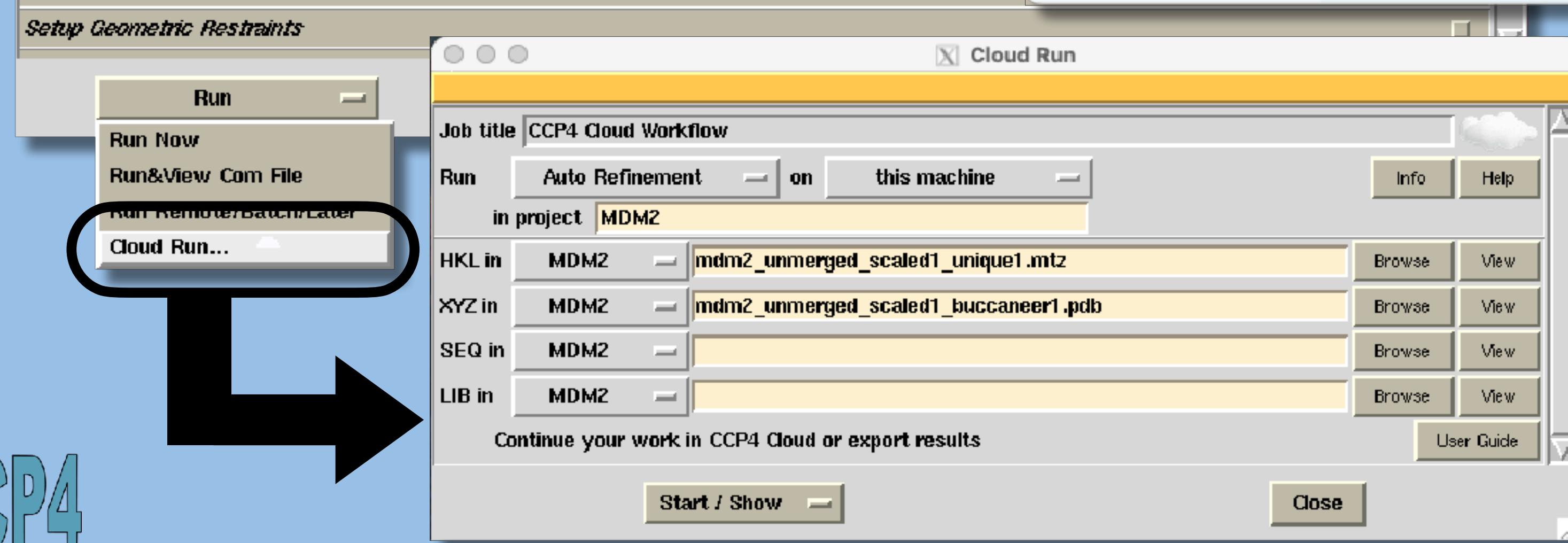
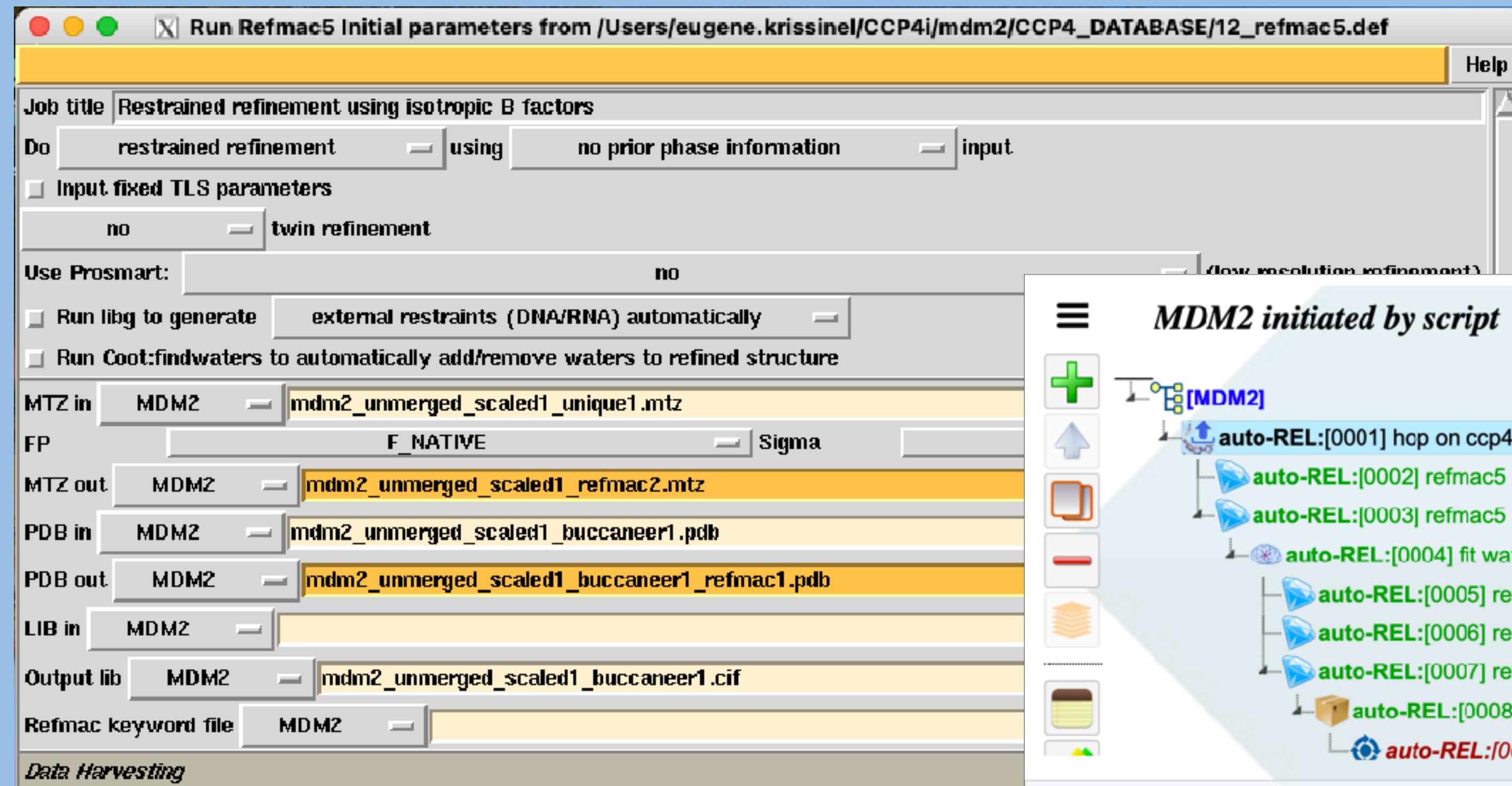
Retype password: confirm password

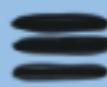
CloudRun Id: 6v45-lxyo-gswi-noa1

Licence agreement: academic

Feedback agreement: accepted (1)

Software authorisations: manage







## Task Reference

Task Reference

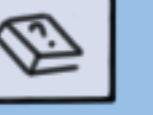
Input  Output

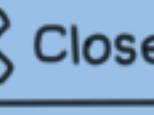
Task name  
Task's logo

job description:

output id:

Structure revision



    Close

▼ Parameters

**CCP4 Cloud 1.8 documentation**[1. Automatic workflows](#)[2. Data Import](#)[3. Structure Prediction](#)[4. Data Processing](#)[5. Asymmetric Unit and Structure Revision](#)[6. Automated Molecular Replacement](#)[7. Molecular Replacement](#)[8. Fragment-Based Molecular Replacement](#)[9. Experimental Phasing](#)**10. Density Modification**[10.1. Density Modification with Parrot](#)[10.2. Phase Refinement and Dynamic Density Modification with ACORN](#)[9.2. SHELXCD](#)[9.3. SHELXE](#)[11. Refinement and Model Building](#)[12. COOT](#)[13. Ligands](#)

# 10. Density Modification

[Show Source](#)

The electron density map is generally calculated from amplitudes measured experimentally and obtained phases. Density modification (DM) methods are necessary to improve the phases in order to obtain an interpretable map. DM has the effect of selecting the correct phase from the two phase possibilities. Thus, in the case of SAD and SIR the improvements in the map can be very dramatic. It may also be applied after molecular replacement to reduce bias towards the search model. Phase improvement is performed using solvent flattening, histogram matching, and optionally non-crystallographic symmetry averaging.

There are two families of approaches to density modification: [classical](#) methods and [statistical](#) methods.

[Classical](#) method includes two major steps:

- density modification to impose a physical constraint in real space
- structure factor merging to combine the resulting information with the experimental data in reciprocal space.

The result of these iterations can be used to redetermine input parameters, such as heavy atom positions, molecular envelopes, and noncrystallography symmetry operators. These parameters will then lead to a new set of initial phases, which in turn are improved by density modification, defining a larger cycle of iterations.

[Statistical](#) methods provide a more sound theoretical basis to the problem of phase improvement and as a result reduce the problems of bias associated with classical density-modification methods. This improvement is achieved by:

- the expression of the additional information to be introduced to the electron-density map in terms of probability distributions and then carrying those distributions into reciprocal space, rather than working with a single map representing a single sample from the phase probability distributions.

# Job dialog

localhost:53552

developer [0019] refmacat -- completed

Input  Output

Report Main Log Service Log Errors

[0019] Verdict

Refinement summary

	Achieved	Expected
R-factor	0.1737	
R <sub>free</sub>	0.2046	< 0.212
Bond length rms	0.0116	0.01-0.02
Clash score	27.91	< 4.3
Ramachandran outliers	0.0	
MolProbity score	2.36	

Fair enough. Overall quality of the structure could be better, either part of structure is missing or geometrical quality is poor

- Clash Score is critically high; model contains severe clashes.

MolProbity clash score of 27.9 for the structure seems quite high (median clash score for your resolution is 4.3). Please increase the weight for the VDW repulsion by setting up 2.0 or higher (we recommend 2.0) for the 'VDW repulsion weight' parameter. Value for the restraints weight is subject to optimisation.

Clone job with suggested parameters *suggested parameters will be shown in italic blue*

auto-REL:[0046] refmacat -- R=0.1768 R<sub>free</sub>=0.2064 MolProbity=1.86  
auto-REL:[0048] refmacat -- R=0.1781 R<sub>free</sub>=0.2067 MolProbity=1.68

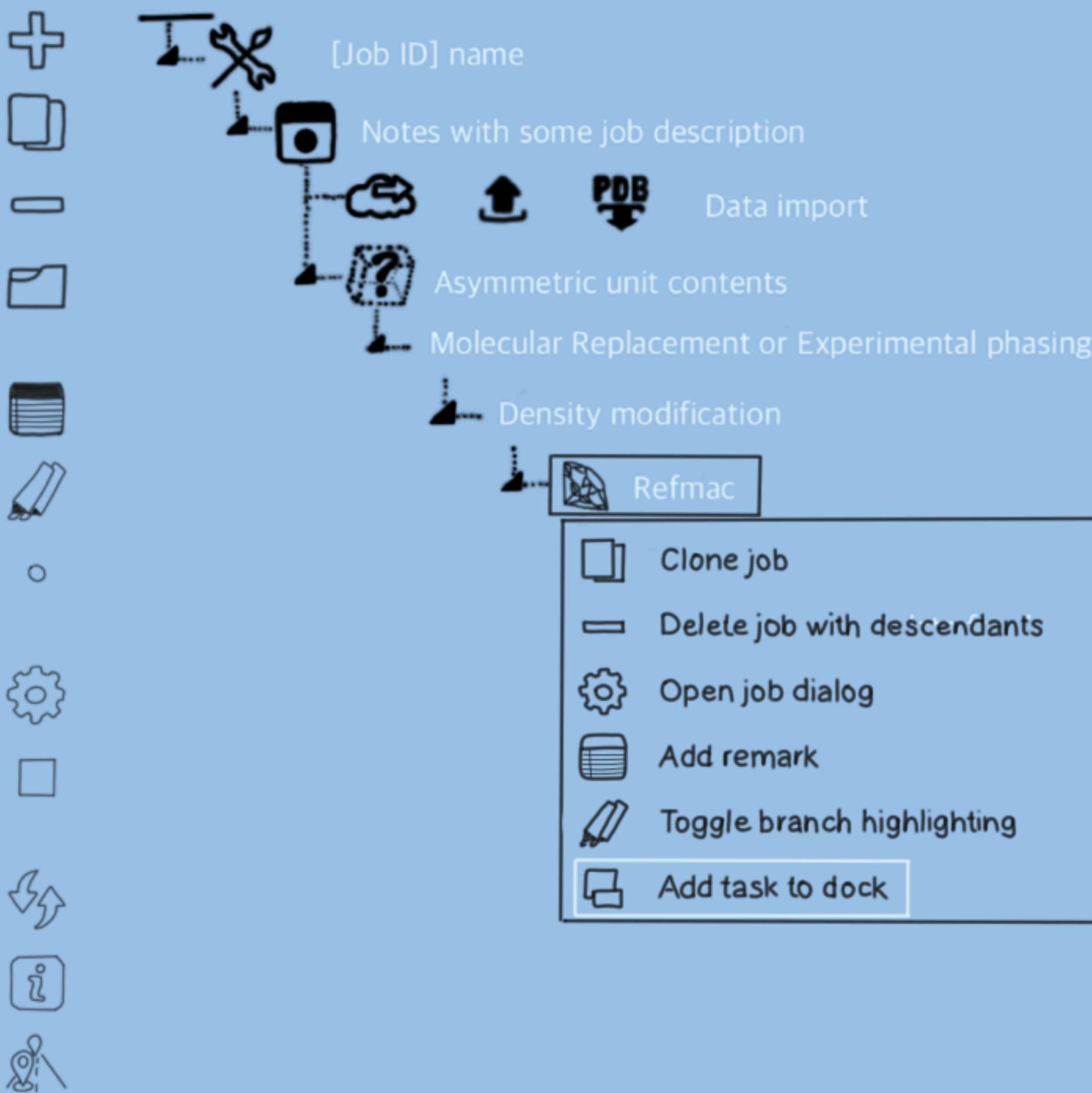
Powered by CCP4 v.8.0.017

CCP4

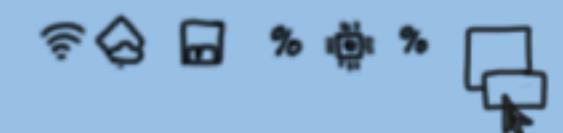
CCP4 Cloud v.1.7.018 [10.01.2024]



User's name



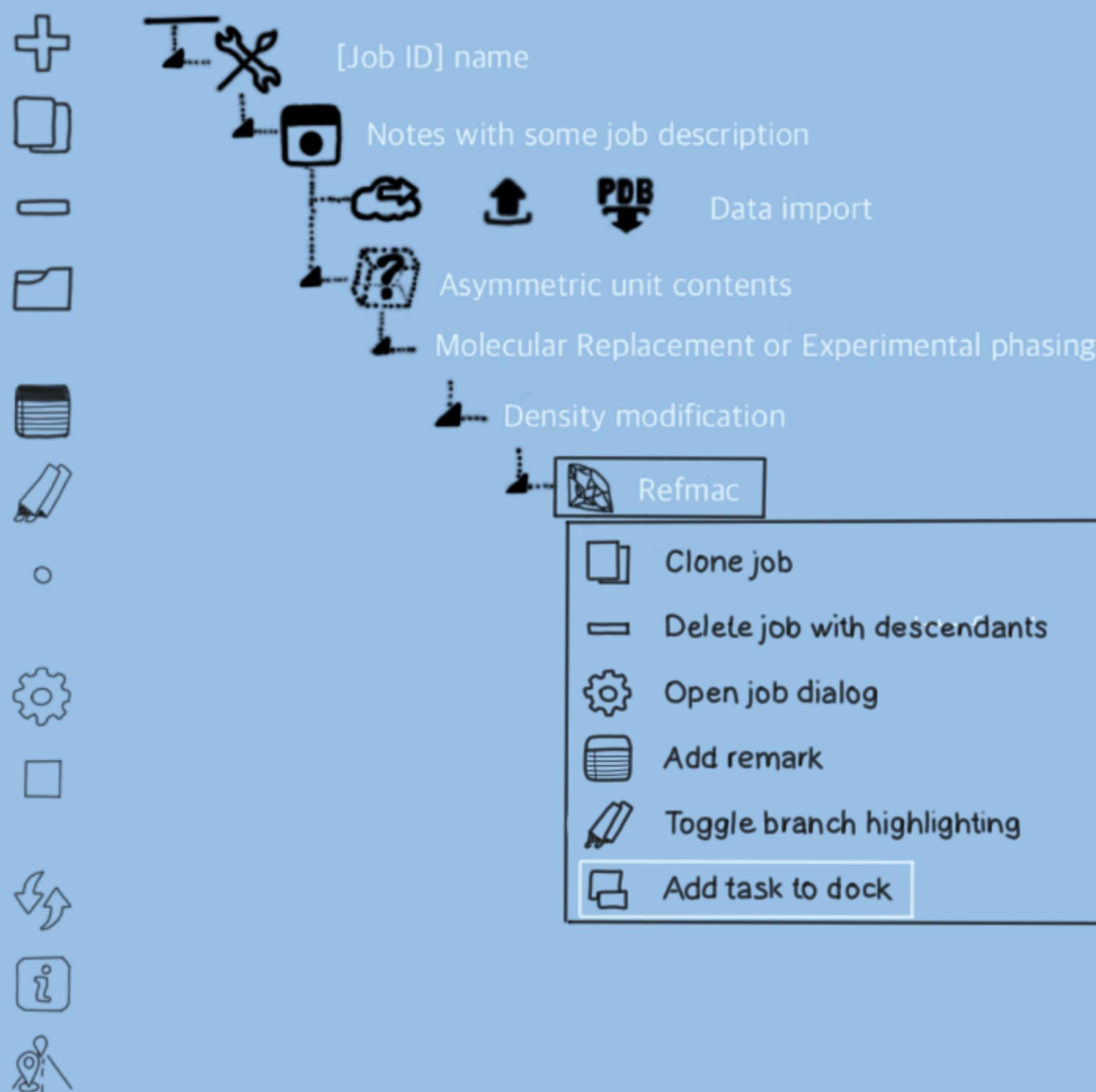
Tasks dock



User's name



Toggle task dock



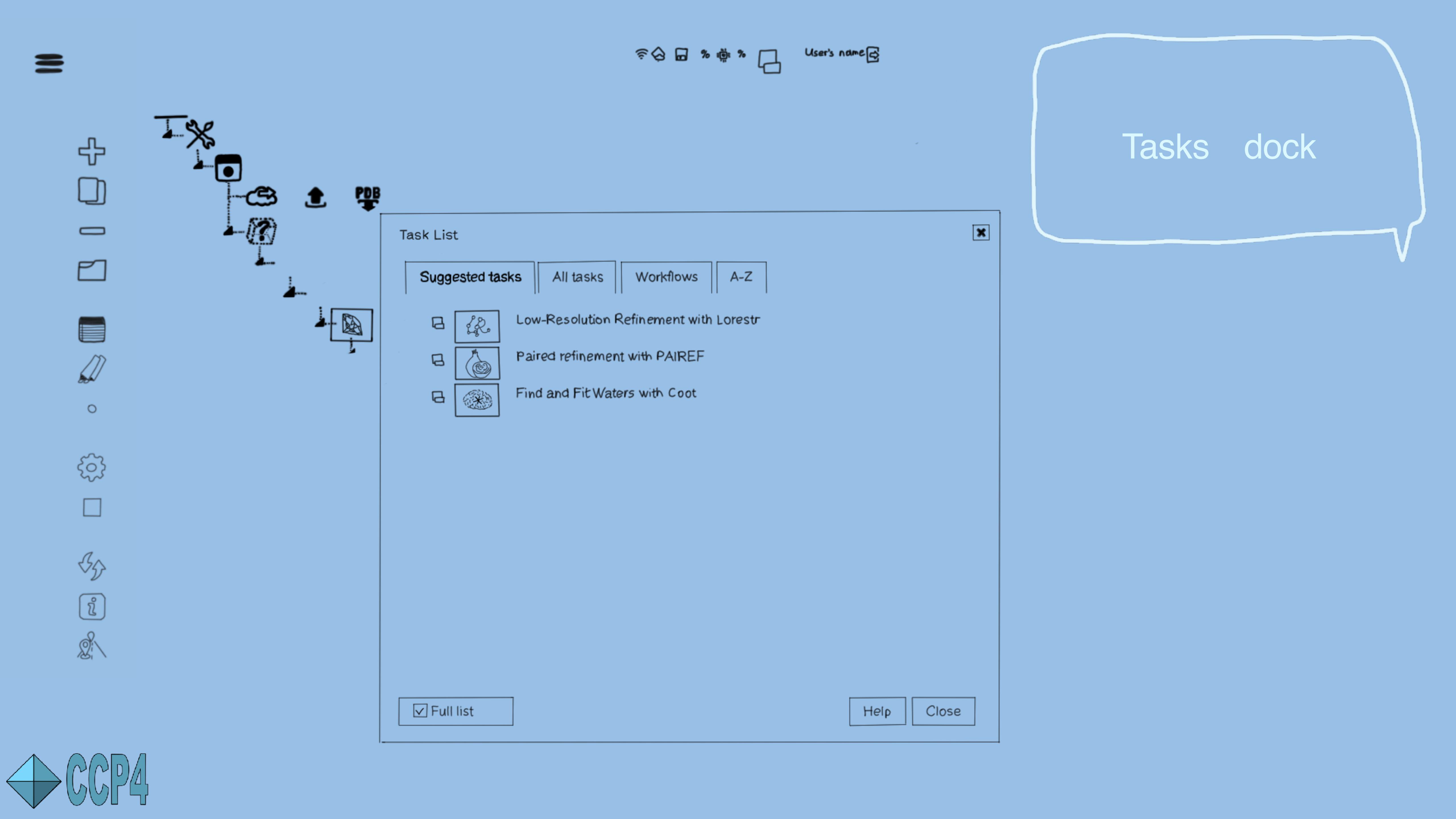
Tasks dock

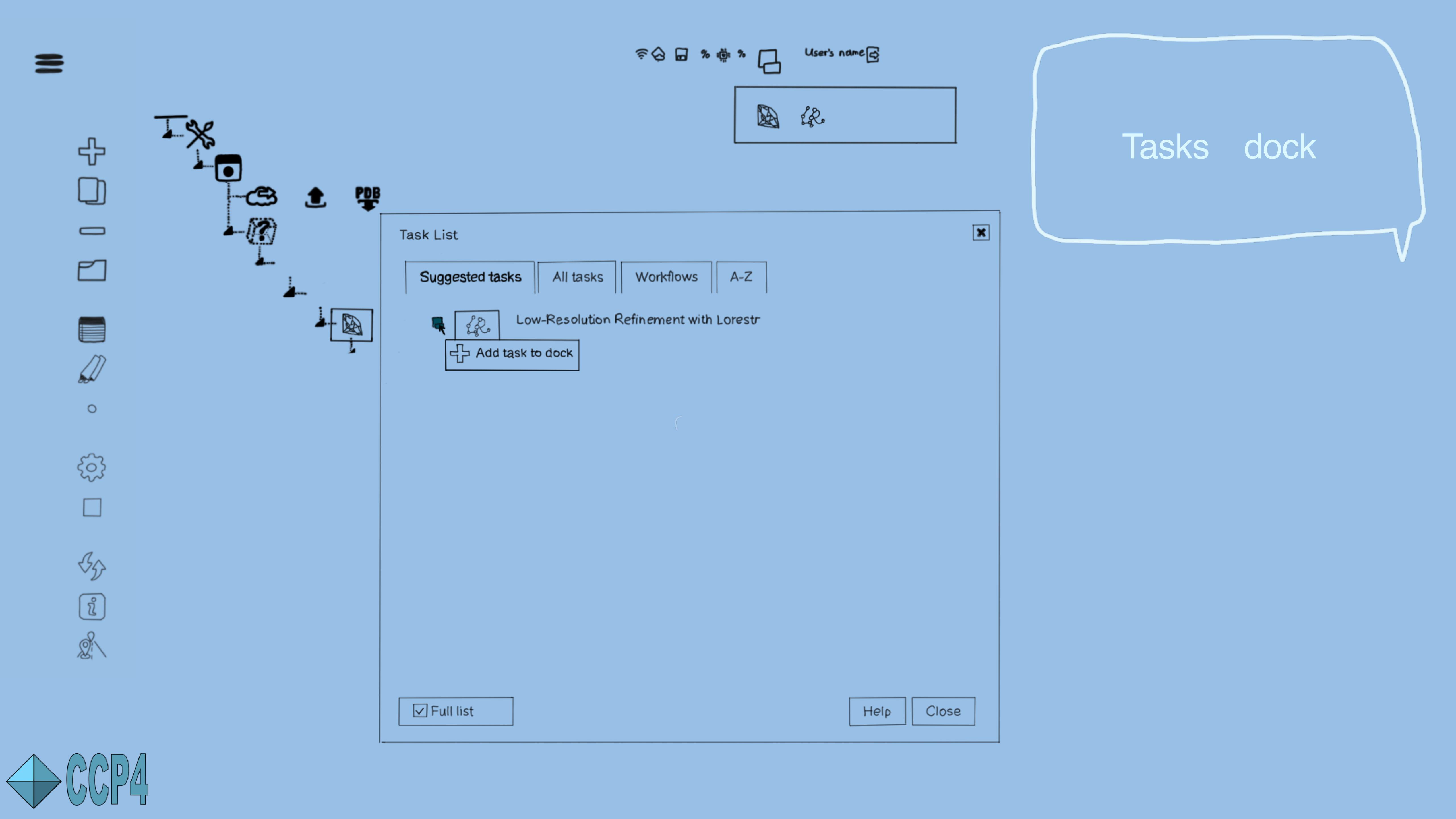


Wi-Fi % User's name

- [Job ID] name
- Notes with some job description
- Data import
- Asymmetric unit contents
- Molecular Replacement or Experimental phasing
- Density modification
- Refmac
  - Clone job
  - Delete job with descendants
  - Open job dialog
  - Add remark
  - Toggle branch highlighting
  - Add task to dock

Tasks dock





cloud ccp4.ac.uk

Press (fn) F to exit full screen

Maria Fando

**standart**

(fando):[DLS23\_demo\_02]

- [0001] import from cloud storage - Imported: HKL (1) Structure (1) XYZ (3) Sequence (1)
- [0003] define asymmetric unit contents -- 3 molecules in ASU, Solv=39.1%
- [0004] prepare model
- [0006] prepare single-chain MR model(s) from xyz -- 1 model(s) generated (molrep protocol)
- [0009] phaser MR --  $N_{sol}=1$  LLG=95 TFZ=11.5 R=0.5504 R<sub>free</sub>=0.5489**
- [0012] prepare single-chain MR model(s) from xyz
- [0005] split model
- [0007] slice -- 3 models generated
- [0008] slice -- 3 models generated
- [0010] phaser MR --  $N_{sol}=1$  LLG=1433 TFZ=29.3 R=0.379 R<sub>free</sub>=0.3885**
- [0011] refmacat -- R=0.3464 R<sub>free</sub>=0.3409 MolProbity=4.76

Powered by CCP4 v.8.0.017

CCP4

UKRI Research Complex at Harwell

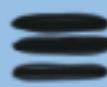
iris

CCP4 Cloud v.1.7.018 [10.01.2024]

Copy-Paste tasks

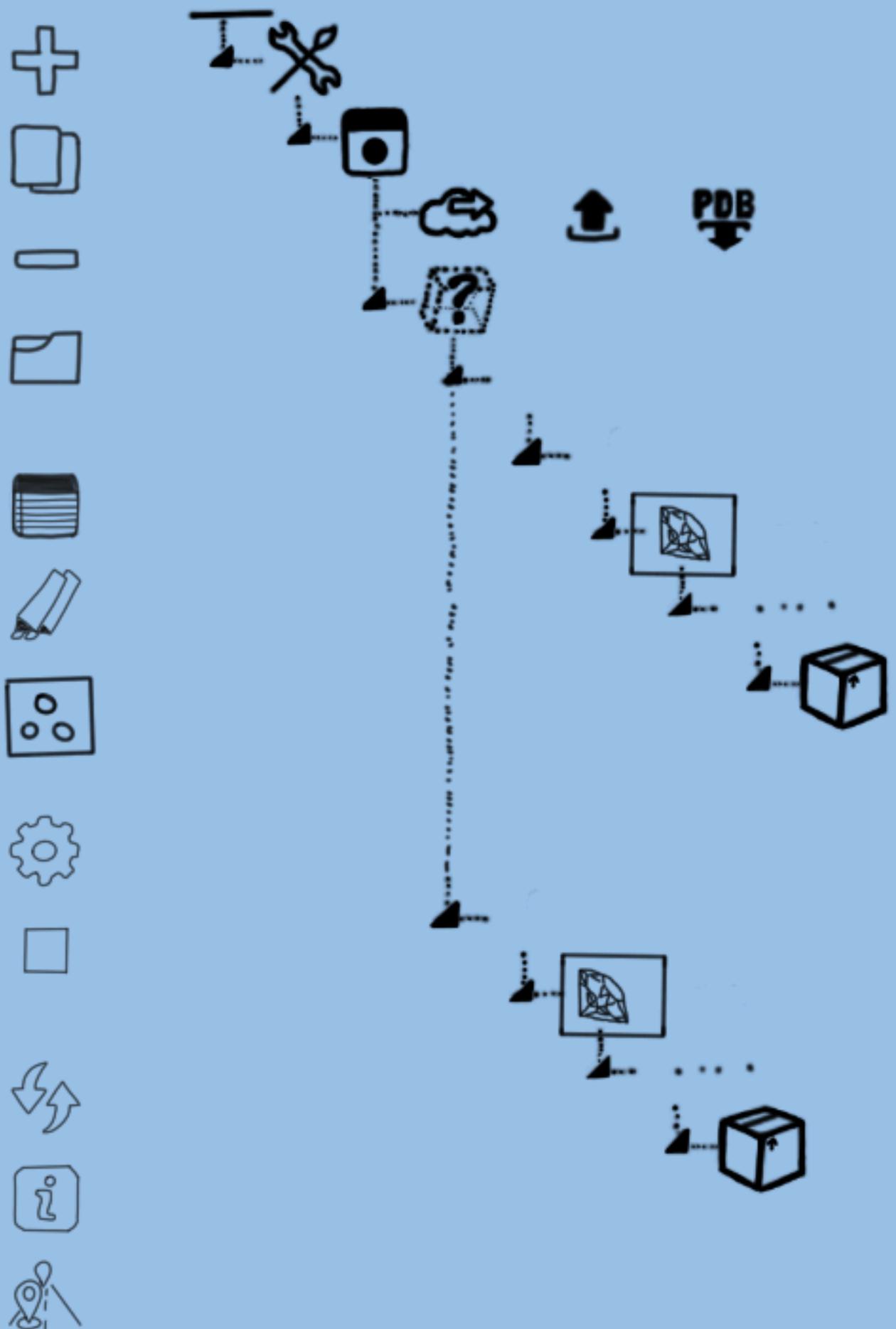
Multiple selection





Wi-Fi ☀️ 📡 % 🚧 %

User's name



Multiple selection

## Multiple selection

localhost:53552    maria

### developed project

(fando):[seacoast\_0]

- [0001] import from cloud storage -- imported: HKL (1) Structure (1) XYZ (1) Sequence (1)
- [0003] define asymmetric unit contents -- 1 molecule in ASU, Solv=62.4%
- [0004] slice -- 1 model generated
- [0008] phaser MR -- N<sub>sol</sub>=1 LLG=583 TFZ=22.6 R=0.486 R<sub>free</sub>=0.484
- [0009] modelcraft -- Compl=95.0%, R=0.201 R<sub>free</sub>=0.225
  - auto-REL:[0013] Refinement and ligand fitting automatic workflow -- workflow started
  - auto-REL:[0014] refmacat -- R=0.1901 R<sub>free</sub>=0.2135 MolProbity=1.61
    - auto-REL:[0017] fit waters -- N<sub>waters</sub>=211 R=0.1747 R<sub>free</sub>=0.2068 MolProbity=2.44
      - auto-REL:[0019] refmacat -- R=0.1737 R<sub>free</sub>=0.2046 MolProbity=2.36
      - auto-REL:[0021] refmacat -- R=0.1747 R<sub>free</sub>=0.2034 MolProbity=2.1
      - auto-REL:[0022] refmacat -- R=0.1772 R<sub>free</sub>=0.2037 MolProbity=1.88
      - auto-REL:[0024] refmacat -- R=0.1803 R<sub>free</sub>=0.2071 MolProbity=1.72
    - auto-REL:[0026] PDB validation report -- pdb report obtained
      - auto-REL:[0029] Automated Workflow has finished successfully (look inside for comments)
- [0005] morda -- R=0.2305 R<sub>free</sub>=0.2565
- [0012] modelcraft -- Compl=94.7%, R=0.202 R<sub>free</sub>=0.231
  - auto-REL:[0035] Refinement and ligand fitting automatic workflow -- workflow started
    - auto-REL:[0036] refmacat -- R=0.1918 R<sub>free</sub>=0.2177 MolProbity=1.69
    - auto-REL:[0040] refmacat -- R=0.1867 R<sub>free</sub>=0.2107 MolProbity=1.48
  - auto-REL:[0042] fit waters -- N<sub>waters</sub>=198 R=0.1721 R<sub>free</sub>=0.1999 MolProbity=1.95
    - auto-REL:[0044] refmacat -- R=0.1761 R<sub>free</sub>=0.2070 MolProbity=2.17
    - auto-REL:[0046] refmacat -- R=0.1768 R<sub>free</sub>=0.2064 MolProbity=1.86
    - auto-REL:[0048] refmacat -- R=0.1781 R<sub>free</sub>=0.2067 MolProbity=1.68

Powered by CCP4 v.8.0.017    CCP4 Cloud v.1.7.018 [10.01.2024]

Download Project

cloud ccp4.ac.uk

## My Projects/SEA COST 2024

Open Add Rename Clone Move Delete Export Import Join Tutorials Help

ID	Name	R <sub>free</sub>	Disk (MBytes)	CPU (hours)	Date Created	Last Opened
seacoast	developed project	0.196	615.3	7.5145	2024-01-28	2024-01-29

Powered by CCP4 v.8.0.017

CCP4 MRC Harwell Research Complex at Harwell iris

CCP4 Cloud v.1.7.018 [10.01.2024]

[0012] modelcraft -- completed

• Input • Output

Report Main Log Service Log Errors

<i>Nwaters</i>	118
<i>R-factor</i>	0.202
<i>R<sub>free</sub></i>	0.231
<i>Completeness</i>	94.7%
<i>EDCC</i>	0.947
<i>Clash score</i>	6.59

• all scores are optimal for auto-build procedure.

• all scores are optimal for auto-build procedure.

[0012] Built Structure <sup>i</sup>

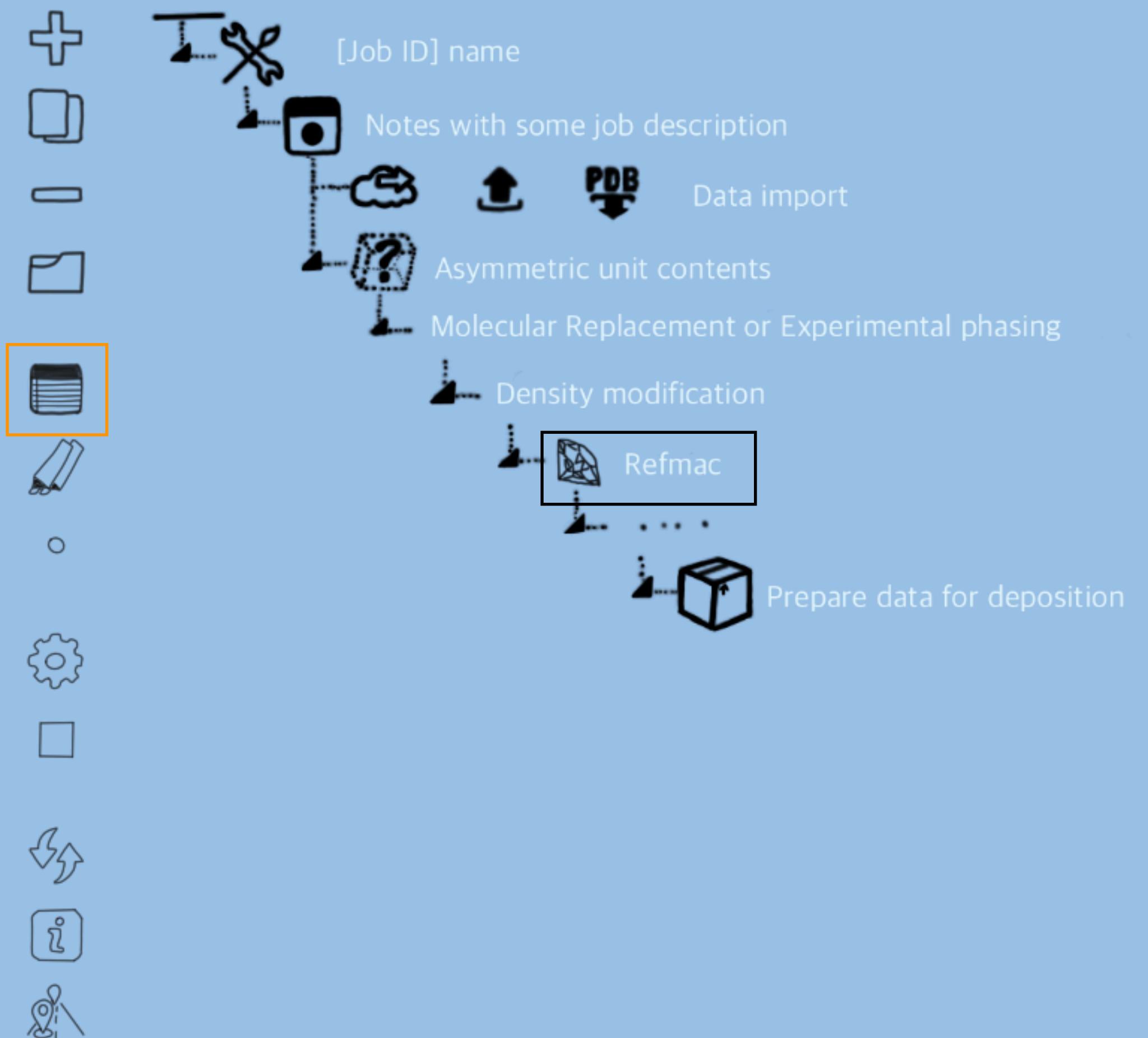
Assigned name: [0012-01] modelcraft /structure/

Structure and electron density UglyMol ViewHKL Display

0012-01\_modelcraft.pdb Export

0012-01\_modelcraft.mtz Export

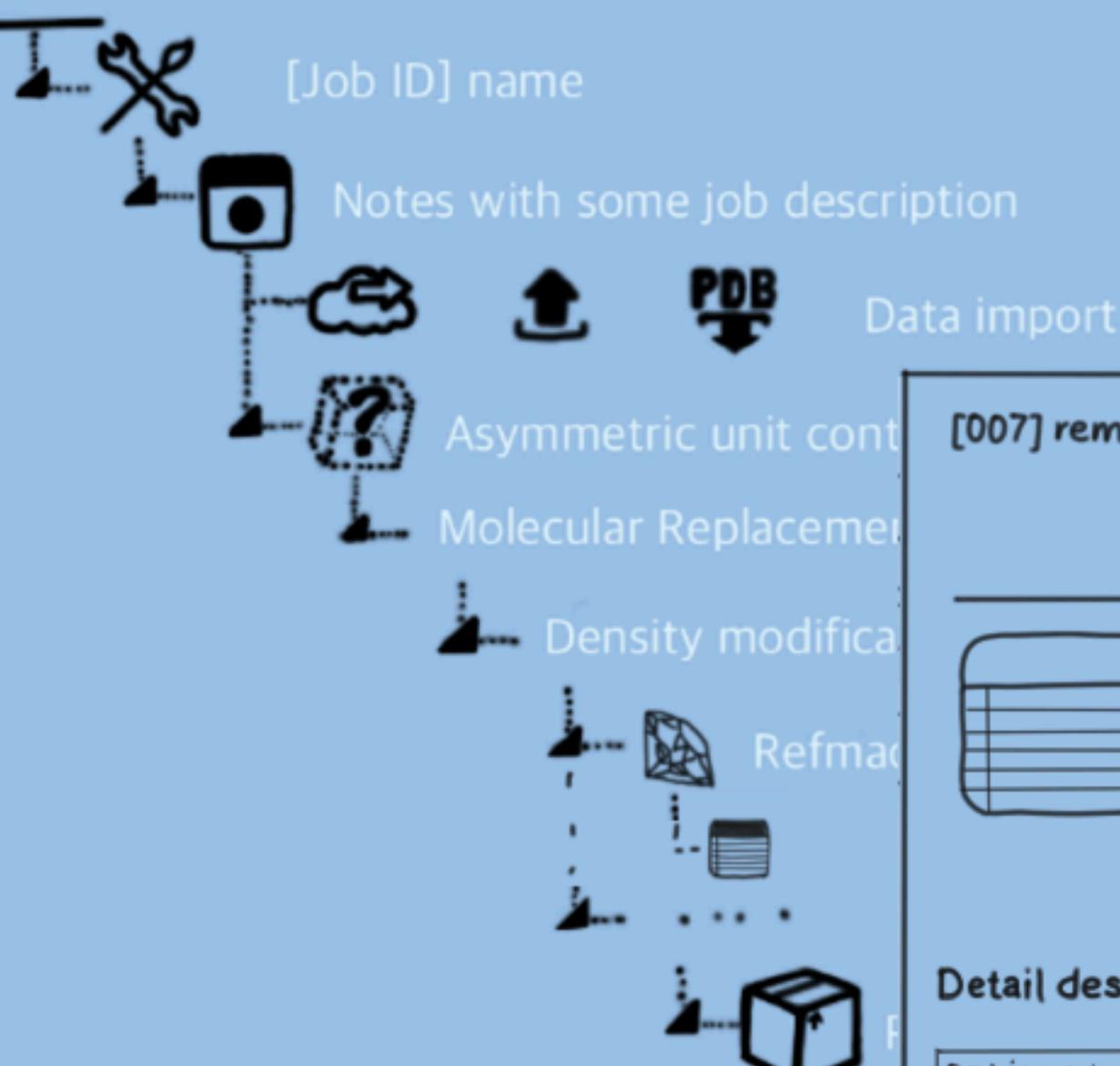
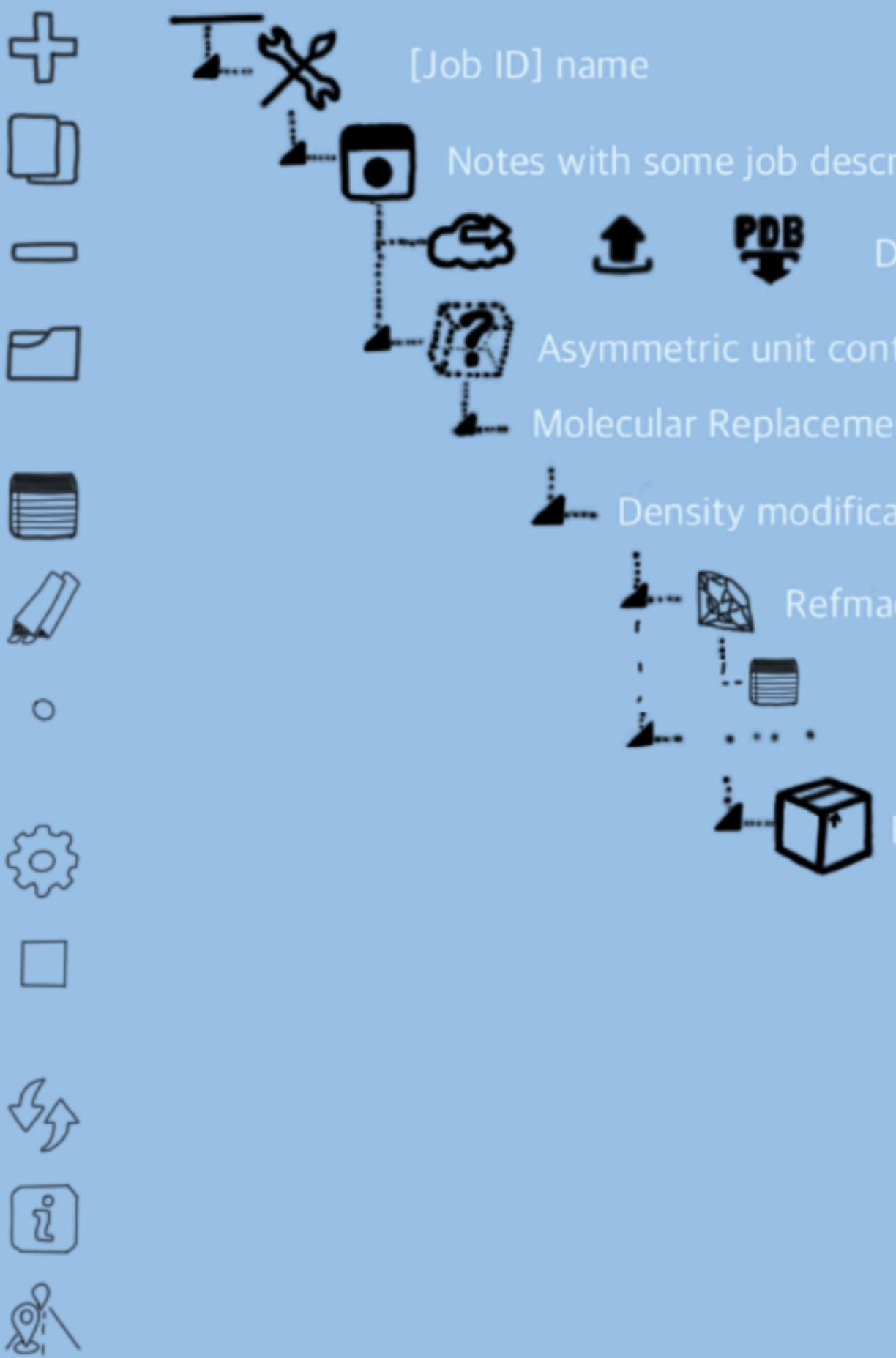
Download data



Remarks



User's name



[007] remark

Custom remark

Remark title:

Detail description

Optional detail description may be placed here

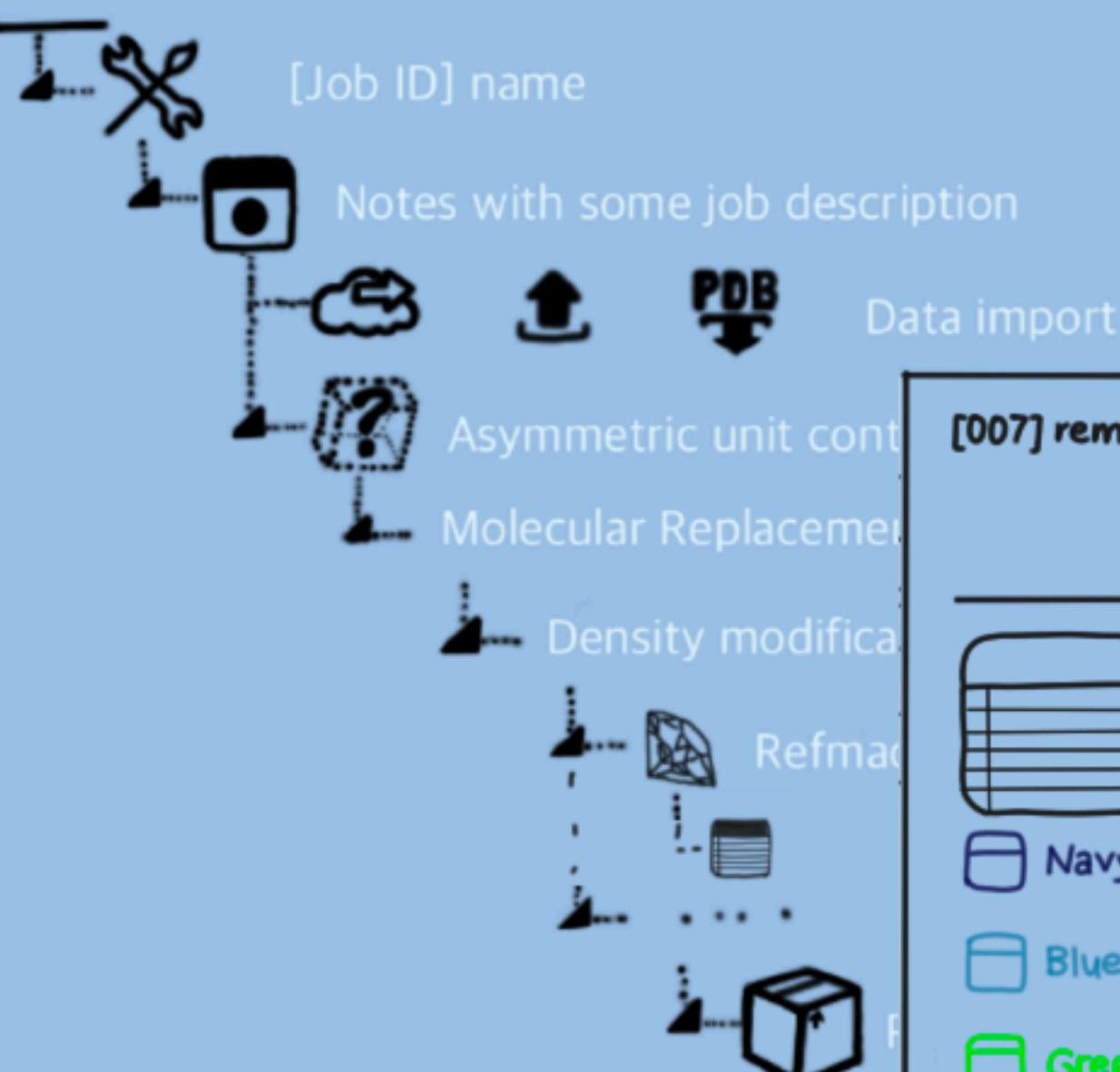
Icons at the top of the dialog: +, -, i, Close.

Remarks



Wi-Fi %

User's name



[007] remark

Custom remark

Remark title:

Navy

Blue

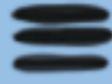
Green

Cyan

description may be placed here

Document link

Remarks



Wi-Fi %

User's name



[Job ID] name

Notes with some job description



Data import

Asymmetric unit cont.

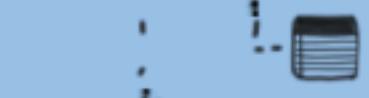
Molecular Replacement



Density modification



Refinement

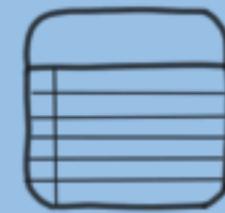


...



Structure

[007] remark



Custom remark

Remark title:



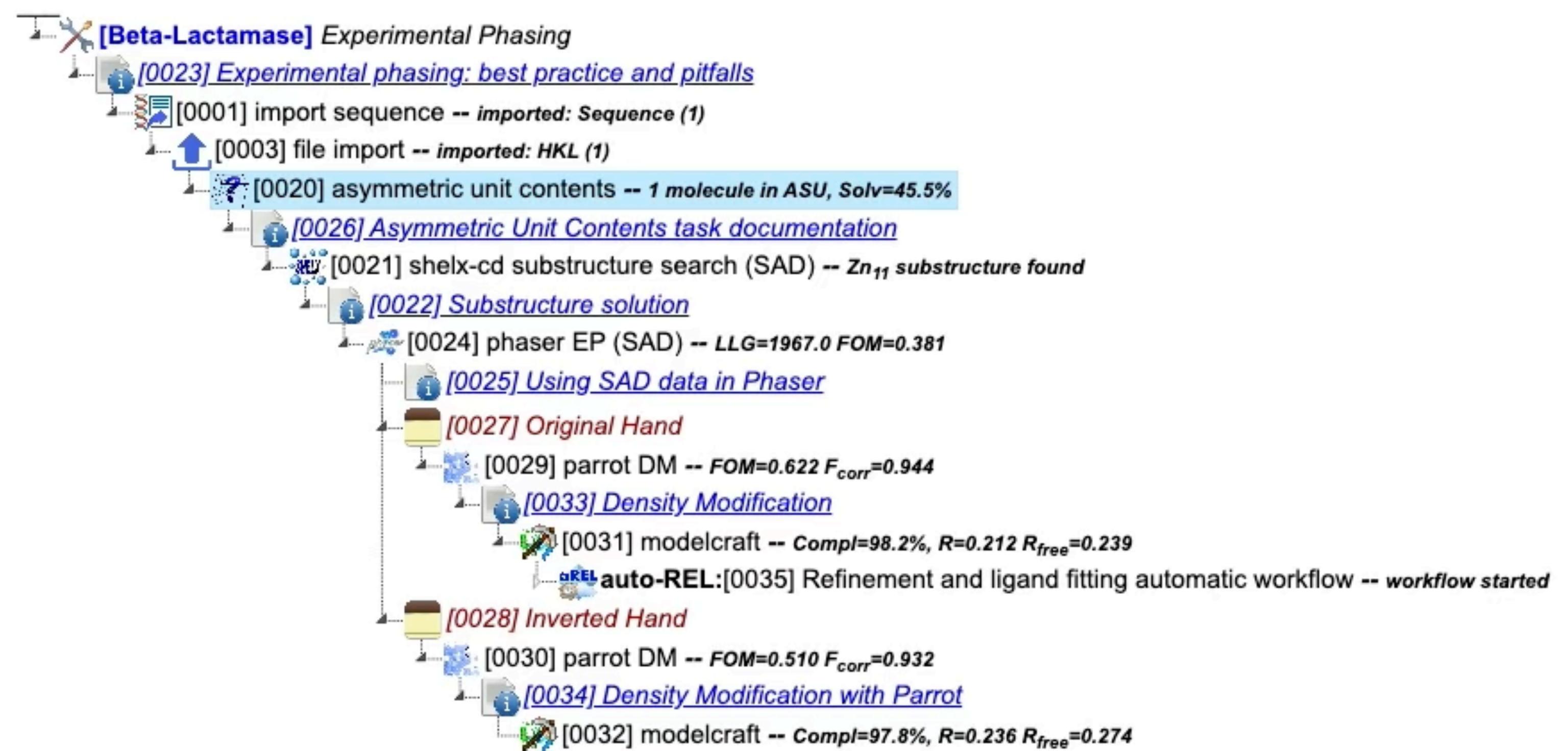
Set Document Link

Link type:

- No link
- Web page
- DOI reference

Remarks

## Experimental Phasing



# Archive

☰ **CCP4 Cloud Archive** ⌂ 77% 0% 0% Maria Fando ↗

Open Access Rename Clone Delist Delete Export Import Join Tutorials Help

Archive ID	ID	Name	R_free	Disk (MBytes)	CPU (hours)	Date Created	Last Opened
------------	----	------	--------	---------------	-------------	--------------	-------------

There are no projects in folder "CCP4 Cloud Archive".

Use "Add" button to create a new Project;  
"Import" button for importing a project exported from CCP4 Cloud;  
"Join" button for joining project shared with you by another user;  
or "Tutorials" button for loading tutorial/demo projects;  
or click on page title or folder icon in it to change the folder.

**Access CCP4 Cloud archive**

**Access CCP4 Cloud Archive**

Access project with Archive ID:

Access Cancel

Powered by CCP4 v8.0.007 CCP4 Cloud v1.7.008 [04.01.2023]

# Archive

Online Help

CCP4 Cloud 1.7 documentation

CCP4 Cloud 1.7 documentation

Search

CCP4 Cloud 1.7 documentation

## 4. CCP4 Cloud Archive

CCP4 Cloud projects can be archived for long-term storage, free access and making external references. This article describes the archiving procedure and working with archived projects.

**Note**

Functionality, described in this article, requires appropriate CCP4 Cloud configuration.

**Contents**

- 4. CCP4 Cloud Archive
  - 4.1. General description and use cases
  - 4.2. Before archiving
  - 4.3. Archiving procedure
  - 4.4. Accessing projects in CCP4 Cloud Archive
  - 4.5. Revising projects in CCP4 Cloud Archive
- 4. CCP4 Cloud education capabilities
- 6. Questions and Answers
- 7. Troubleshooting
- 8. CCP4 Cloud Version Log

4.1. General description and use cases

CCP4 Cloud archive is a collection of projects referenced by stable identifiers, Archive IDs. Upon archiving, the project is moved to a designated area in CCP4 Cloud storage, and the corresponding disk quota is released for the project owner. Archived projects are frozen in their state at the time of archiving; no jobs can be deleted from them. [However, new jobs and project branches can be added and the project author can archive thus revised projects under the same Archive ID.](#)

The main purpose of project archiving is to provide supplementary information for scientific publications and other reports, where structure solution may be demonstrated by quoting the corresponding Archive ID. Projects may also be archived for sharing structure solution experience and practices, especially in difficult cases, and for general education purposes. In institutional or laboratory setups, CCP4 Cloud archives may be used for organising work results and preserving data and the history of extended

Back Forward Return Detach Close





Archive

## Example

**CCP4 Cloud Archive ID:** **CCP4-RNASE** (could be published in a paper on web-site etc.)

**Access URL:**

<https://cloud ccp4.ac.uk/archive/access.html?id=CCP4-RNASE>

**Consider archiving completed projects in CCP4 Cloud when publishing your work**

- share your knowledge and findings
- regain your storage quota in CCP4 Cloud

# Share Project

The image shows two CCP4 Cloud windows side-by-side.

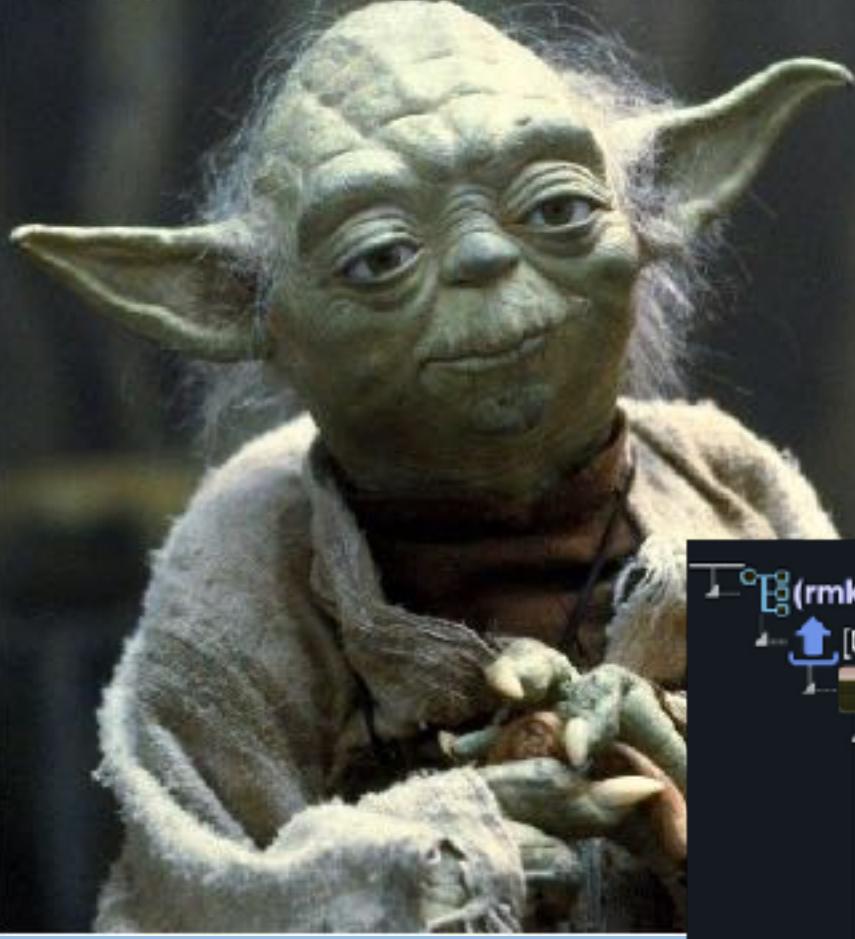
**Left Window: 'auto'**

- Shows a detailed log of an automated workflow named 'WF\_demo'.
- Workflow steps include: auto-MR, simbad, auto-MR, auto-MR, simbad, modelcraft, xyz Util, auto-MR, refmacat, fit waters, refmacat, refmacat, refmacat, refmacat, refmacat, PDB validation report, and a final message stating "Automated Workflow has finished successfully (look inside for comments)".
- Metrics shown: CC<sub>1,2</sub>=0.998, R<sub>meas\_all</sub>=6.070, R<sub>meas\_pro</sub>=0.068, Res=1.25-61.93 SpG=P 61 2 2.

**Right Window: 'All projects'**

ID	Name	R <sub>free</sub>	Disk (MBytes)	CPU (hours)	Date Created	Last Opened
(tutorial)s):T2_006	Determining the Structure of Twinned Crystals Using Molecular Replacement	15.3	0.0011	2023-09-20	2024-01-19	
1ejg	1ejg	0.1394	217.5	12.0802	2022-10-07	2024-01-19
A4.1.1	Solving protein-nucleotide complex with Phaser and Arp/wArp (NUCE)	0.3605	79.8	0.911	2022-12-28	2024-01-19
D02	Staged solution of Insulin structure with EP on sulphur atoms	0.1888	164.4	1.6017	2019-12-10	2024-01-19
Mva	Mva CMP	0.1898	2685.8	22.5195	2018-05-17	2024-01-19
hem	hemoglobin	0.1875	2698	10.5676	2022-08-02	2024-01-19
[eugene]:mcm2	MDM2 protein bound to the inhibitor nutlin 3A	0.2377	773.1	5.8365	2023-08-07	2024-01-19
mpro_x0692	SARS CoV-2 main protease with bound ligand MR	0.3144	660.8	5.321	2021-07-29	2024-01-19
(andrey):nz4pv-twinn	Pv NZ4 twinned	0.224	848.5	4.6465	2023-08-23	2024-01-19
le	ret4ae4y	0	0	2024-01-18	2024-01-18	
MCCS_2	try	0.2108	962.4	16.3739	2023-05-04	2024-01-09
Morda	Morda	0.5152	488.6	35.981	2021-06-24	2024-01-09
[martinmalay]:hnkrp1glyco	hnkrp1glyco	0.2236	632.3	0.6742	2023-05-05	2023-12-08
(setests):aepWFTest	aepWFTest	0.235	308.9	0.9115	2023-11-10	2023-11-13
Beta-Lactamase	Experimental Phasing	0.2068	557.8	7.1933	2021-11-18	2023-11-10
[paul.bond]:mbiutidea	Model Building Tutorial	0.238	1622.0	24.6082	2023-10-17	2023-11-09
[eugene]:dna	DNA	0.2258	51.9	1.3758	2019-12-03	2023-11-07
(tutorial)s):T4_002	Refinement using REFMAC5 - Part 2: Twin Refinement	0.3173	2133.8	14.2268	2021-12-08	2023-10-19
[rmk65]:T1145	T1145	0.2902	1815.5	126.7775	2022-10-24	2023-10-17
[olga.moroz]:disp37	disp37	0.2105	2596.8	2.2586	2023-06-20	2023-08-25
NULL	NULL initiated by script	0.171	58.9	0.324	2023-01-12	2023-08-23
(tutorial)s):T4_006	Moorhan Tutorial 1: Fix up the Cyclin-Dependent Kinase	6.1	0.0004	2023-05-11	2023-08-21	
[eugene]:arcimboldo-tests	Arcimboldo tests	58.2	15.1193	2021-02-22	2023-08-17	
dip_test	test	0.3343	108.6	0.6546	2023-03-28	2023-08-17
AF_workflow	demo	0.2874	249	7.7189	2022-12-20	2023-08-16
ranker	try	80.7	0.0027	2023-04-04	2023-08-15	
[monjoe]:DeoxyHb	deoxy horse hemoglobin, 07032021	0.1507	591	7.144	2022-09-20	2023-07-27
Demo1	Demo	0.2458	120.1	0.1905	2021-07-13	2023-05-24
T4_004	Paired refinement with PaRef	477.5	0.0937	2023-05-15	2023-05-15	

JOINED THE DARK SIDE HE HAS



Dark theme

E(rmk65):[AF-workflow]

[0001] file import -- Imported: HKL (1) XYZ (1) Sequence (1)

[0002] Upload reflection data, sequence and AF model

[0026] modelcraft -- completed

0026-01\_modelcraft Structure and electron density

This is uglymol not coot. H shows help.

Input • Output

Report Main Log Service L

Build summary

$N_{\text{residues}}$	134
$N_{\text{waters}}$	5
R-factor	0.255
$R_{\text{free}}$	0.295
Completeness	78.8%
EDCC	0.092
Clash score	12.1

[0026] Built Structure<sup>1</sup>

Assigned name: [0026-01] modelcraft

Structure and electron density

[0026] Structure Revision

Inspect Name: "R0026.01: modelcraft"

[0026] Quality Assessment

B-Factors Analysis

af-MR:[0052] phaser MR --  $N_{\text{ref}}=1$  LLG

af-MR:[0053] refmac5 -- R=0.4253 R<sub>free</sub>

af-MR:[0054] modelcraft -- Compr=8.8% R=0.202 R<sub>free</sub>=0.3124

af-MR:[0059] refmac5 -- R=0.2475 R<sub>free</sub>

af-MR:[0060] refmac5 -- R=0.2462 R<sub>free</sub>=0.3081

af-MR:[0061] fit waters --  $N_{\text{waters}}=29$

Dark Mode Tune-up

Dark Mode parameters

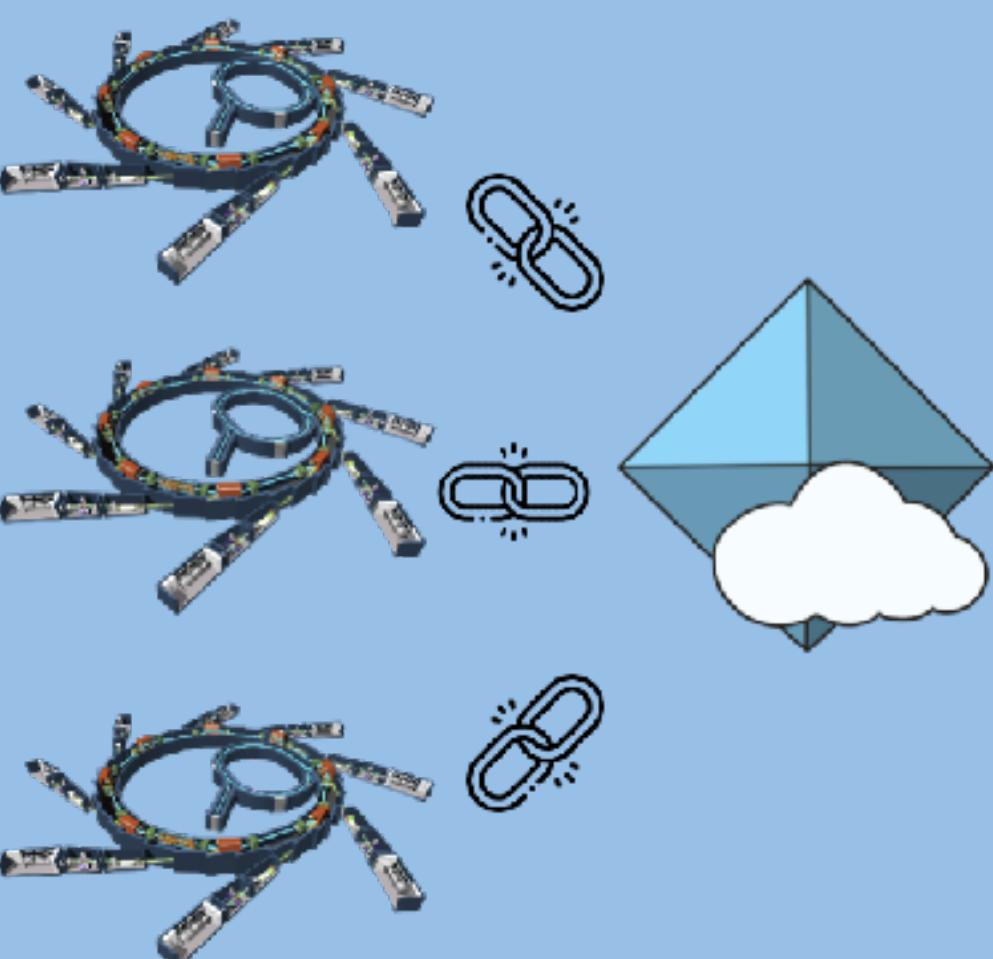
Preferred mode: Dark

Invert Sepia HUE Saturation Contrast Brightness Gray scale

Save mode Reset mode

A 3D molecular structure visualization showing a protein backbone (yellow sticks) and side chains (green sticks) overlaid with a blue electron density mesh. A small green arrow points towards the structure. A 'Dark Mode Tune-up' panel is open on the right, containing sliders for various color and contrast parameters.

# Data link



Home Calendar Logout

diamond

Data Collections > i04 > mx37045-37

Proposals mx37045 Projects Unit Cell Search Feedback Help (PDF)

Following a filesystem upgrade in the recent shutdown, accessing some historical files and reprocessing data through ISPyB may be affected for a short while - please bear with us. Run 3 runs to 8th August. MX Users please ship dewars from 10th June. Please report any SynchWeb / ISPyB issues to your local contact. X

### Data Collections for mx37045-37 on i04

The raw data from this visit have been archived. You can no longer reprocess data or view full-sized diffraction images.

+ Assign Contouring  Summary  Auto Processing  Visit Stats  Beam  Down  Sample Changer  Reseeding

Search

Data Collections  Grid Boxes  Full Collections  Auto Integrated  Phasing  Processing Errors  Wavelengths  Edge Boxes  MCA Spectra  Robot Actions  Sample Actions  Favourites

15 Page < ( 1 2 3 4 5 6 7 > )

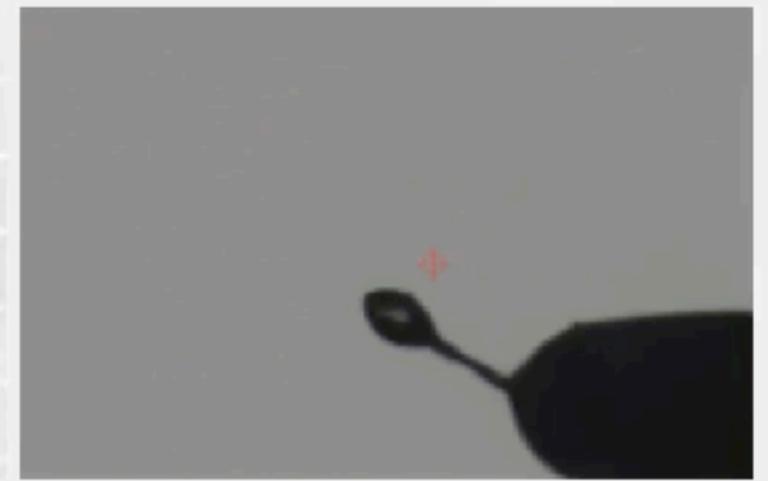
2023-12-14 09:11:08 - EG\_sealmyoglobin/Seal\_28/Seal\_28\_2\_master.h5

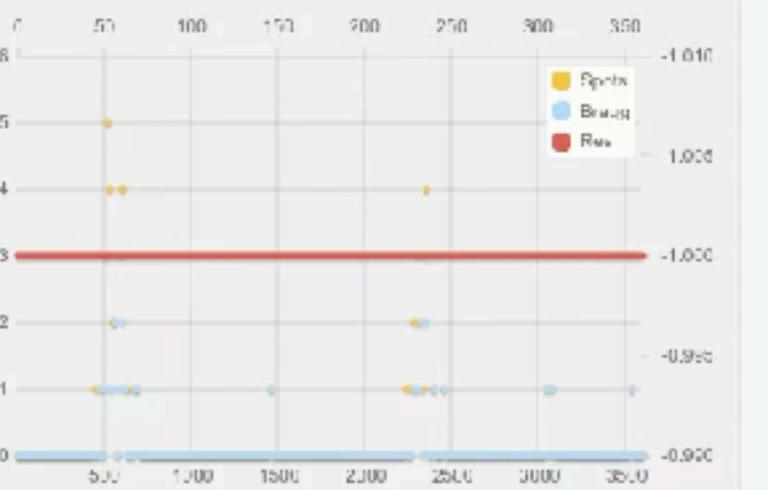
Sample: Seal\_28 Flux: 9.00e+11  
O\_Start: 0.0° O\_End: 0.10°  
O\_Overlap: 0.0° Nu. Images: 3600  
Resolution: 1.29Å Wavelength: 0.9507Å  
Exposure: 0.0066s Dose: 1.60MGy  
Transmission: 100.00% Beamsize: 56x75μm  
Type: SAD

Comments: (522,-361,131) Xray centring boxes: [30.6a (0a), 97, 124.4a (0a), 42] Aperture: Large

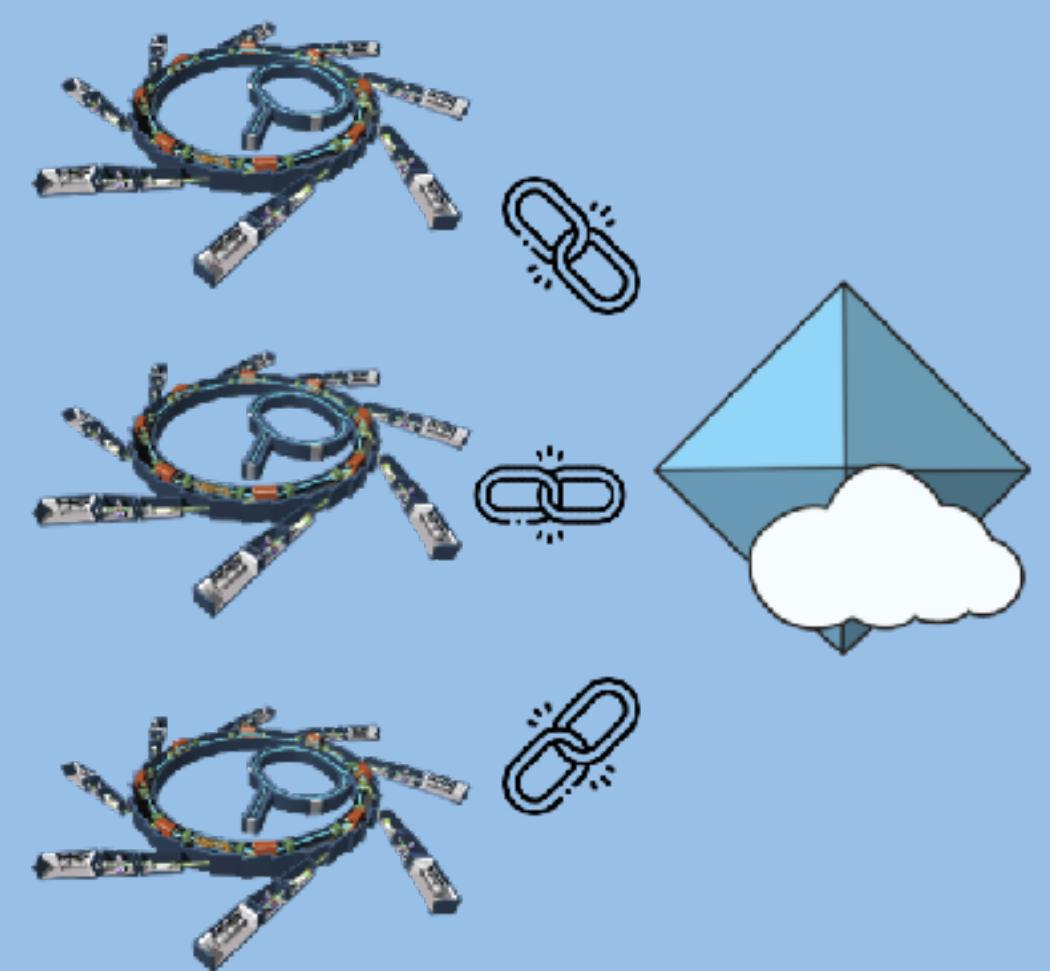
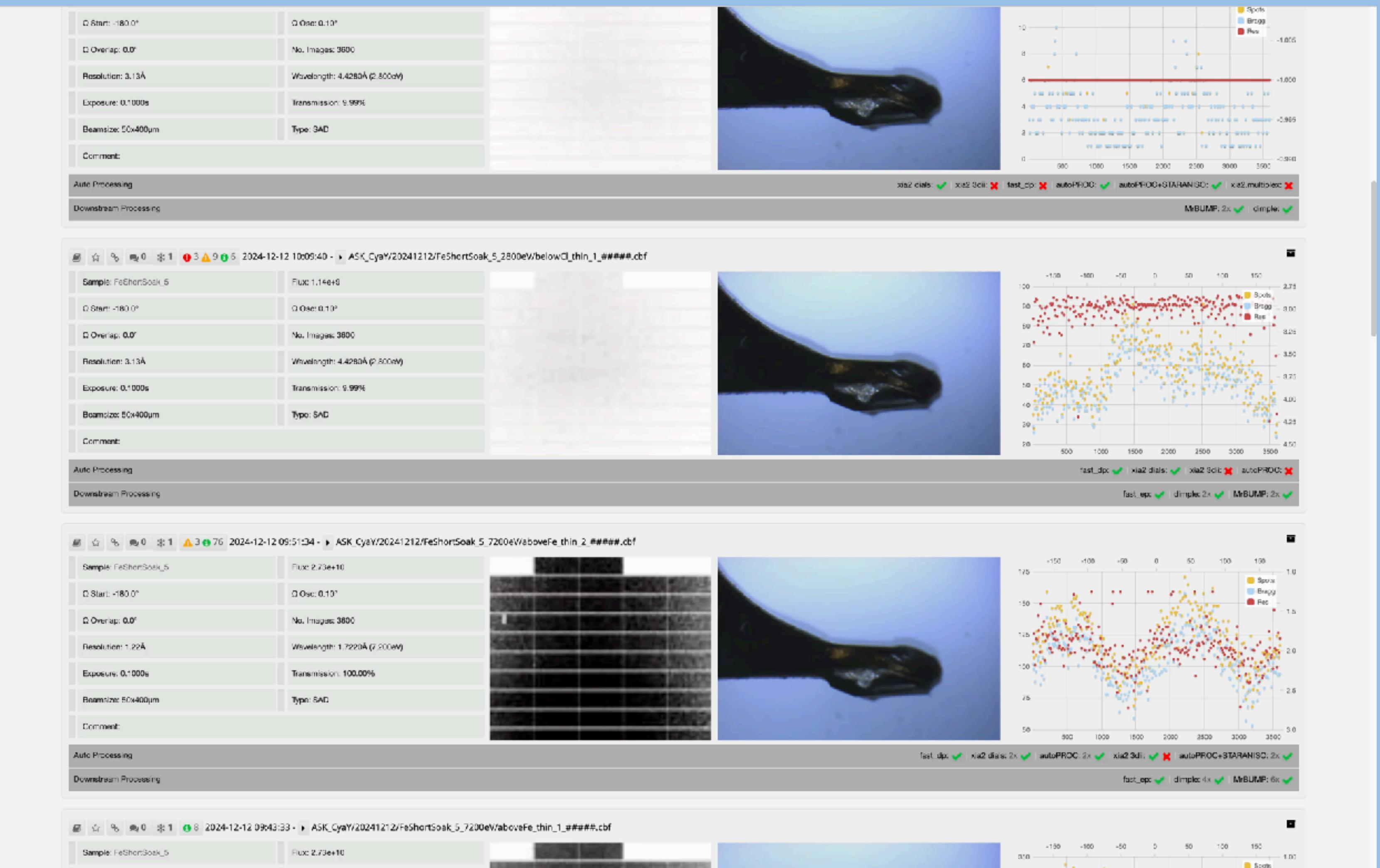
Auto Processing feel\_dps: X xia2\_dials: X autoPROC: X xia2\_3dii: X

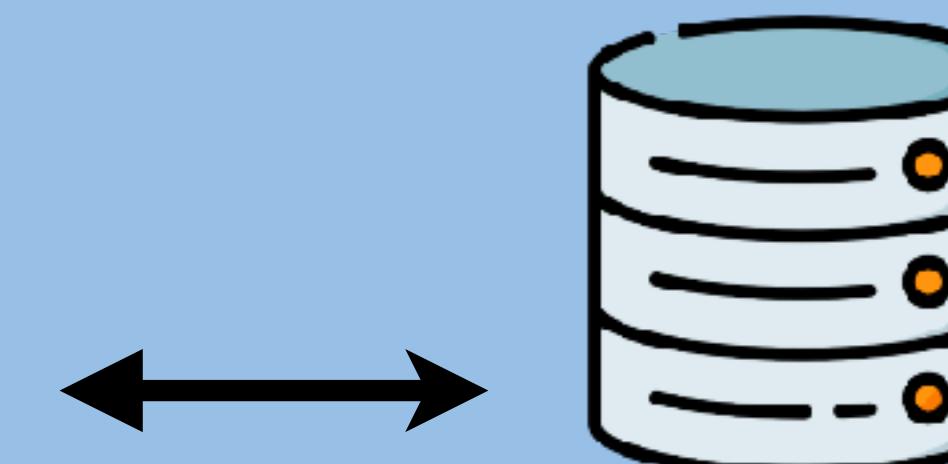
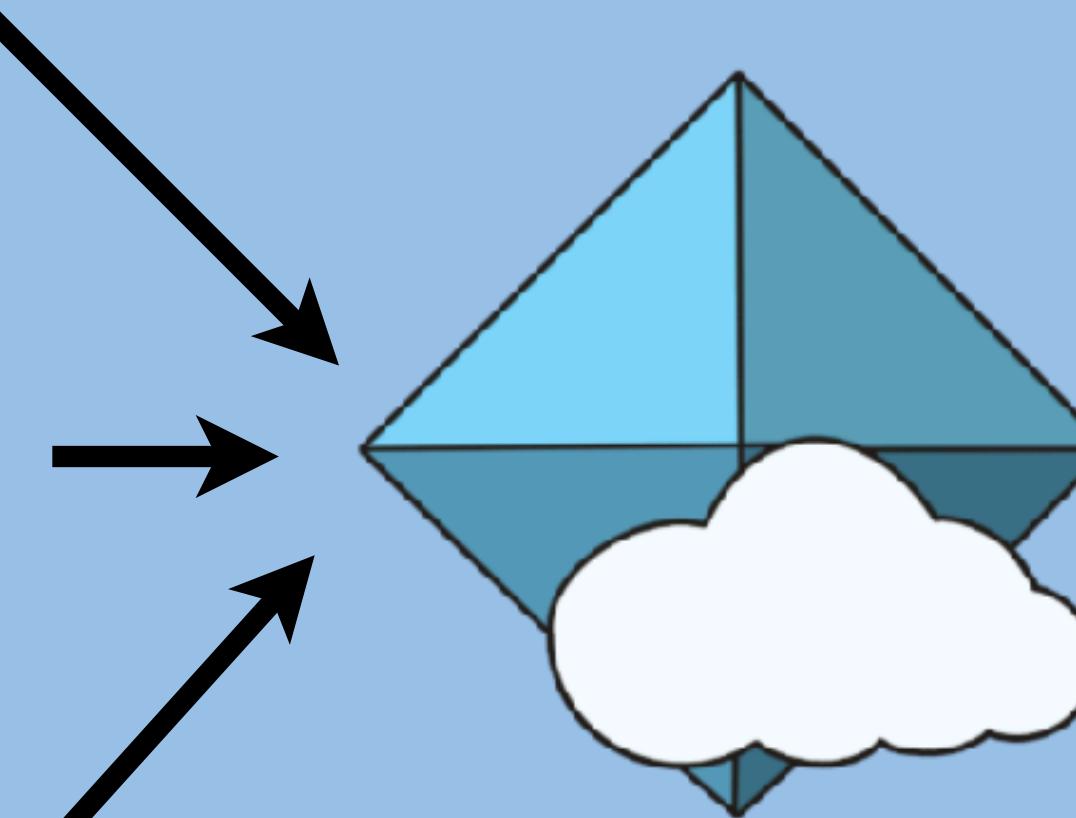
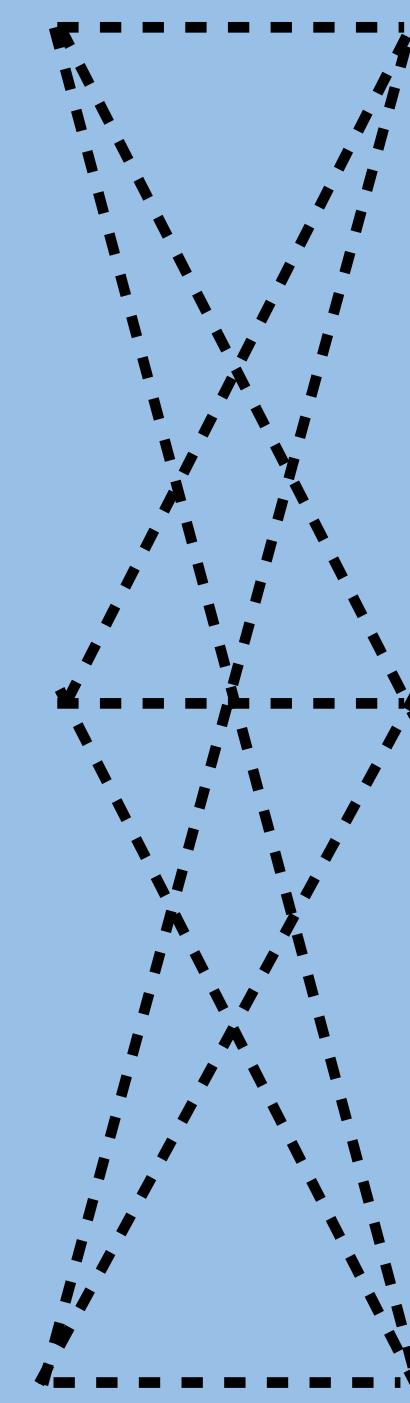
Downstream Processing No processing results





# Data link





WORLDWIDE  
**wwPDB**  
PROTEIN DATA BANK

*Research Labs*



*Imaging Facilities*



*Structure Solution*



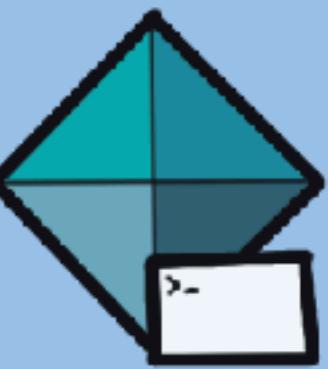
*Data Bank*



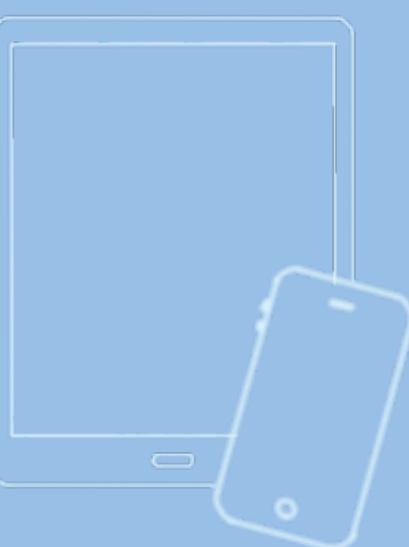
*Utilisation*



Key features

A large, light blue rectangular callout box with a black border and a white interior. It is positioned below the character and to the right of the laptop. The text inside the box is as follows:

24/7 access to considerable computing resources,  
maintained software setup and data backup



Key features

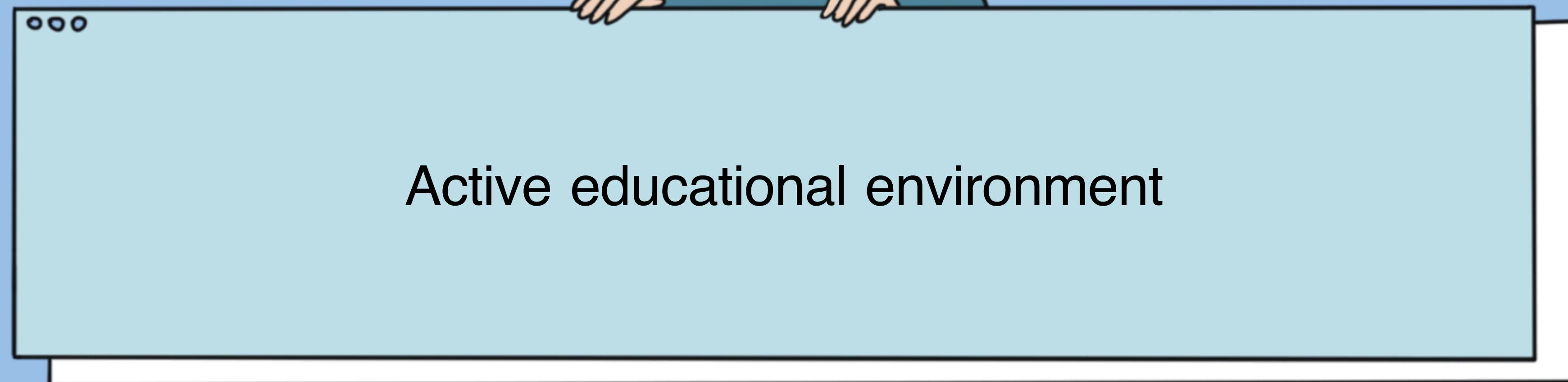


Cross-platform compatibility and high accessibility



Key features

Active educational environment



# Acknowledgments

STFC, CCP4, Harwell, UK:

**Eugene Krissinel, Andrey Lebedev, Oleg Kovalevskyi, Jools Wills, Ronan Keegan, Charles Ballard, Ville Uski, Jools Wills**

Newcastle Uni UK:

**Martin Noble**

Uni Southampton UK:

**Ivo Tews**

MRC/LMB, Cambridge, UK:

**Robert Nicholls**

EMBL-EBI, Hinxton, UK:

**John Berrisford**

Uni Leiden, The Netherlands:

**Navraj Pannu, Pavol Skubak**

Global Phasing Ltd, Cambridge, UK:

**Marcin Wojdyl, Clemens Vonrhein**

Uni York, UK:

**Stuart McNicholas, Filomeno Sanchez Rodriguez, Paul Bond**

Uni Liverpool, UK:

**Adam Simpkin, Jens Thomas**

Uni Birmingham, UK:

**Christopher Oliver**

**CCP4, STFC & RCaH**

**CCP4 Collaboration,  
CCP4 developers**

**CCP4 Cloud users  
Worldwide**

**CCP4 School hosts**

**Ed Lowe**

Oxford University

**Andy Purkiss**

*Francis Crick Institute, London*

**Grzegorz Chojnowski**

*EMBL-Hamburg*

**Arnaud Basle**

*Newcastle University*

**Michael Isupov**

*University of Exeter*

**Biotechnology and Biological Sciences Research Council (BBSRC) UK**

*Fantastic work environment,  
support and dissemination*

*Contribution of task reports,  
general support and  
valuable feedback*

*Trial use and feedback on development  
versions of CCP4 Cloud*

*Using CCP4 Cloud as a  
teaching platform*

*Creating  
Oxford\_UG course*

*Setup and  
maintenance  
of CCP4*

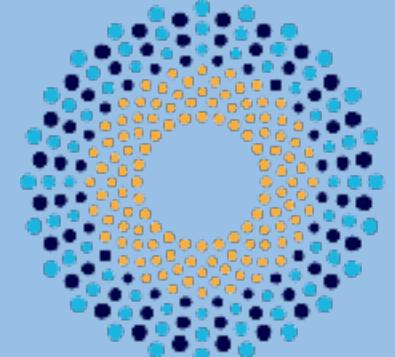
*Cloud*

*instances in  
their home  
labs*

*Research grant  
BB/L0070317/1  
(2014-2019)*



Research Complex  
at Harwell



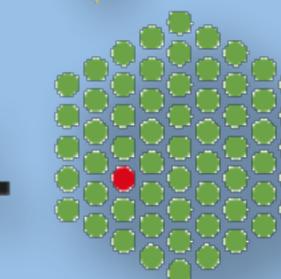
**iris**



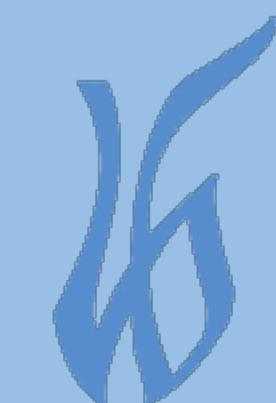
Science and  
Technology  
Facilities Council



**EMBL**



European Molecular  
Biology Laboratory



Biotechnology and  
Biological Sciences  
Research Council

*Research grant  
BB/L0070317/1 (2014-2019)*

