

# **Welcome!**

**8th DLS-CCP4 Data Collection and  
Structure Solution Workshop**

# Welcome to the Virtual Space!

In order to make the Workshop most efficient, help tutors and each other, please:

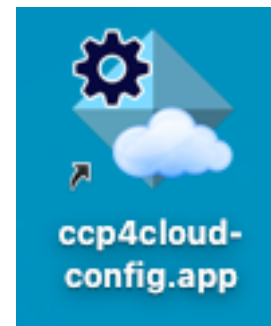
- **Use your full name** when on Zoom/Slack, so that others know who you are
- **During a talk/presentation:**
  - ~ *Ensure your video/audio are off*
  - ~ *Post questions in the chat*
- In any other moment:
  - ~ *Feel free/you are encouraged to keep your video and audio on*
  - ~ *Just speak up to ask a question*
- What we expect – our **code of conduct**:
  - ~ The Diamond-CCP4 Data Collection and Structure Solution Workshop is an inclusive event where people should feel comfortable sharing their work, opinions, and perspectives. All of us commit to engaging with each other mindfully to ensure an environment that promotes shared learning and collaboration.

# How to get the most out of the workshop

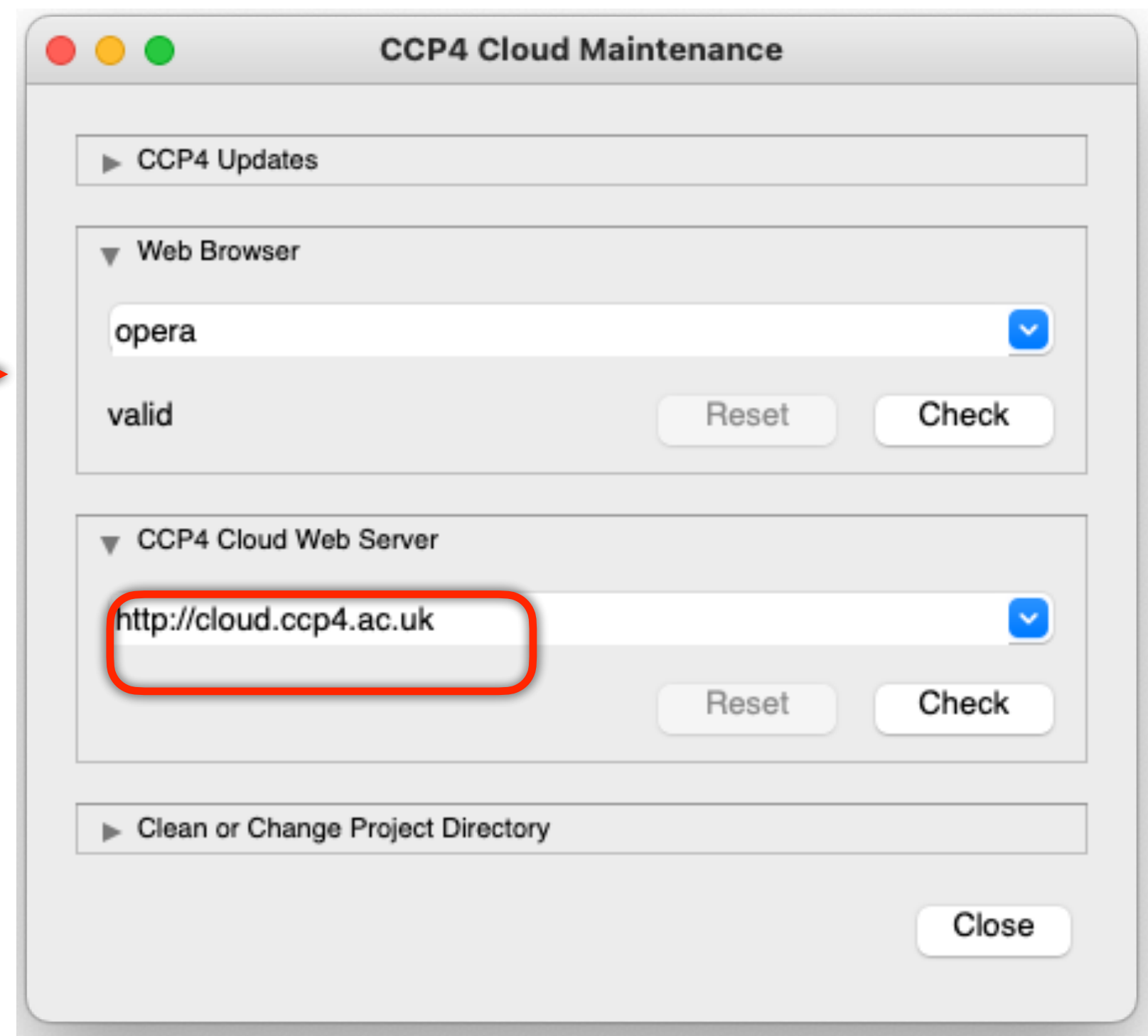
- **Ask questions!** The tutors are experts and developers of the software you will use. They are not all available for the full week, please approach them if you need help.
- **Talk to your each other.** The attendees at the course have various levels of expertise and scientific backgrounds. You may learn from each other and not just the tutors.
- **Take your time.** You will get the most out of the tutorials if you work through each step carefully and think about what you are doing
- **Course materials** will be uploaded to the website [https://www.ccp4.ac.uk/schools/DLS-2021/course\\_material.php](https://www.ccp4.ac.uk/schools/DLS-2021/course_material.php), so don't feel you have to copy every slide. You will have them available at the end of the workshop.

# A few more points of the moment

- **If you still have problems with software setup and data upload:** post a message to the # help-computer channel on the Slack and we will help you out.
- **Your posters:** please upload them to *your own Slack channel*. Each upload will start a thread, in which the poster discussion will then take place asynchronously by Slack chat
- **CCP4 Cloud:** set http protocol in local configuration:



https can be used when connecting directly from browser. This will be corrected in next CCP4 update.





If progress you make during the workshop leads to published results we ask that you please acknowledge this in your papers. We will link to them on our website. This helps us to keep delivering similar workshops in the future.

*We wish you every success with your projects!*



Collaborative Computational Project No. 4  
Software for Macromolecular X-Ray Crystallography



[Course home](#)

[2021 home](#)

[Programme](#)

[Event information @ DLS](#)

[Course material](#)

## DLS-CCP4 Data Collection and Structure Solution Workshop *November 29th – December 10th 2021*



### Workshop Announcement

We are very pleased to announce the eighth joint Diamond-CCP4 MX workshop for graduate students, postdocs and early career scientists. As last year, the event remains online due to the COVID-19 pandemic. Data collection will take place at Diamond Light Source, on the Harwell Oxford campus in Oxfordshire, UK.

All aspects of structure solution will be covered during the workshop, from data collection through to phasing, refinement and validation.

- Lectures and tutorials will be delivered by experts in the field
- One day of data collection time will be provided at Diamond's excellent MX beamlines



DLS-CCP4 Data Collection and Structure Solution Workshop  
November 30 - December 10, 2020, Diamond Light Source Ltd., UK

# ***Introduction to CCP4: Project and Software***

Eugene Krissinel & Ronan Keegan

CCP4, Research Complex at Harwell  
Didcot, Oxfordshire, UK

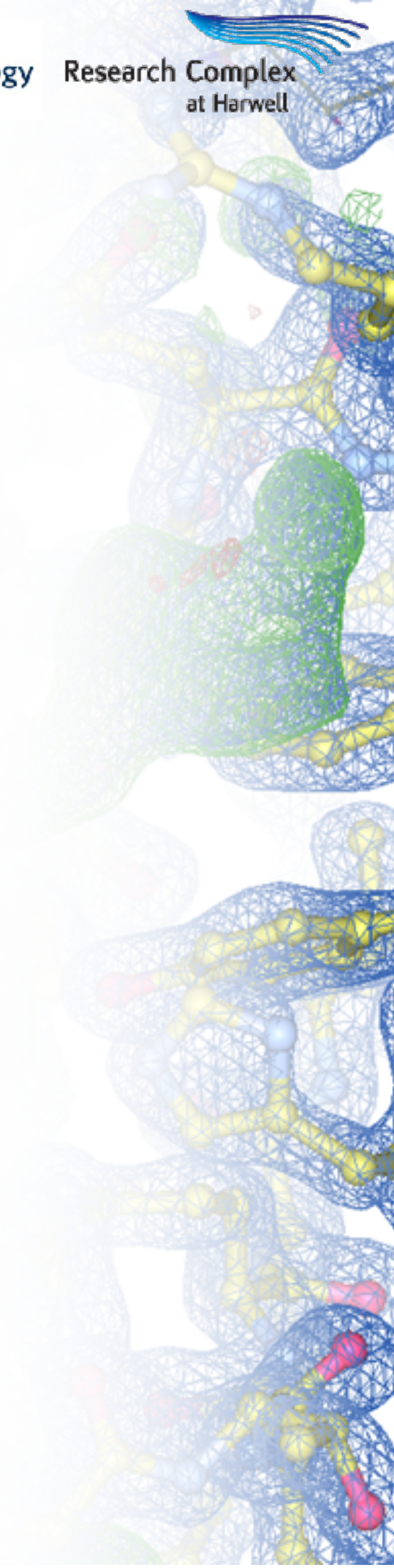


Science & Technology  
Facilities Council



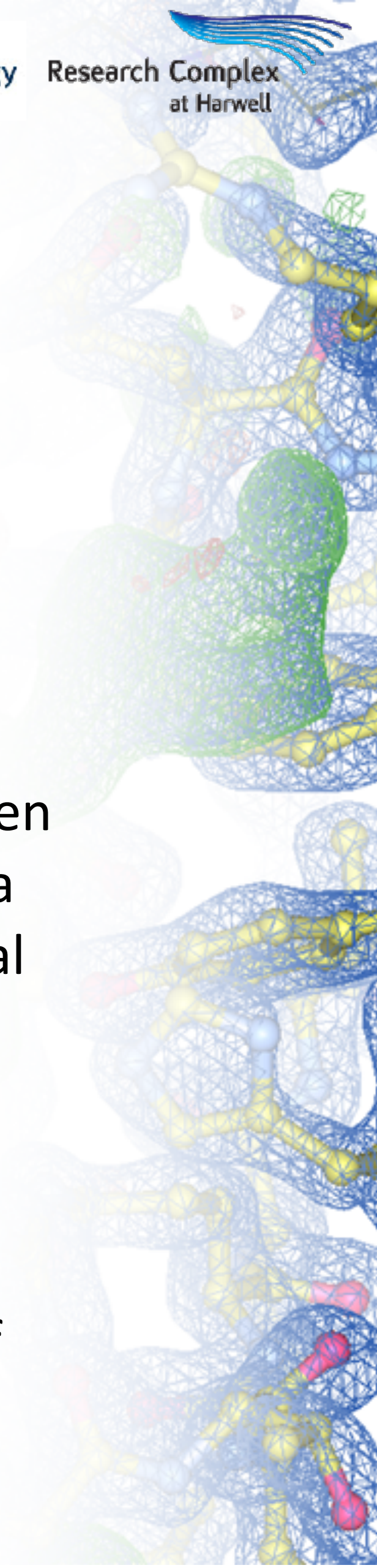


# A Project with History



# What is CCP4?

- CCP4 stands for “*Collaborative Computational Project No. 4 in Protein Crystallography*”
- One of several CCPs set up in the UK to advance and support scientific software developments
- CCP4 was formally set up in **1979** to support collaboration between researchers working on MX software in the UK, and to assemble a comprehensive collection of software to satisfy the computational requirements of the relevant UK groups
- Funded by the Biotechnology and Biological Sciences Research Council (BBSRC) and industrial licensing
- The project is coordinated at Scientific Computing Department of the Science and Technology Facilities Council (STFC)





# Main Activities

- Today CCP4's main activities are:
  - ❖ Supporting the development and distribution of a comprehensive suite of software for performing structure solution in macromolecular crystallography
  - ❖ Providing educational and training events to users of the software including schools/workshops where users can get access to expert assistance with structure solution problems
  - ❖ Providing other resources to the user community including the CCP4BB mailing list, Wiki's and access to web/cloud-based computational resources



# Main CCP4 Groups

## ● *Oxford*

- ~ CCP4 core team – software development, maintenance, distribution, educational outreach and CCP4 online resources
- ~ Diamond – data processing developments (DIALS)

## ● *Cambridge*

- ~ MRC/LMB – software development for refinement (REFMAC) and data processing (MOSLFM, Aimless, etc.)
- ~ Uni. of Cambridge – Phaser development team for phasing software

## ● *University of York*

- ~ Software developments (CCP4mg, Buccaneer, Privateer)
- ~ CCP4 GUI-2 developments





# Main CCP4 Groups

- *University of Liverpool*

- ~ AMPLE (ab-initio MR)
- ~ SIMBAD (sequence-less MR)

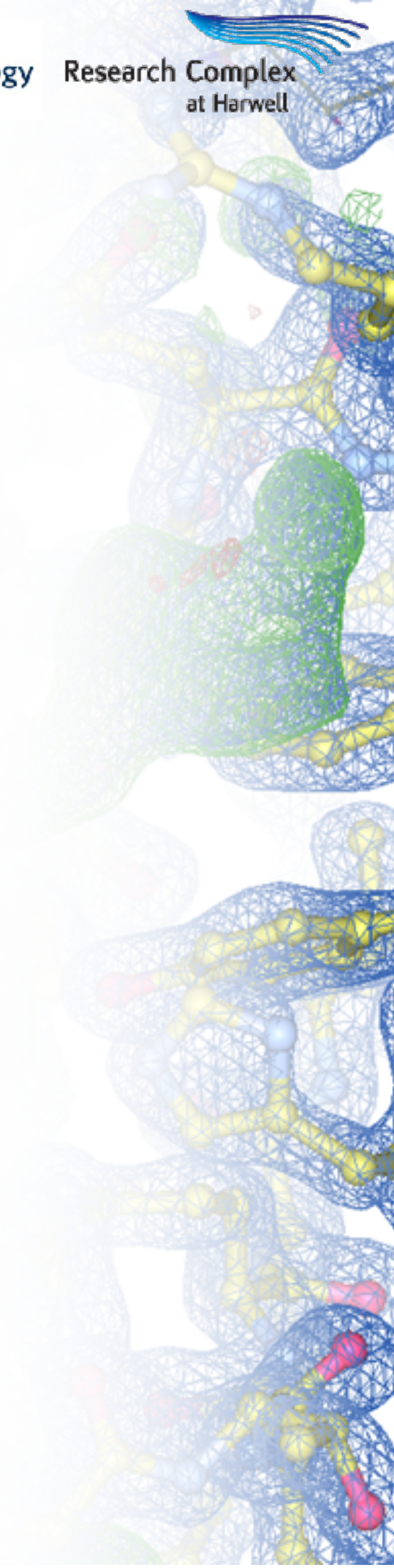
- *Associated projects*

- ~ ARP/wARP (Model building, EMBL-Hamburg)
- ~ PDB redo (Validation and completion, NKI, the Netherlands)
- ~ SHELX (Experimental phasing, Goettingen and Barcelona)
- ~ Arcimboldo (Fragment-based MR, Barcelona)
- ~ Crank-2 (Automated experimental phasing, University of Leiden, The Netherlands)





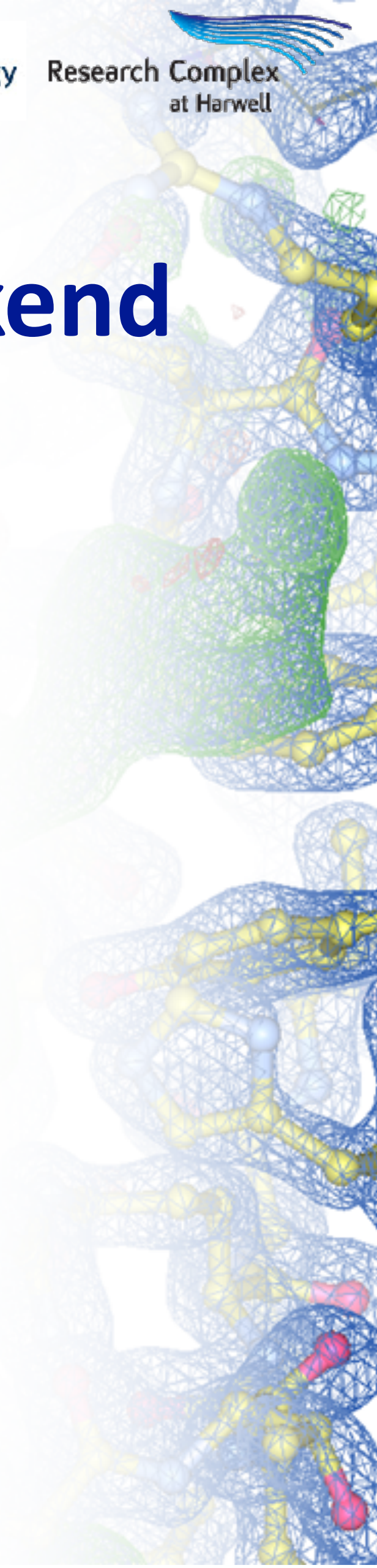
# Educational Outreach





# CCP4 Main Event: the Study Weekend

- Takes place every January in the UK
- Each year tackles a different topic:
  - ~ Data processing
  - ~ Experimental phasing
  - ~ Molecular replacement
  - ~ Model building and refinement
  - ~ Related topics: Complementary methods (EM, NMR, SAX etc.), Structure analysis, Complexes, Ligands, Databases
- Lectures streamed live on the internet





# CCP4 Study Weekend

- Proceedings published in special edition of **Acta Cryst. D**

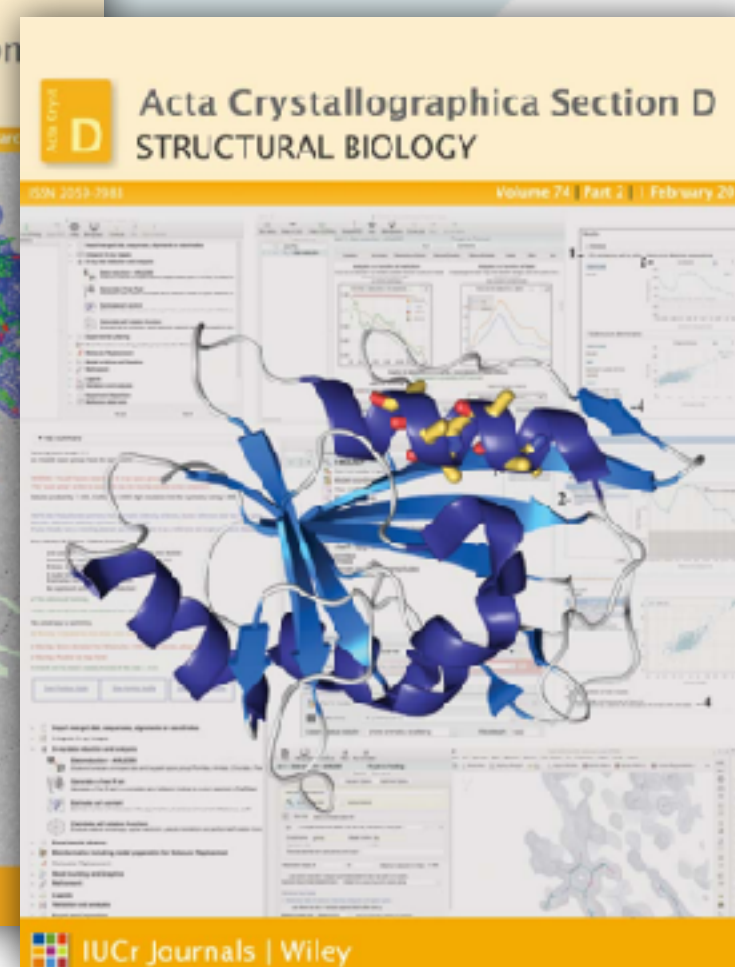
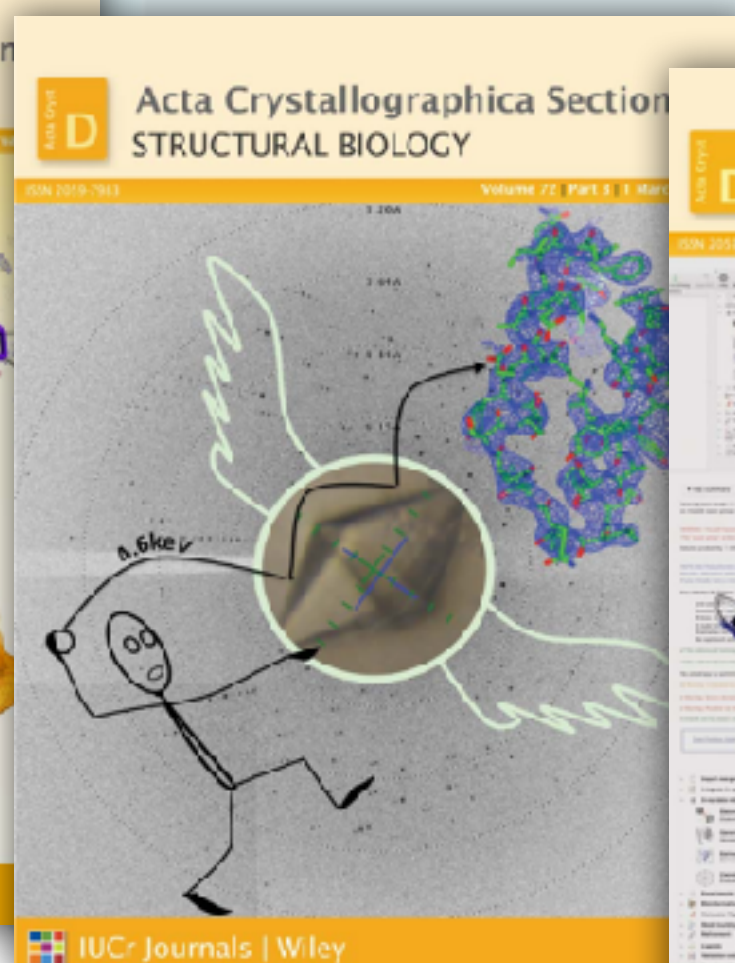
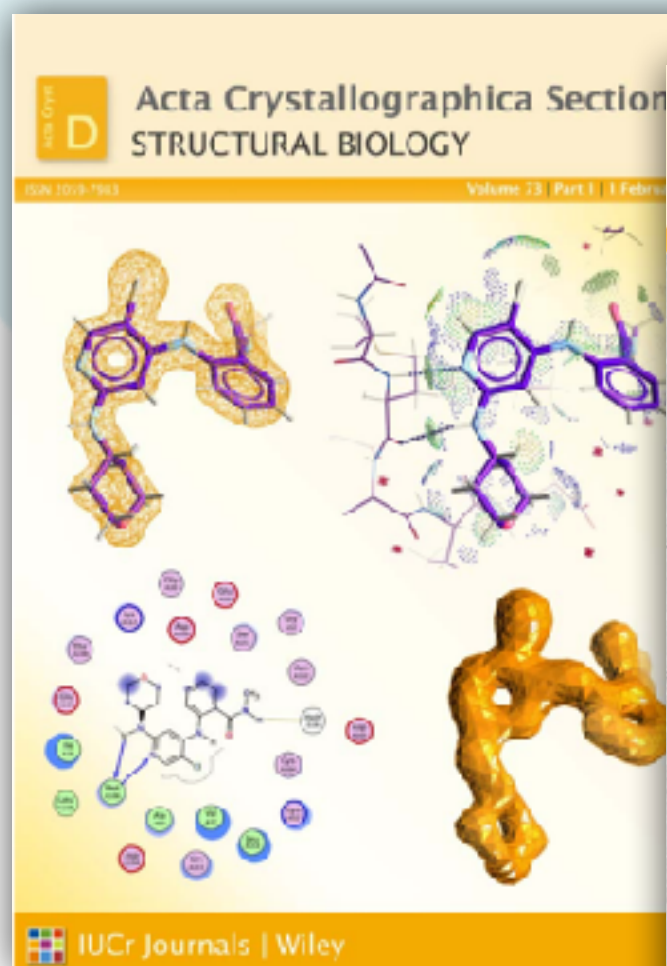
2017: *“From crystals to structure with CCP4”*

2018: *“Multi and Serial Crystal Data Collection and Processing”*

2019: *“Molecular Replacement”*

2020: *“Model Building”*

2021: *“Integrating Structural Biology”*





# CCP4 Schools and Workshops

- Main aim is to give education and expert help to researchers working with collected crystal data
- Some schools also provide expert help with collecting crystal data (APS, Hamburg, Diamond)
- Applicants with challenging crystals and/or data are given strong consideration but this is not mandatory
- Software developers from CCP4, Phenix (APS Workshop), SHELX, ARP/wARP, XDS and HKL as well as others give lectures, tutorials and are also available to help with data processing and data solution throughout the meetings

<https://www.ccp4.ac.uk> – Courses & Events



# CCP4 users around the world



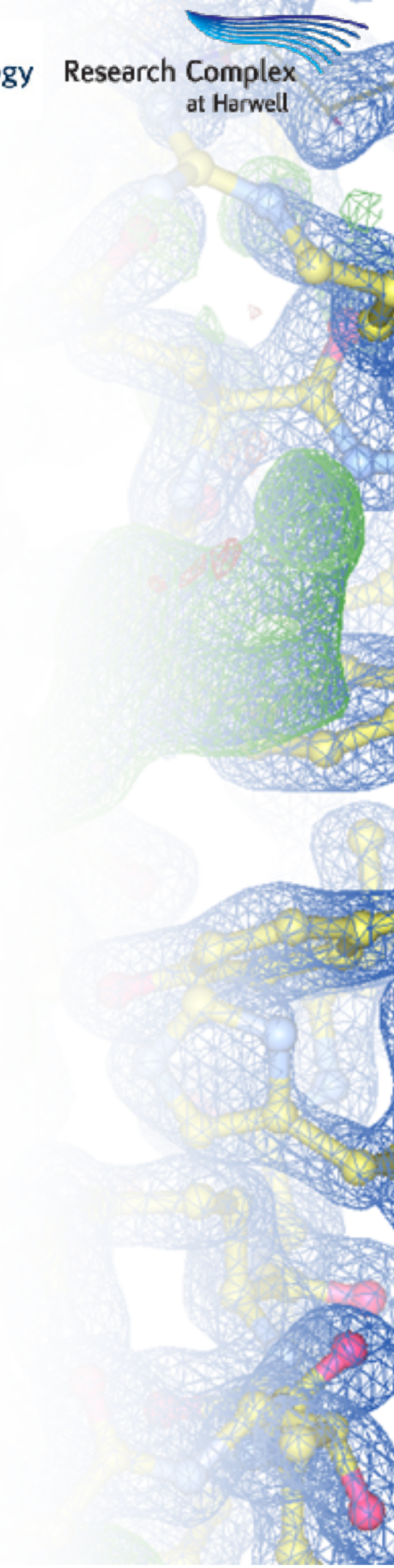


# CCP4 Resources

- CCP4BB mailing list — bulletin board, news, expert help and advice
- CCP4 help desk — [ccp4@ccp4.ac.uk](mailto:ccp4@ccp4.ac.uk) — bug reports, problems with software
- CCP4 wiki @ Konstanz: — <http://strucbio.biologie.uni-konstanz.de/ccp4wiki/index.php/Crystallography> (thanks to Kay Diederichs)
- CCP4 web site — <https://www.ccp4.ac.uk> (downloads, documentation, news and more)
- CCP4 Cloud manuals:  
<https://cloud.ccp4.ac.uk/manuals/html-taskref/index.html> (task manual)  
<https://cloud.ccp4.ac.uk/manuals/html-userguide/index.html> (user guide)

Documentation is a public resource and contributions are welcome!

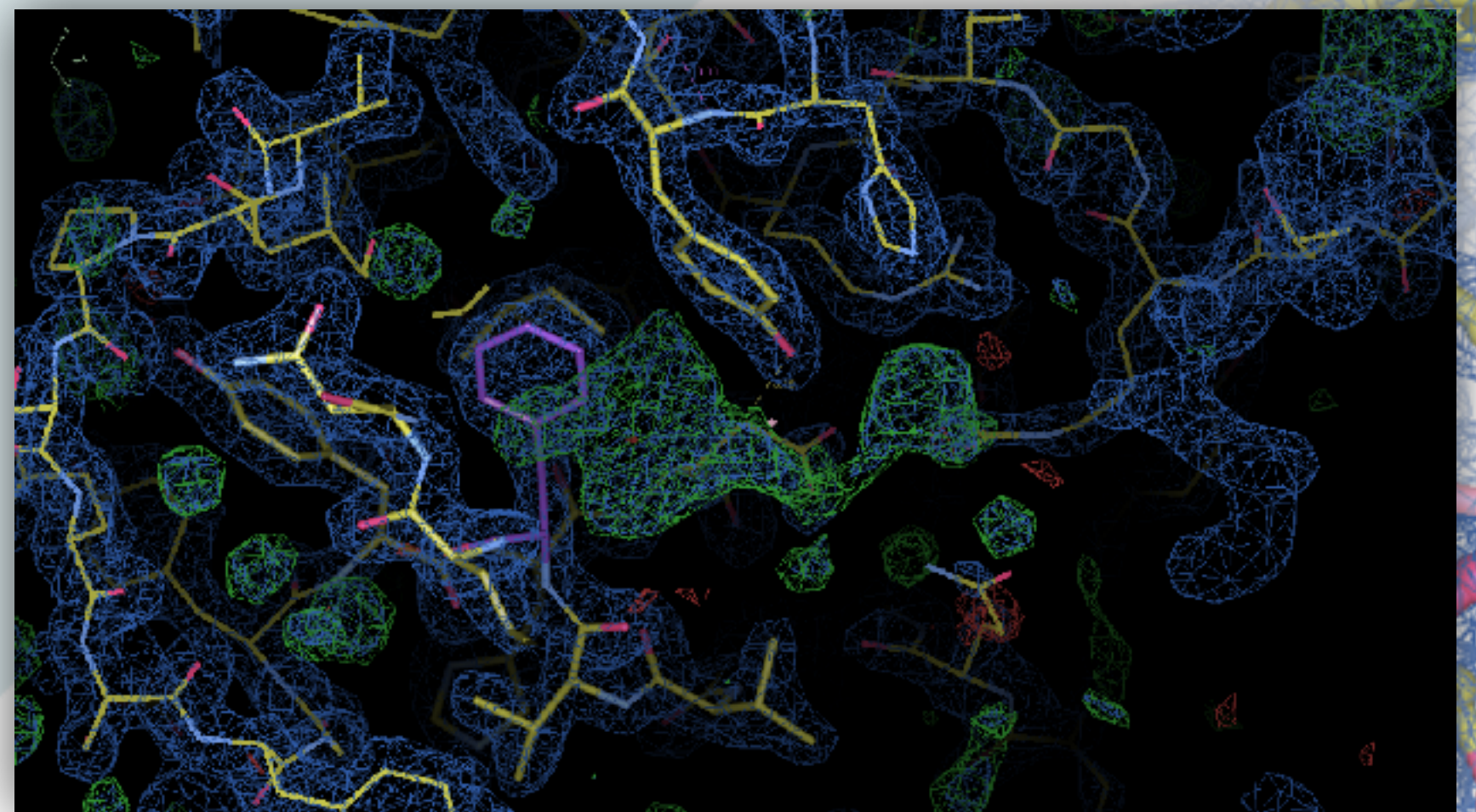
# Crystallography in nutshell





# Structure Solution in Essence

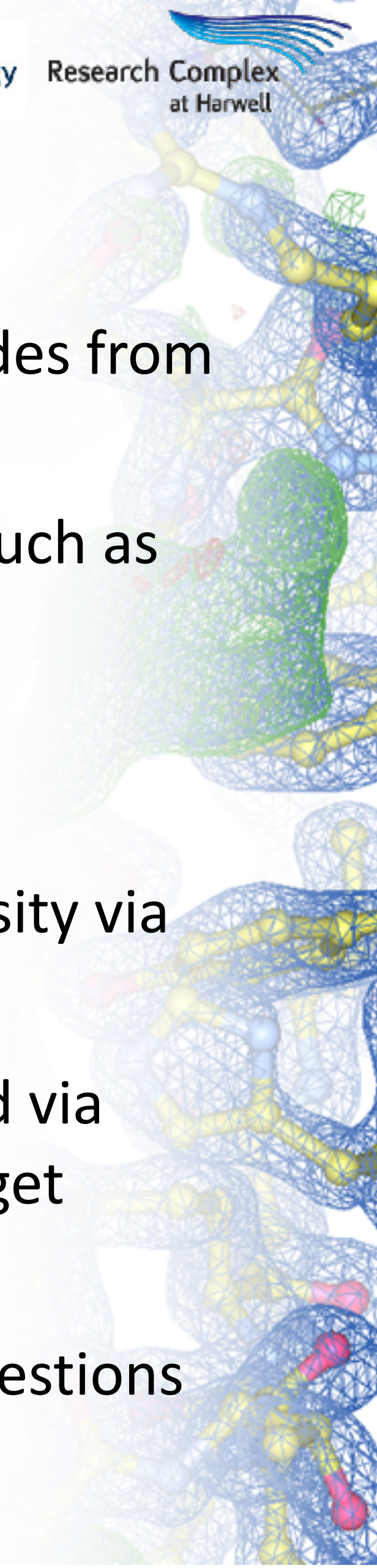
- As an ultimate goal, one would like to generate an atomic model for their target
- This could be achieved by applying the inverse Fourier transform to experimental structure factors (which are Fourier transform of the structure's atomic coordinates) if they were known or could be indeed obtained in an experiment
- In reality, the X-ray diffraction experiment gives only moduli, ***but not phases***, of structure factors
- Therefore, phases need to be elicited by other means





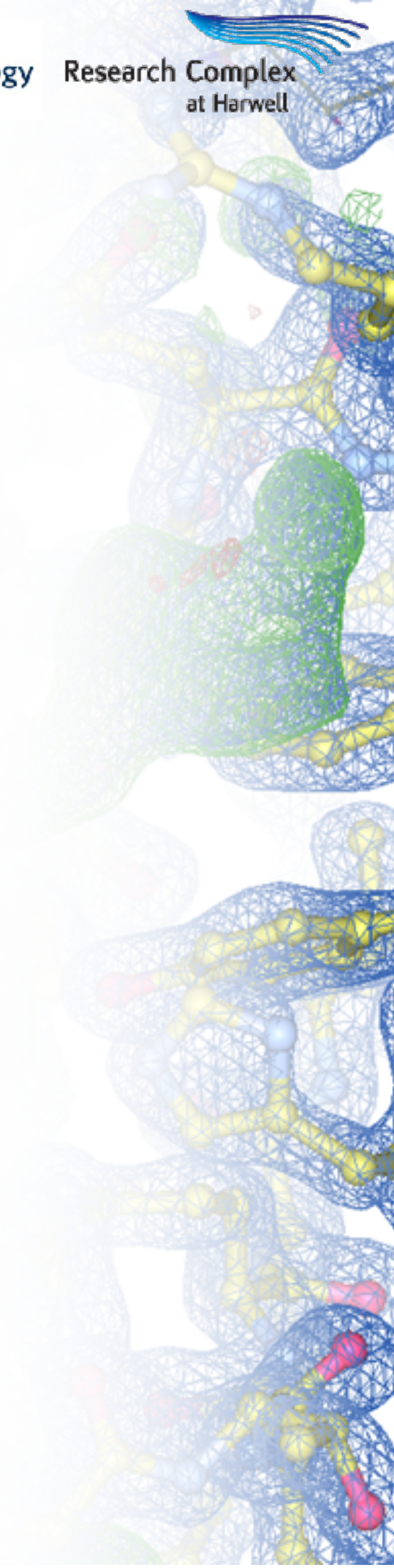
# Structure Solution Pathway

- As a first step, one needs to derive structure factor amplitudes from the intensities of spots in X-ray images
- Next, phases need to be approximated by using methods such as
  - ~ Experimental Phasing: SAD, MAD, SIRAS etc.
  - ~ Molecular Replacement
  - ~ Combination of the above
- Then, structure factors can be converted into electron density via *inverse Fourier transform*
- The obtained electron density map needs to be interpreted via model building and refinement to produce a model for target structure
- The model needs to be analysed to answer biochemical questions and deposited in the PDB



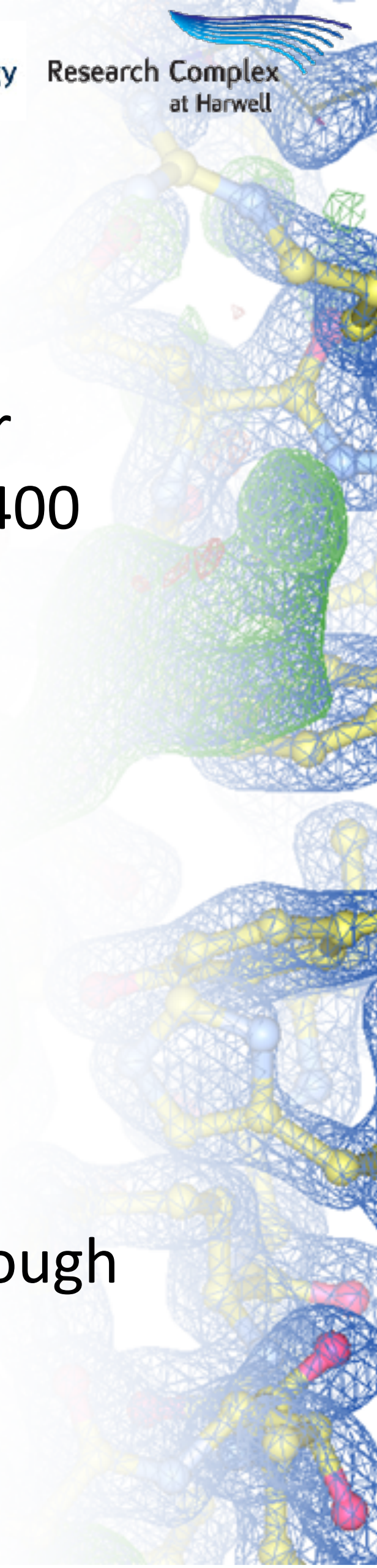


# The Software



# The CCP4 Software Suite

- The CCP4 Suite is a comprehensive suite of software for macromolecular crystallography and it contains about 400 program components
- New versions of the suite are released about every 12 months
  - ~ New programs
  - ~ Major updates to existing programs
  - ~ Other new features such as changes to CCP4i interface
- Revisions to the current release are made available through the CCP4 updates manager





# CCP4 Scope

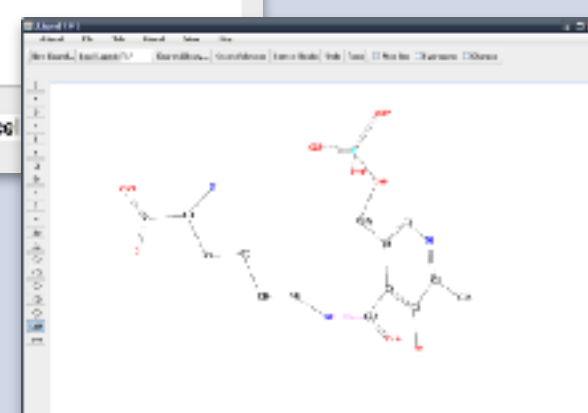
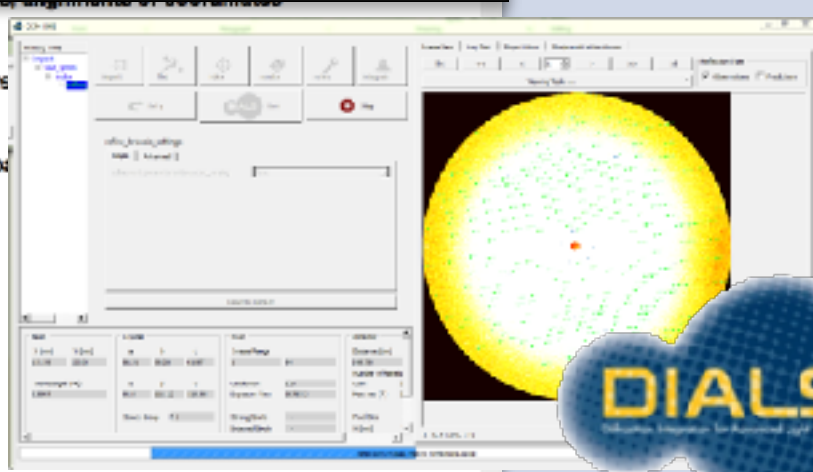
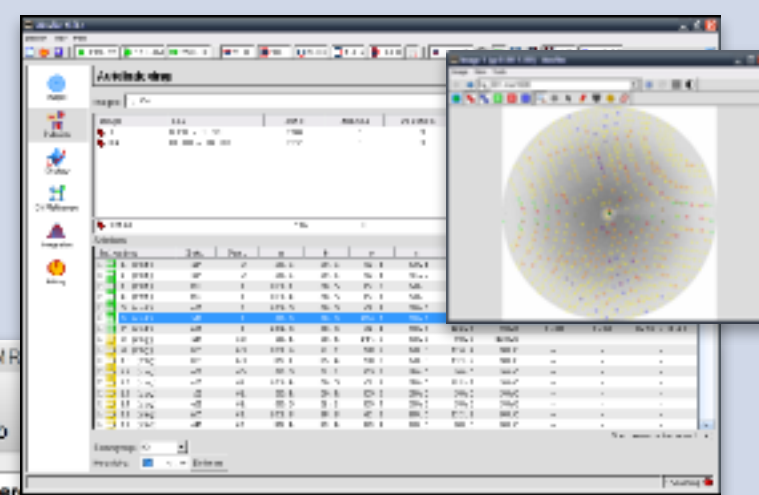
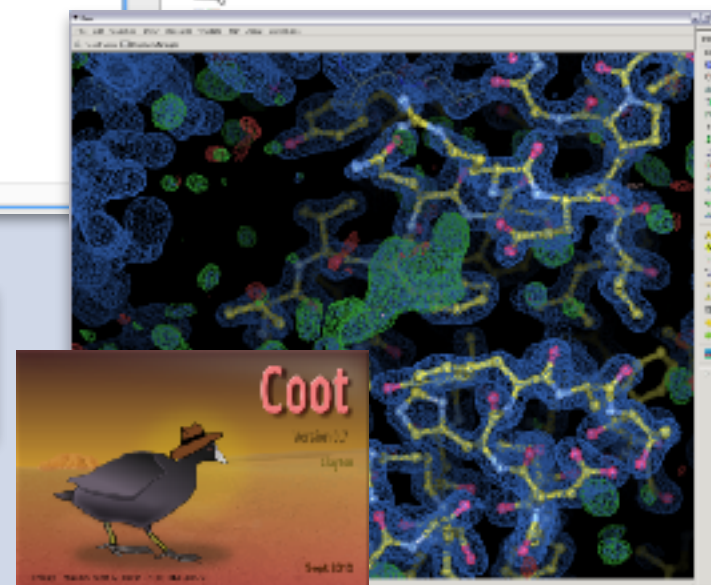
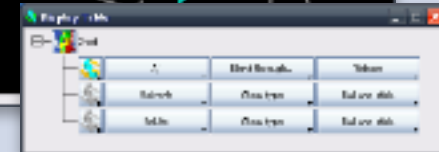
## CCP4 Software

Task menu View in Coot View in CCP4mg Export MTZ Help Bibliography Clone job

Job list Project directory

JobFile Evaluation

- 6 Molrep
- 4 Refinement - REFMAC5  $R=0.49$   $R_{free}=0.58$
- 3 Molrep
- 2 Import a coordinate set - optional se...  $nRes=168$
- 1 Import merged



PDB\_REDO

Crystallisation

Data Collection

Data Processing  
and Reduction

Experimental  
Phasing

Molecular  
Replacement

Density  
Modification

Model Building

Refinement

Structure Analysis

Deposition

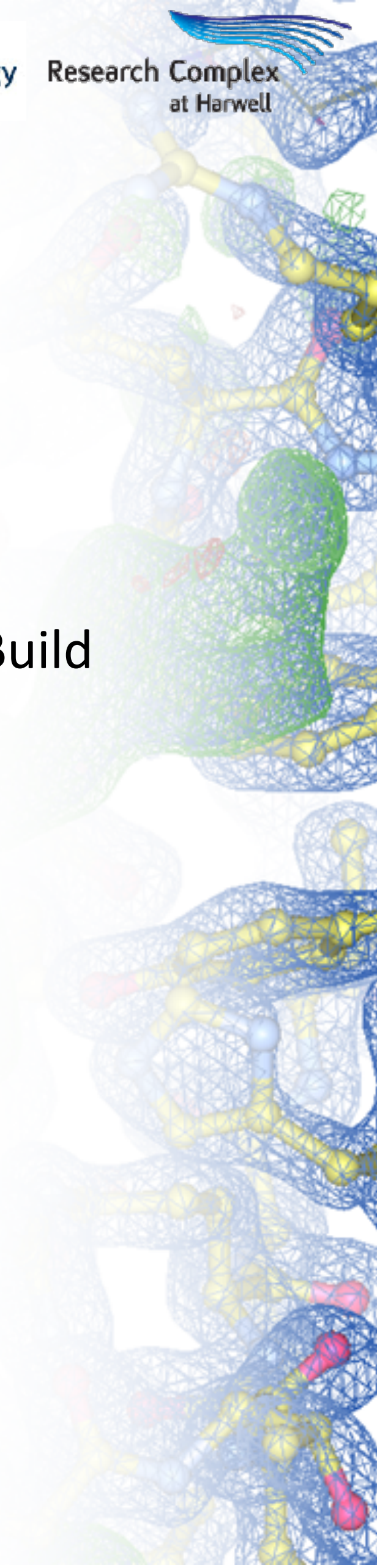
SHELX

7.3  
ARP  
wARP

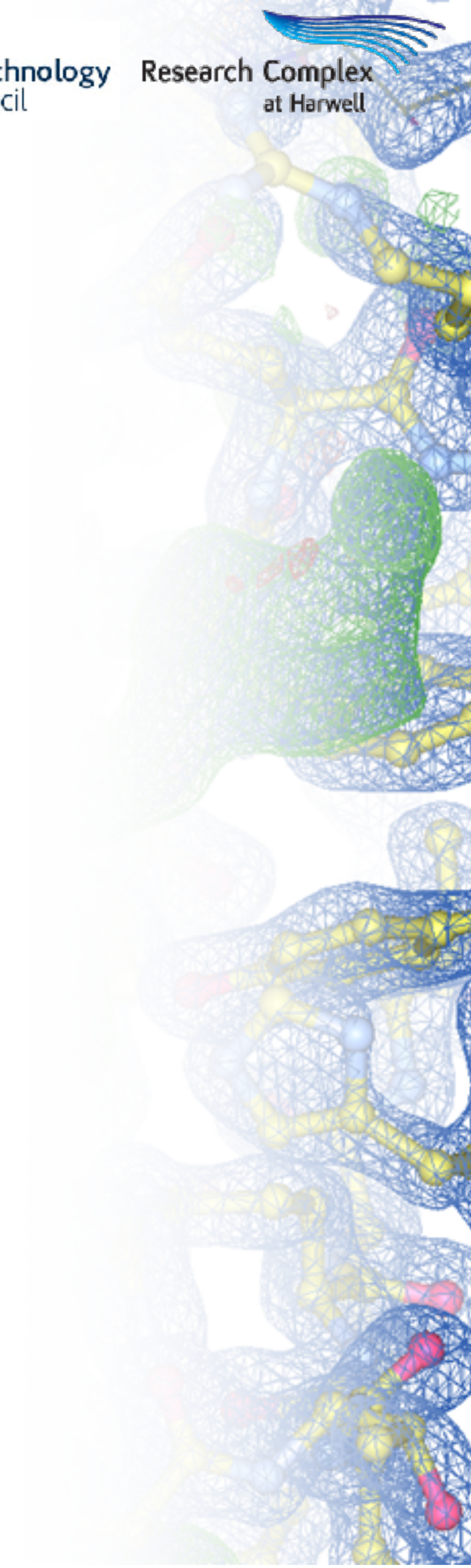


# CCP4 Releases

- Current release version — CCP4 7.1.008
- Recent programs:
  - ~ SHELX, DIALS, MorDA, Arcimboldo, CCP4i2, CCP4 Cloud, CCP4Build
  - ~ QtPISA, Aimless, Dimple, AMPLE, SIMBAD, Zanuda, ProSMART, Nautilus, AceDRG, Privateer, Feckless and other
  - ~ In collaboration with the EMBL-Hamburg, ARP/wARP model building software is now rolled with CCP4 Suite
- Continuing development of major components:
  - ~ Phaser, Refmac, Mosflm/iMosflm, Crank-2, MrBUMP
- Newer infrastructure
  - ~ Build system, Setup Manager and Updates Manager

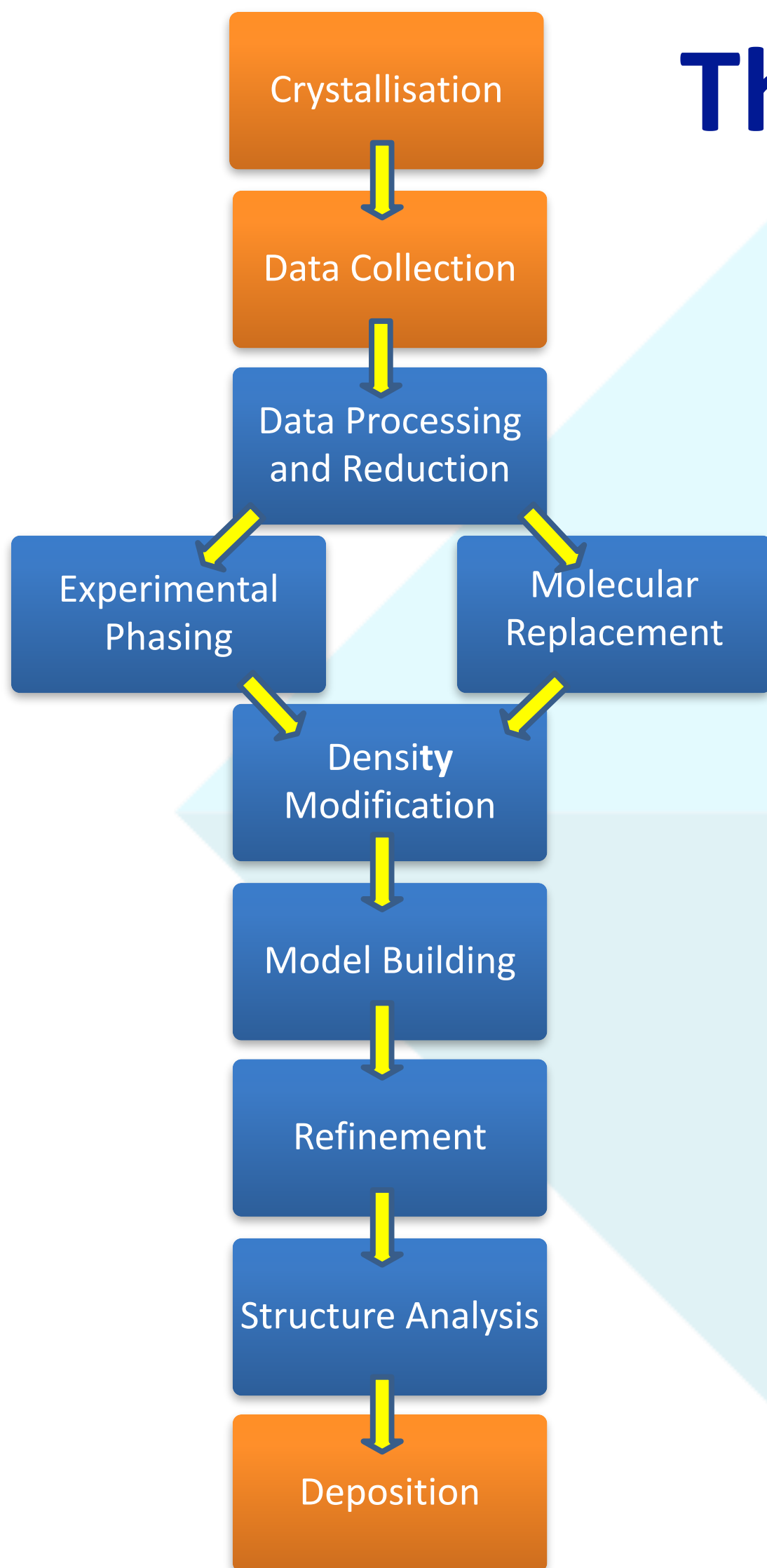


# Using CCP4





# The Structure Solution Stages



## Automated\*

Xia-2

MrBump, Balbes, MorDA,  
Crank-2, Simbad, Ample

Buccaneer, CCP4Build,  
Arp/wArp

Lorestr, Dimple

PDB Deposition module

## Fundamental\*

XDS, DIALS, Aimless,  
DUI, XDSCui, iMosflm

Phaser, Molrep, ShelxCD,  
Sculptor, Chainsaw

Parrot, Acorn, ShelxE

Coot, AceDrg, jLigand

Refmac, Prosmart

Zanuda, PISA, Gesamt

\* only selected representative programs are shown



# Programs' use and Projects

- Crystallographic projects may be very complex
  - ~ over 100 programs may need to be used
  - ~ sometimes, 100s jobs may need to be run
- All CCP4 programs can be used from command line
  - ~ [+] gives full control of programs and access to all parameters
  - ~ [-] difficult to memorise all options and parameters
  - ~ [-] difficult to keep 100s and 1000s files organised
  - ~ [-] may be difficult to analyse the structure solution pathway *post factum*
- Most frequently used programs are available through graphical interfaces
  - ~ [+] greatly simplifies manipulation with data and program parameters
  - ~ [+] arranges work in **Projects**, easier to navigate, analyse and make decisions
  - ~ [+] take care of many petty jobs such as routine format conversions, map preparations and other
  - ~ [-] may give access only to a subset of most frequently used program parameters
  - ~ [-] may not exist for a particular program of interest



# Command Line Operation

## Example:

*refmac5 HKLIN my.mtz HKLOUT output.mtz XYZIN my.pdb XYZOUT output.pdb*

## Keywords:

- Most CCP4 programs take “keywords” as command options through standard input to the program
- Gives access to all options of the program and the most fine-grained control
- Can be provided through ccp4i using “**Run & view com file**”

## Scripting:

- Repetitive tasks can be scripted
- Pipelines of programs can be created in a script

**Command  
line**

```
f2mtz hklin ${1} hklout shelxe-output.mtz << eof
```

```

TITLE      ample
cell       ${cell}
symm       ${symm}
labout     H K L F FOM PHI SIGF
CTYPOUT    H H H F W P Q
pname      ample
dname      ample
END
```

**Keywords**



# Command Line Operation

- CCP4 program keyword descriptions are found in documentation pages online or in the suite (`$CCP4/html/INDEX.html`):



The screenshot shows a web browser window with the address `www.ccp4.ac.uk/html/aimless.html#keywords`. The page title is "KEYWORDED INPUT - DESCRIPTION". It explains that keywords are case-insensitive and lists available keywords: ANALYSIS, ANOMALOUS, BINS, DUMP, EXCLUDE, INITIAL, INTENSITIES, NAME, ONLYMERGE, OUTPUT, PARTIALS, REFINER, REJECT, RESOLUTION, RESTORE, RUN, SCALES, SDCORRECTION, TIE, TITLE. It then details the "RUN" command, including subkeys like ROTATION, BATCH, BECTOR, BROTON, and SECONDARY, with their respective functions and default values.

**KEYWORDED INPUT - DESCRIPTION**

In the definitions below "|" encloses optional items, "[" delineates alternatives. All keywords are case-insensitive, but are listed below in upper-case. Anything after "!" or "#" is treated as comment. The available keywords are:

[ANALYSIS](#), [ANOMALOUS](#), [BINS](#), [DUMP](#), [EXCLUDE](#), [INITIAL](#), [INTENSITIES](#), [NAME](#), [ONLYMERGE](#), [OUTPUT](#), [PARTIALS](#), [REFINER](#), [REJECT](#), [RESOLUTION](#), [RESTORE](#), [RUN](#), [SCALES](#), [SDCORRECTION](#), [TIE](#), [TITLE](#)

**RUN <Nrun> BATCH <b1> to <b2>**

Define a "run": Nrun is the Run number, with an arbitrary integer label (i.e. not necessarily 1,2,3 etc). A "run" defines a set of reflections which share a set of scale factors. Typically a run will be a continuous rotation around a single axis. The definition of a run may use several RUN commands. If no RUN command is given then run assignment will be done automatically, with run breaks at discontinuities in dataset, batch number or Phi. If any RUN definitions are given, then all batches not explicitly specified will be excluded.

**SCALES [<subkeys>]**

Define layout of scales, ie the scaling model. Note that a layout may be defined for all runs (no RUN subkeyword), then overridden for particular runs by additional commands.

Subkeys:

**RUN <run\_number>**  
Define run to which this command applies: the run must have been previously defined. If no run is defined, it applies to all runs

**ROTATION <Nscale> | SPACING <delta\_rotation>**  
Define layout of scale factors along rotation axis (i.e. primary beam), either as number of scales or (if SPACING keyword present) as interval on rotation [default SPACING 5]

**BATCH**  
Set "Batch" mode, no interpolation along rotation (primary) axis. This option is compulsory if a ROT column is not present in the input file, but otherwise the ROTATION option is preferred. WARNING: this option is not optimised and may take a very long time if you have many batches

**BECTOR ON | OFF**  
Switch Bfactors on or off. The default is ON.

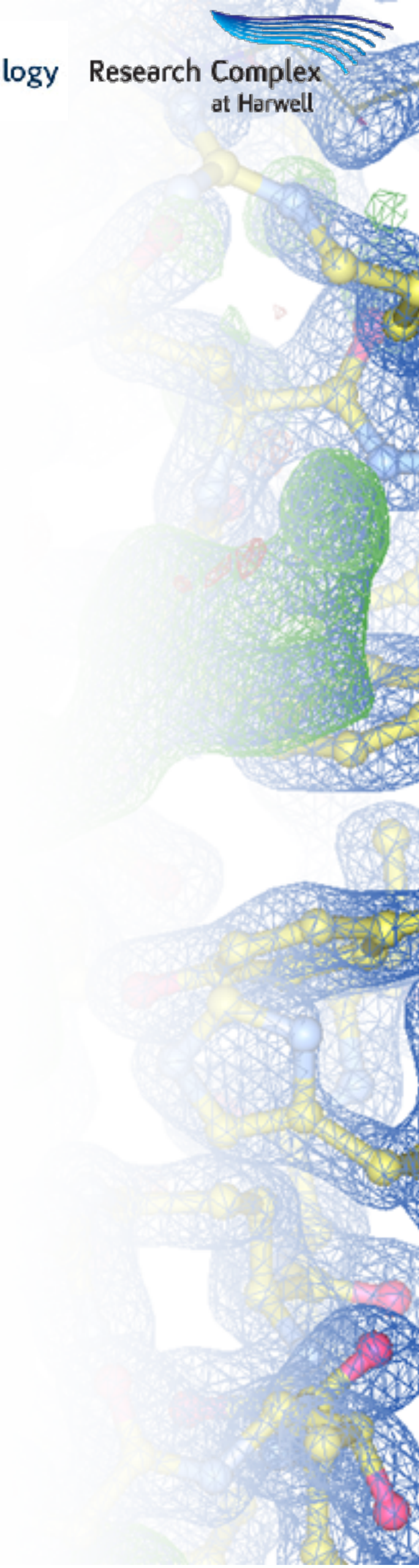
**BROTON <Ntime> | SPACING <delta\_time>**  
Define number of B-factors or (if SPACING keyword present) the interval on "time": usually no time is defined in the input file, and the rotation angle is used as its proxy [default SPACING 20].

**SECONDARY [<Lmax>]**  
Secondary beam correction expanded in spherical harmonics up to maximum order Lmax in the camera spindle frame. The number of parameters increases as  $(L_{max} + 1)^2$ , so you should use the minimum order needed (eg 4 - 6, default 4). The deviation of the surface from



# The CCP4 user interface(s)

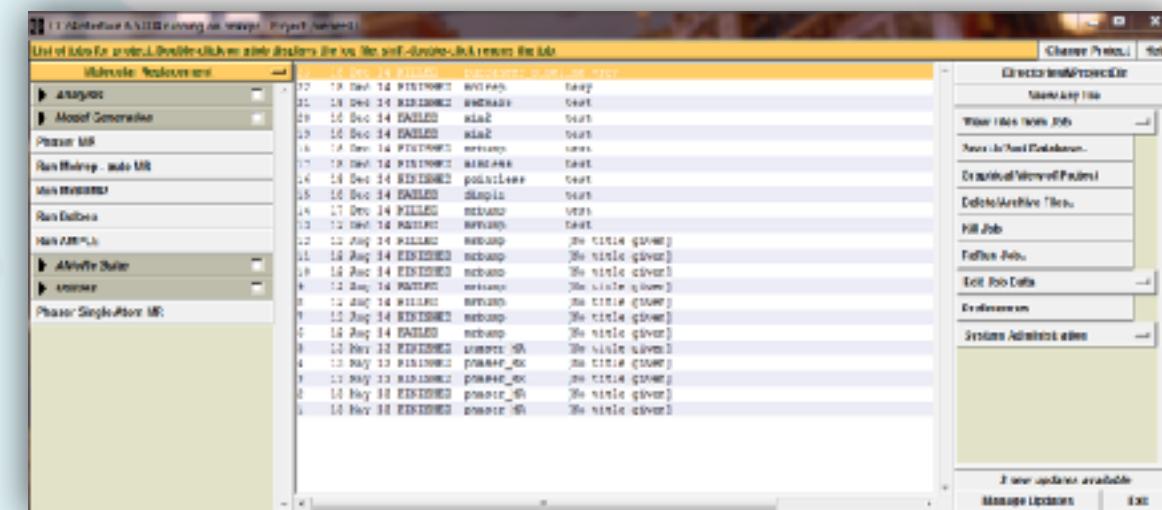
- Three main interfaces to the CCP4 suite



# The CCP4 user interface(s)

- Three main interfaces to the CCP4 suite

1. **CCP4i** – original interface developed around 2000

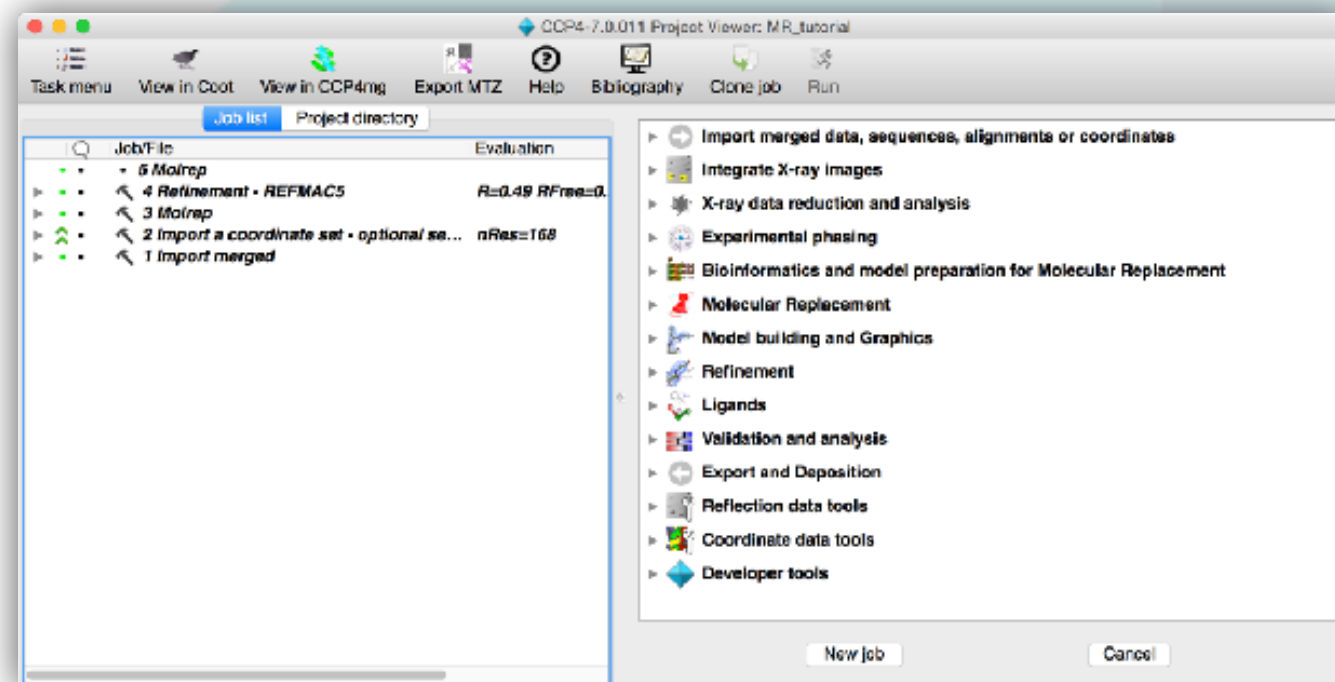
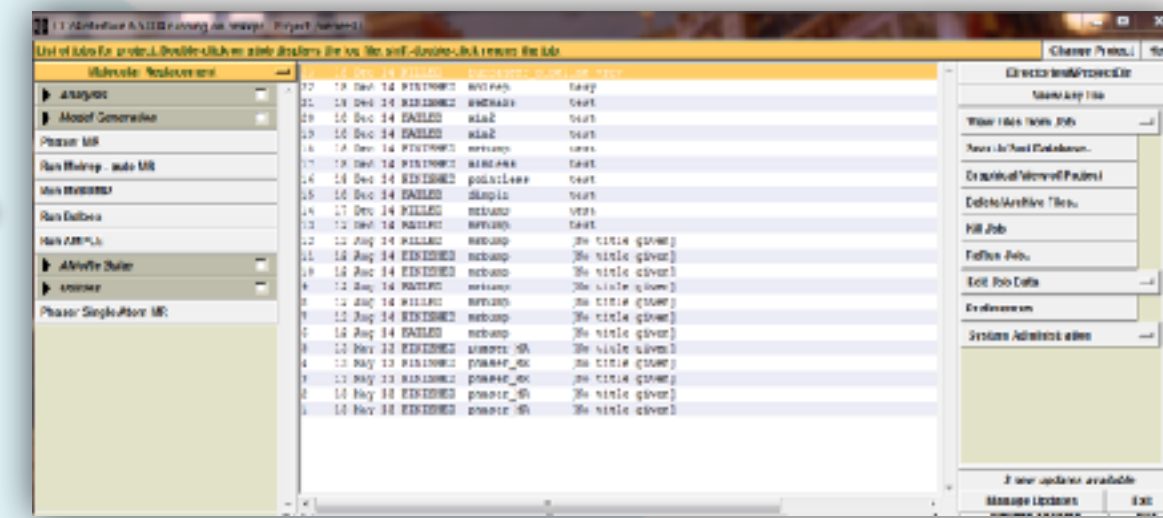




## The CCP4 user interface(s)

- Three main interfaces to the CCP4 suite

1. **CCP4i** – original interface developed around 2000



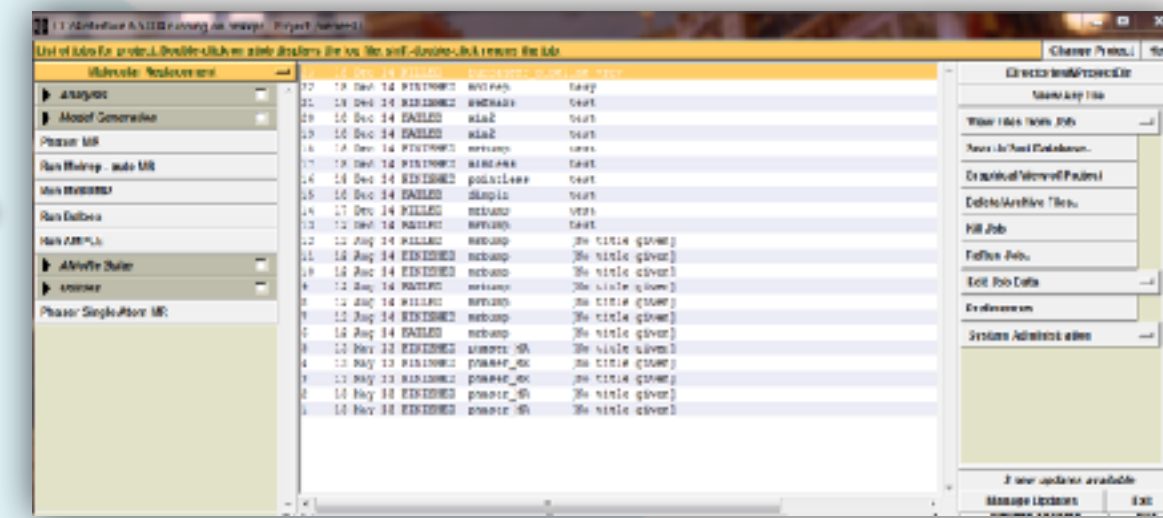
2. **CCP4i2** – new graphical desktop interface (2016)



# The CCP4 user interface(s)

- Three main interfaces to the CCP4 suite

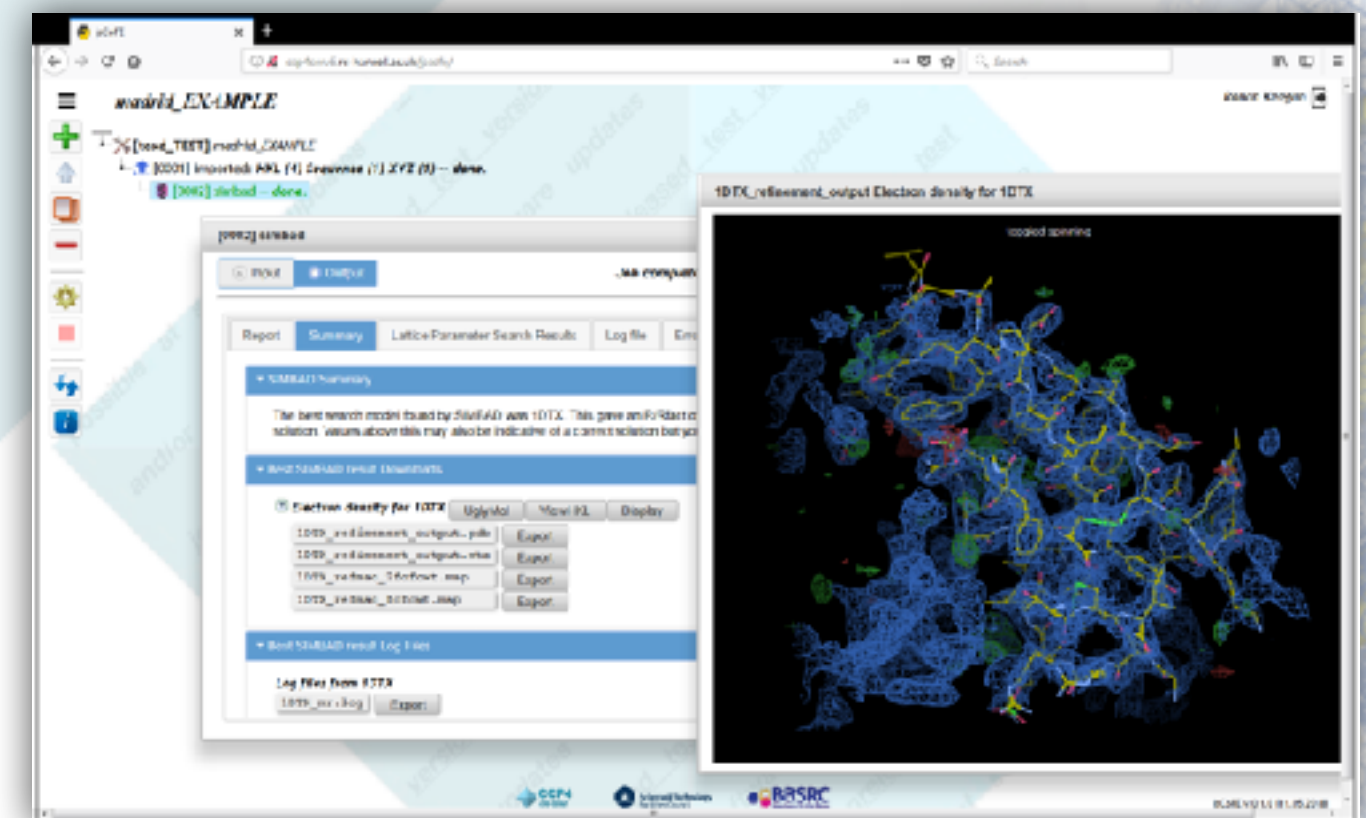
1. **CCP4i** – original interface developed around 2000



2. **CCP4i2** – new graphical desktop interface (2016)



3. **CCP4 Cloud**, browser based (2019)

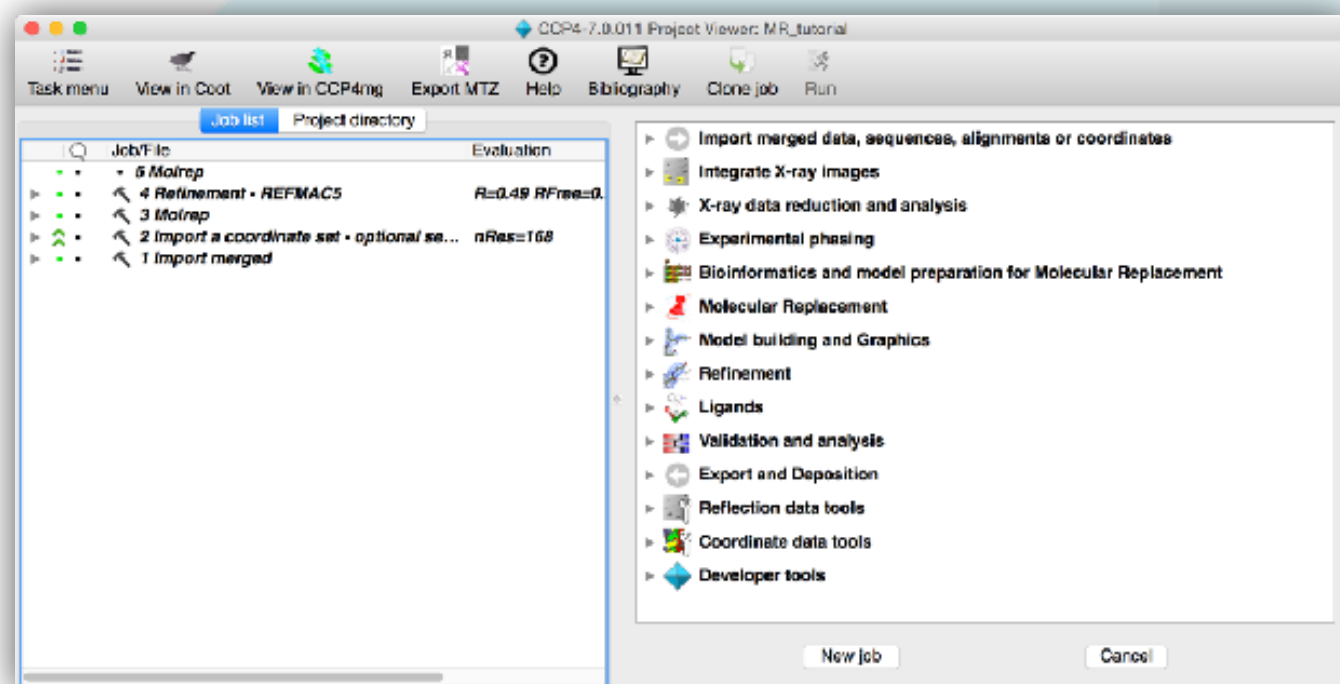
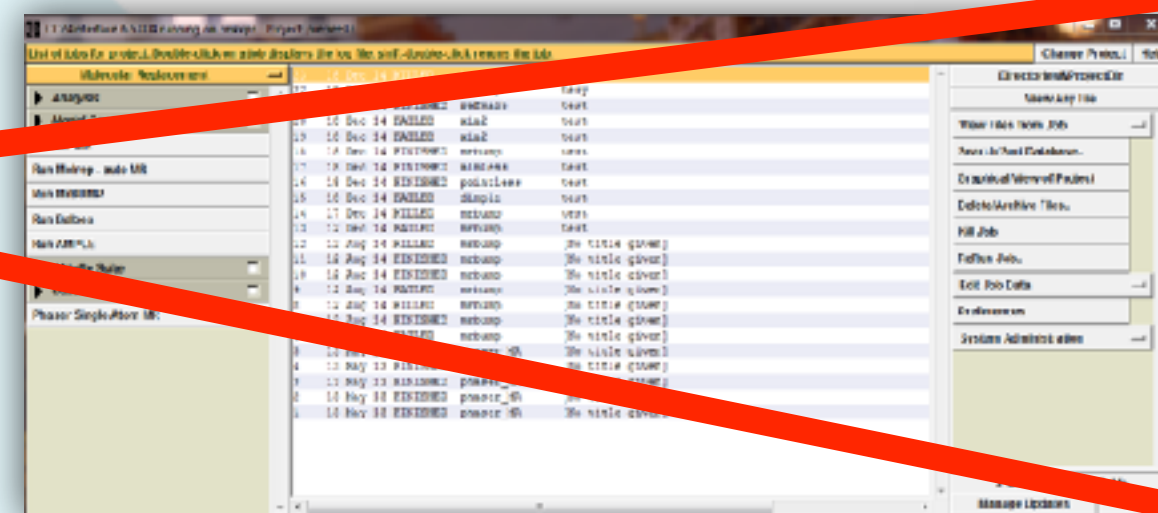




# The CCP4 user interface(s)

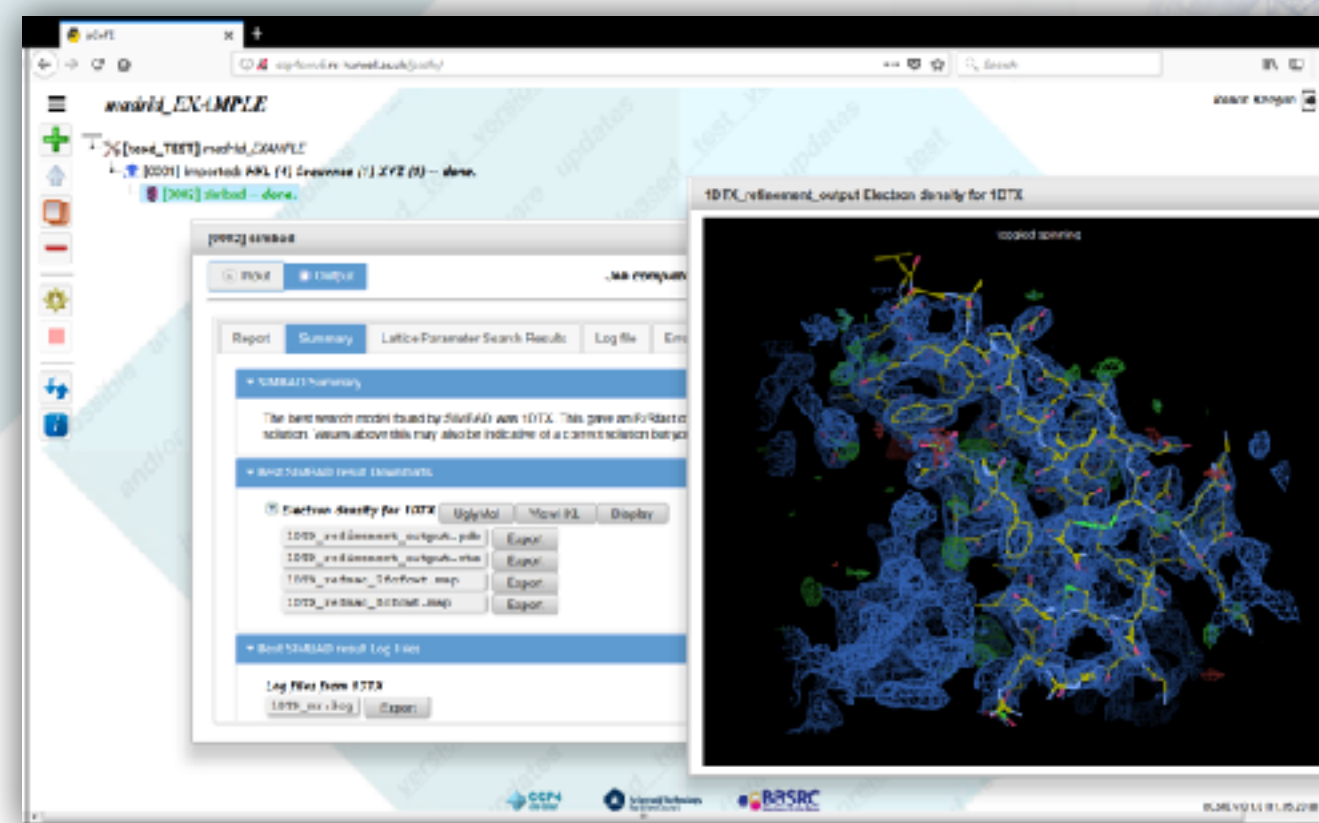
- Three main interfaces to the CCP4 suite

1. **CCP4i** – original interface  
developed around 2000  
*deprecated*



2. **CCP4i2** – new graphical  
desktop interface (2016)

3. **CCP4 Cloud**, browser  
based (2019)





# Documentation in CCP4i2



CCP4-7.1.018 Use Phaser to carry out molecular replacement — CCP4i2 documentation

Back Forward Find Reload Help Open tab

file:///Applications/ccp4-7.1/share/ccp4i2/docs/sphinx/build/html/tasks/phaser\_pipeline/index.html

Welcome to CCP4i2's documentation! — CCP4i2 documentation Use Phaser to carry out molecular replacement — CCP4i2 documentation

## Molecular replacement

- Automated Molecular Replacement from target sequence
- Use Phaser to carry out molecular replacement
  - Workflow
  - Input
  - Molecular replacement - MOLREP
  - SYMMETRY MATCH MODEL TO REFERENCE
  - Molecular replacement with fragments (Fragon)
  - Morda Installation
- Density Modification
- Model building and graphics
- Refinement
- Ligands
- Validation and analysis
- Export and Deposition
- Reflection data tools
- Coordinate data tools

## Input

Input data Known structure Keywords Extra steps

Job title

Use data from job 17 Generate a Free R set as input below.

### Reflections 1

Reflections 1 beta\_blip\_P3221: imported by job 1

Resolution range Spacegroups to test Use input spacegroup only

Free R set 17 New set of freeR flags

### Composition 2

For estimating zsymmetric unit contents: Provide no guidance to Phaser

### Search model(s) 3

Show list Click "Show list" if more than one copy or more than one search model

...must be selected

Atom selection No atoms Help

Sequence identity to target: OR structure RMS difference:

CCP4i2 Command Line - i2run  
CCP4i2 Update History  
How to Contribute to the Documentation  
Developer Notes

Figure 1: PHASER MR input front page

*Reflections.(1.1)* Hopefully self-explanatory.

*Resolution range.* Based on the expected LLGs, PHASER will try to search with the best resolution. You may override the maximum resolution that PHASER will attempt here.

*Spacegroups.* Where there is ambiguity, you can invite PHASER to attempt MR in more than one spacegroup: data reduction generally



# Documentation in CCP4 Cloud

- Trying to focus on the scientific content of the task, rather than interface features

The screenshot displays the CCP4 Cloud interface. On the left, a vertical toolbar contains icons for various functions, with the 'Help' icon (a blue circle with a white 'i') circled in red. The main workspace shows a workflow for 'Gamma' with steps: [0001] import from cloud storage, [0002] asymmetric unit contents, [0004] mrparse, [0005] phaser MR, and [0015] refmac5. Below the workflow, the 'Refinement with Refmac' panel is visible, featuring a 'Run' button and a 'Help' icon (a blue book) circled in red. The 'Online Help' window is open, displaying the 'CCP4 Cloud 1.6 documentation' for '10.1. REFMAC5'. The window includes a navigation bar with links to '10. Refinement and Model Building', 'Contents', and '10.2. Buster R'. The main text area contains the title '10.1. REFMAC5' and a paragraph describing the program's purpose: 'REFMAC5 is a program designed for REFinement of MACromolecular structures. It's final step in the process of macromolecular crystal (MX) structure, refinement is carried out to maximize the agreement between the model and the Model parameters that are optimized in the refinement process include atomic coordinates, atomic displacement parameters, scale factors and, in the presence of twinning, twin fraction(s). It uses Maximum likelihood and some elements of Bayesian Statistics. Although refinement procedures are typically designed for the final stages of MX analysis, they are also often used to improve models and to calculate the 'best' electron-density maps for further model (re)building.' Below this, the section '10.1.1. Basic principles of refinement' explains the process of fitting the atomic model into observed X-ray crystallographic data. It states that refinement allows the atomic model to be criticized and analyzed in direct relation to model quality and phase quality, and that the model is defined not only by the PDB file but also by the parameters of the refinement program. Two types of maps are mentioned:  $2F_{obs} - F_{calc}$  (standard electron density) and  $F_{obs} - F_{calc}$  (difference density). A 'Note' box at the bottom of the help window states: 'Data of different quality shall be described differently (the difference in quality tells us about how many statistics for the atom, that why different number parameters of the model could be estimated given particular data).' The bottom of the interface shows a status bar with 'Powered by CCP4 v.7.1.017' and 'CCP4 Cloud v.1.6.024 [02.11.2021]'.

**Gamma**

[gamma] Gamma

[0001] import from cloud storage -- imported: HKL (1) Sequence (1)

[0002] asymmetric unit contents -- 1 molecule in ASU, Solv=41.7%

[0004] mrparse -- 31 MR model(s) prepared (PDB:11, AFDB:20)

[0005] phaser MR --  $N_{sol}=1$  LLG=4256 TFZ=43.5 R=0.2941  $R_{free}=0.2907$

[0015] refmac5

[0015] refmac5 (new)

Input Output Run

**Refinement with Refmac**

job description: refmac5

output id: refmac

**Structure revision**

R0005.01: phaser-mr (anom,protein)/xyz,phases

Resolution range (Å): 34 to 1.79

Refine using: Mean Amplitudes only

**Basic options**

Number of refinement cycles: 10

Overall data-geometry weight: Auto starting value

VDW repulsion weight

Generate H-atoms for refinement: Yes

**Model Parameterisation**

**Online Help**

CCP4 Cloud 1.6 documentation

10.1. REFMAC5

« 10. Refinement and Model Building :: Contents :: 10.2. Buster R

**10.1. REFMAC5**

REFMAC5 is a program designed for REFinement of MACromolecular structures. It's final step in the process of macromolecular crystal (MX) structure, refinement is carried out to maximize the agreement between the model and the Model parameters that are optimized in the refinement process include atomic coordinates, atomic displacement parameters, scale factors and, in the presence of twinning, twin fraction(s). It uses Maximum likelihood and some elements of Bayesian Statistics.

Although refinement procedures are typically designed for the final stages of MX analysis, they are also often used to improve models and to calculate the 'best' electron-density maps for further model (re)building.

**10.1.1. Basic principles of refinement**

refinement is a process of fitting the atomic model into observed X-ray crystallographic data. Allows the atomic model to be criticized and analyzed in direct relation between model quality and phase quality. We need to iteratively improve the model the agreement between  $F_{obs}$  and  $F_{calc}$ .

The model is defined not only about the PDB file, but also should consider the parameters of the refinement program.

We work with two types of maps:

- $2F_{obs} - F_{calc}$  : "standard" electron density - represents crystal contents
- $F_{obs} - F_{calc}$  : difference density - represents differences

**Note**

Data of different quality shall be described differently (the difference in quality tells us about how many statistics for the atom, that why different number parameters of the model could be estimated given particular data)."

Back Forward Return Detach Close

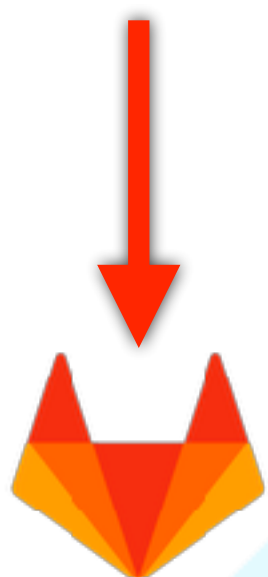
Powered by CCP4 v.7.1.017

CCP4 Cloud v.1.6.024 [02.11.2021]



# Documentation in CCP4

Community  
input and  
effort



GitLab



## Online Help

- 13.3. X-ray cross sections and anomalous scattering factors
- 13.4. Coordinate Utilities
- 13.5. Gemmi
- 13.6. Pairwise Structural Alignment with GESAMT
- 13.7. Structure Superposition with LsqKab
- 13.8. Sequence Alignment with ClustalW
- 13.9. Symmetry Match to Reference Structure with CSymMatch

## Search

- [Search Page](#)

## Authors and Contributors

Task Reference for CCP4 Cloud was prepared by

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Please send documentation-related questions and suggestions to: [CCP4 Cloud Reception](#).

[Back](#)[Forward](#)[Return](#)[Detach](#)[Close](#)



## CCP4 on-line services

<http://www.ccp4.ac.uk/ccp4online>

### Welcome to CCP4 online

Login

Other Options - [Register](#), [Forgot](#)

#### Runnable programs

The following programs and pipelines are available:

##### Balbes

An automated Molecular Replacement pipeline that searches for the correct orientation and position of the components necessary for the structure.

##### MrBUMP

An automated Molecular Replacement pipeline that searches for the correct orientation and position of the components necessary for the structure. It will search from the template structure and apply restraints to the refinement.

##### Zanuda

Space group and crystallographic analysis.

##### jsPISA

Calculation and analysis of protein-protein interfaces.

##### AMPLE

Automated ab initio search.

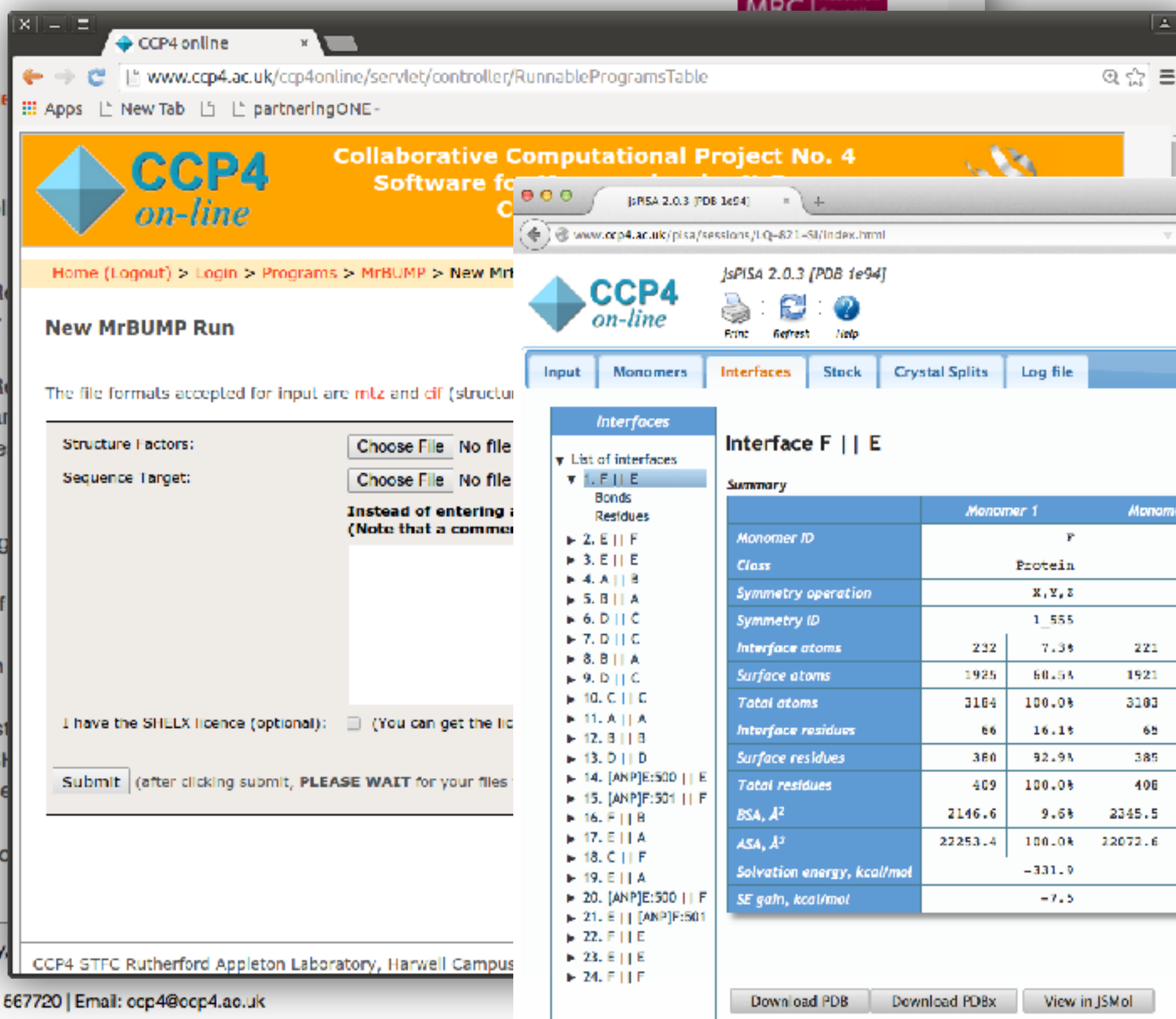
##### SHELX

Automated SHELXC/D/E suite for processing X-ray diffraction data in XDS, Scalepack, SHARP and HKL. If a protein sequence is provided, it will be used to generate a model.

##### CRANK2

Automated structure solution.

**BETA**



**New MrBUMP Run**

The file formats accepted for input are **mtz** and **cif** (structure factors) and **fasta** (sequence target).

Structure factors:  No file  
Sequence target:  No file

Instead of entering a file name, you can enter a PDB ID (Note that a comma is not allowed in the PDB ID)

I have the SHELX licence (optional): ☐ (You can get the licence from [here](#))

(after clicking submit, PLEASE WAIT for your files)

**Interfaces**

List of interfaces

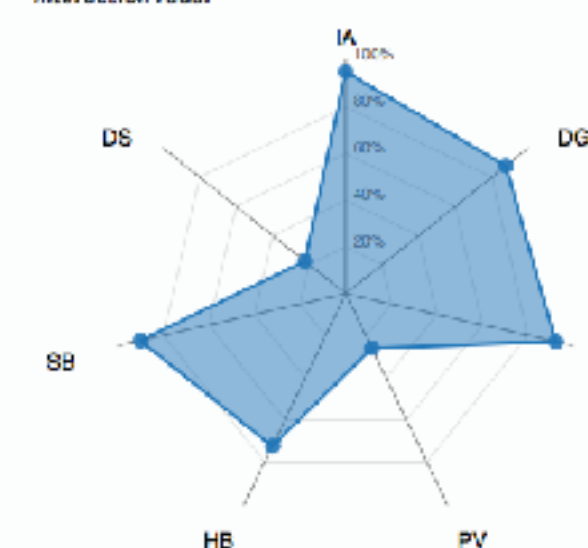
Interface	Monomer 1	Monomer 2
1. F    E	F	E
2. E    F	F	E
3. E    E	F	E
4. A    B	F	E
5. B    A	F	E
6. D    C	F	E
7. D    C	F	E
8. B    A	F	E
9. D    C	F	E
10. C    C	F	E
11. A    A	F	E
12. B    B	F	E
13. D    D	F	E
14. [ANP]E:500    E	F	E
15. [ANP]F:501    F	F	E
16. F    B	F	E
17. E    A	F	E
18. C    F	F	E
19. E    A	F	E
20. [ANP]E:500    F	F	E
21. E    [ANP]F:501	F	E
22. F    E	F	E
23. E    E	F	E
24. F    F	F	E

**Interface F || E**

Summary

	Monomer 1	Monomer 2
Monomer ID	F	E
Class	Protein	Protein
Symmetry operation	x,y,z	x,y,z
Symmetry ID	1_555	1_555
Interface atoms	232	221
Surface atoms	1925	1921
Total atoms	3164	3103
Interface residues	66	65
Surface residues	360	385
Total residues	409	406
BSA, Å <sup>2</sup>	2146.6	2345.5
ASA, Å <sup>2</sup>	22253.4	22072.6
Solvation energy, kcal/mol	-331.9	-334.3
SE gain, kcal/mol	-7.5	-5.0

Interaction radar



Interface parameters

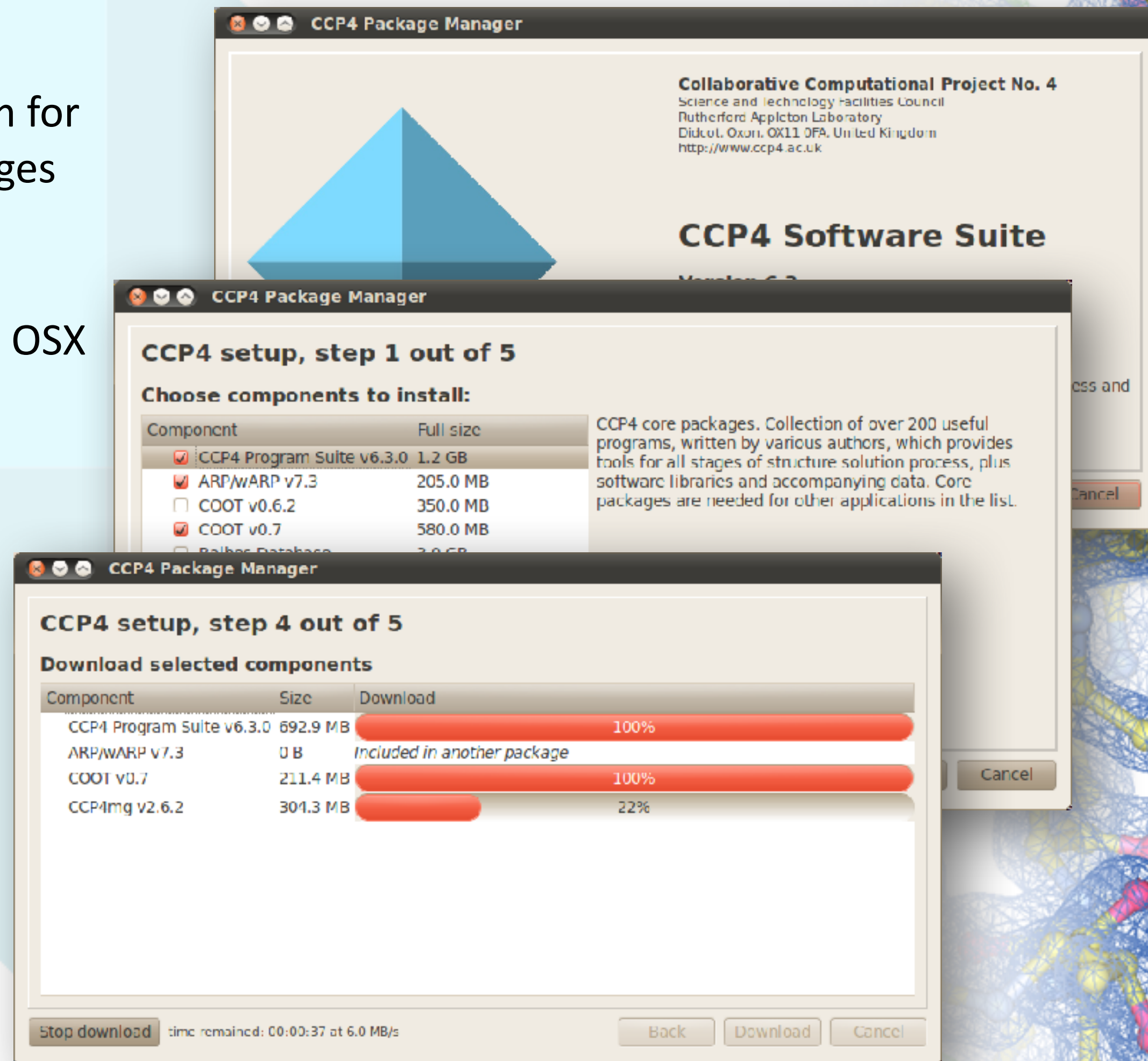
IA : Interface area, Å <sup>2</sup>	2246
DG : Solvation Energy, kcal/mol	-12.46
BE : Total Binding Energy, kcal/mol	-26.65
PV : Hydrophobic P-value	0.3542
HB : Number of Hydrogen Bonds	11
SB : Number of Salt Bridges	25
DS : Number of Disulphide Bonds	0





## CCP4 Setup Manager

- Easy installation mechanism for CCP4 and associated packages (Coot, ARP/wARP, CCP4mg)
- Available on Linux and Mac OSX platforms
- Sets up system variables automatically if you wish

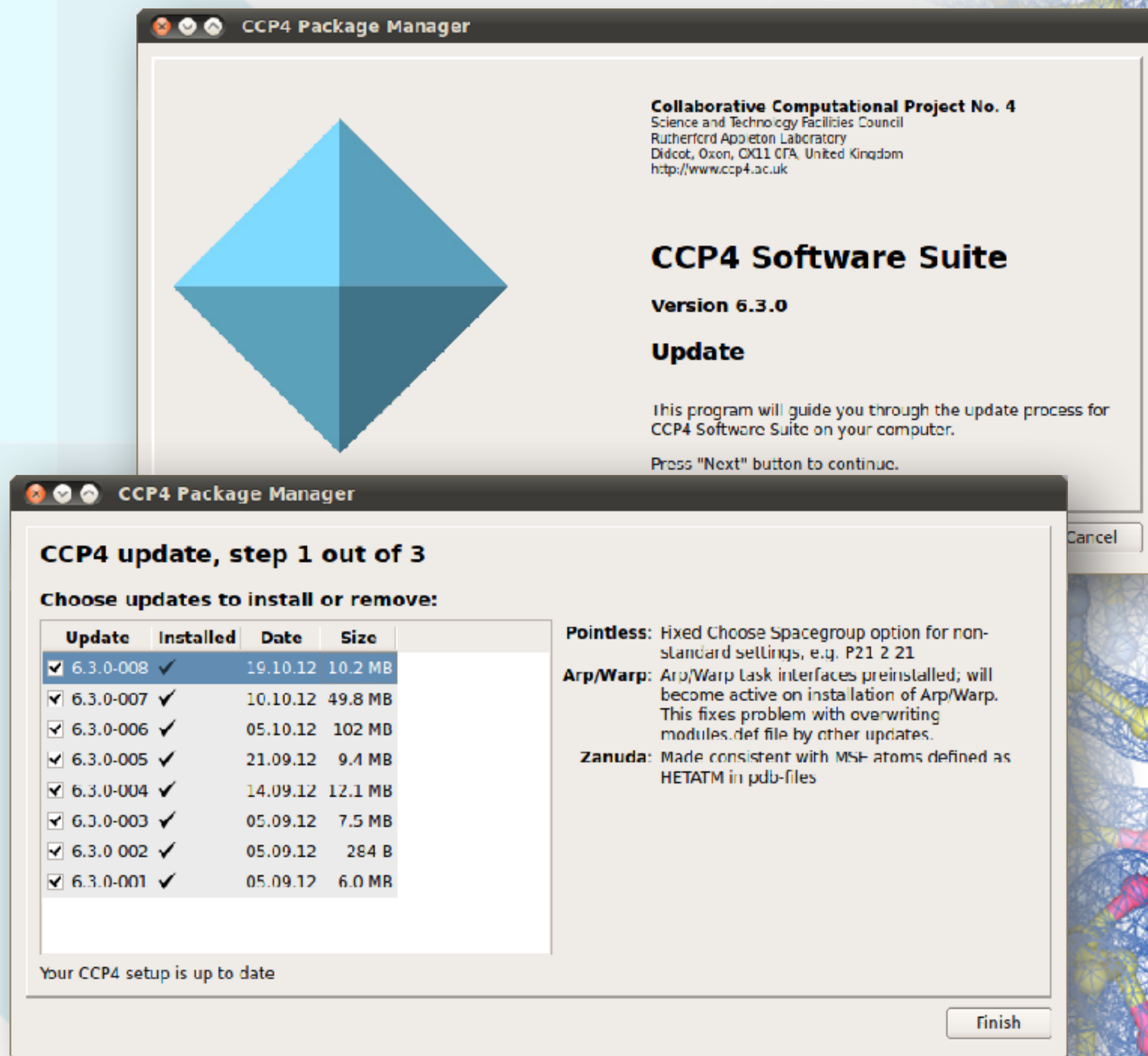






## Update Manager

- Automatically install latest fixes and new features
- Allows for rolling back to previous versions
- Updates made available once every two weeks or as and when they are needed
- Available on Linux, Mac OSX and Windows





# Acknowledgements

**CCP4 Core group:** Andrey Lebedev, Charles Ballard, Ronan Keegan, David Waterman, Marcin Wojdyr, Ville Uski, Karen McIntyre, Oleg Kovalevskyi, Maria Fando, Kyle Stevenson, Tarik Drevon, Martyn Winn

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**Phaser Group:** Airlie McCoy, Randy Read, Rob Oeffner, Gabor Bunkoczi, Massimo Sammito

**YSBL York:** Keith Wilson, Eleanor Dodson, Kevin Cowtan, Liz Potterton, Stuart McNicholas, Paul Bond, Jon Agirre, Huw Jenkins

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**Leiden:** Raj Pannu, Pavol Skubak

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# CCP4 People (core and associated developers)



Martyn  
Winn



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Charles  
Ballard



Ronan  
Keegan



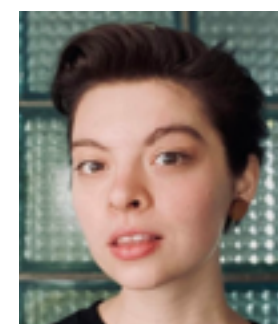
David  
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Lebedev



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Maria  
Fando



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Stevenson



Ville  
Uski



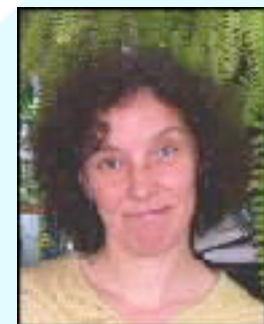
Tarik  
Drevon



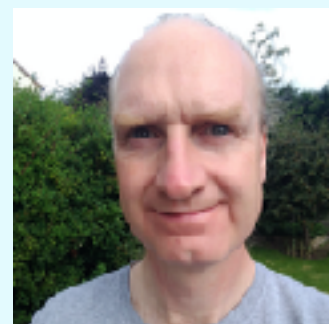
Keith  
Wilson



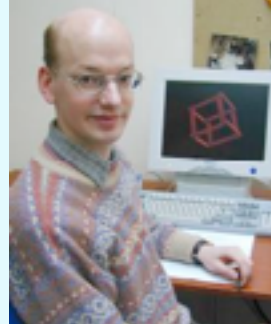
Eleanor  
Dodson



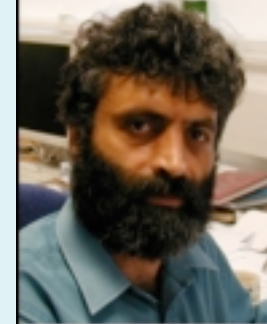
Liz  
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Stuart  
McNicholas



Kevin  
Cowtan



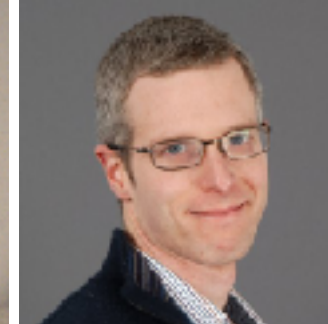
Garib  
Murshudov



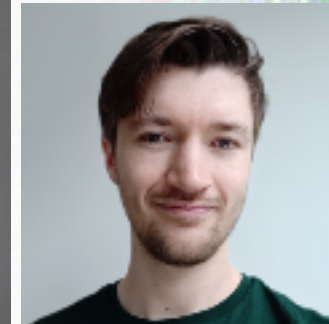
Alexei  
Vagin



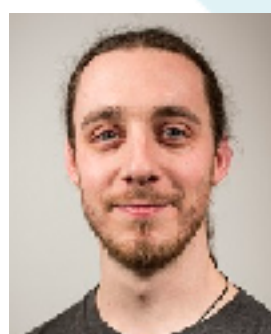
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Long



Hew  
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Adam  
Simpkin



Paul  
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Pavol  
Skubak



Robert  
Nichols



Daniel  
Rigden



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Andrew  
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Harry  
Powell



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Johnson



Jon  
Agirre



Robbie  
Joosten



Randy  
Reed



Isabel  
Uson



Martin  
Noble



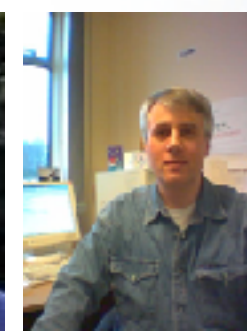
Paul  
Emsley



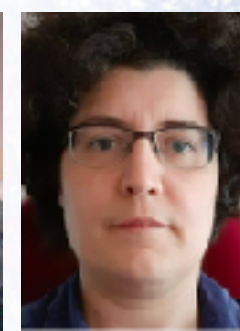
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Pannu



Luis Fuentes-  
Montero



Chris  
Morris



Melanie  
Vollmar