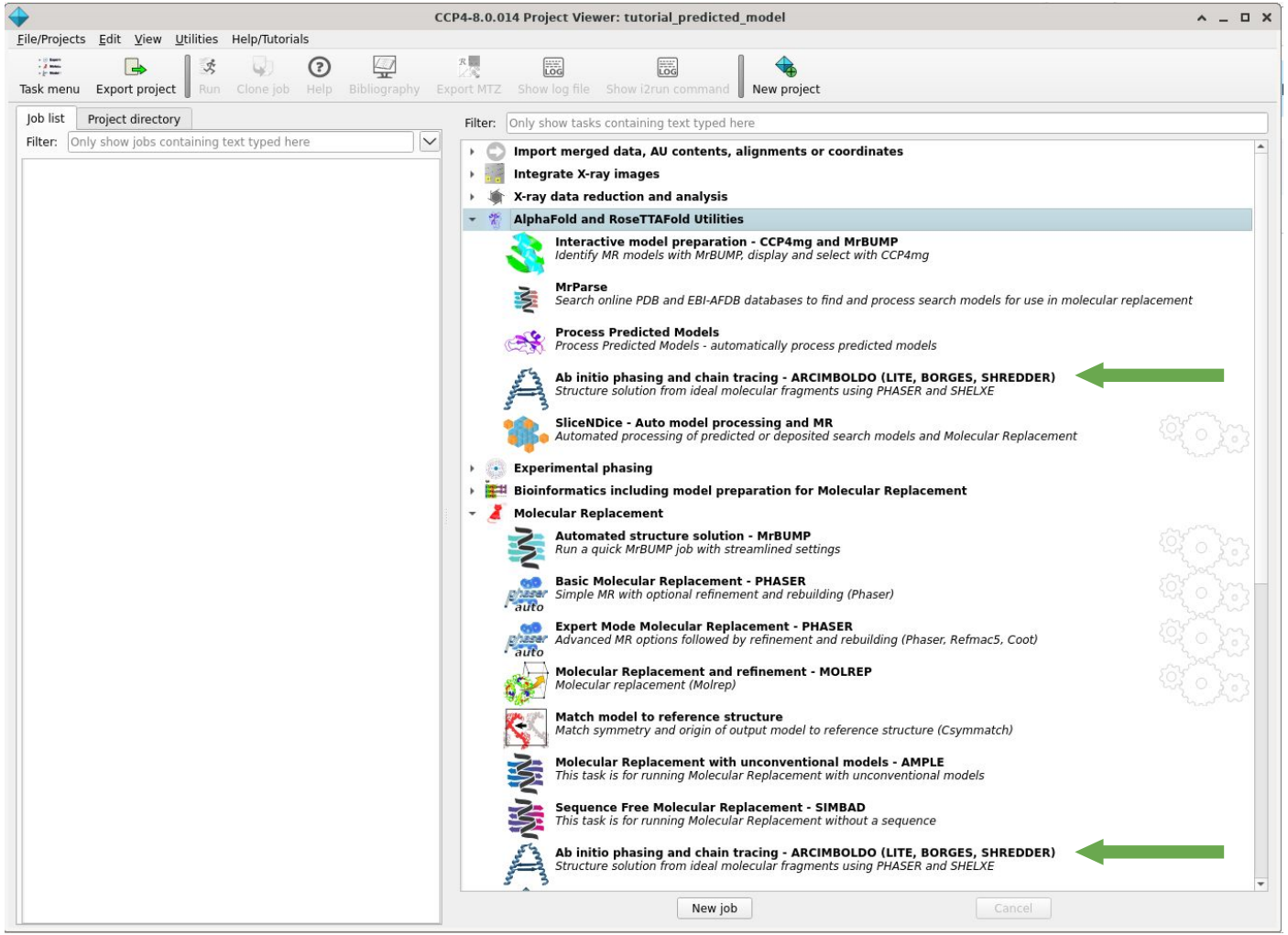
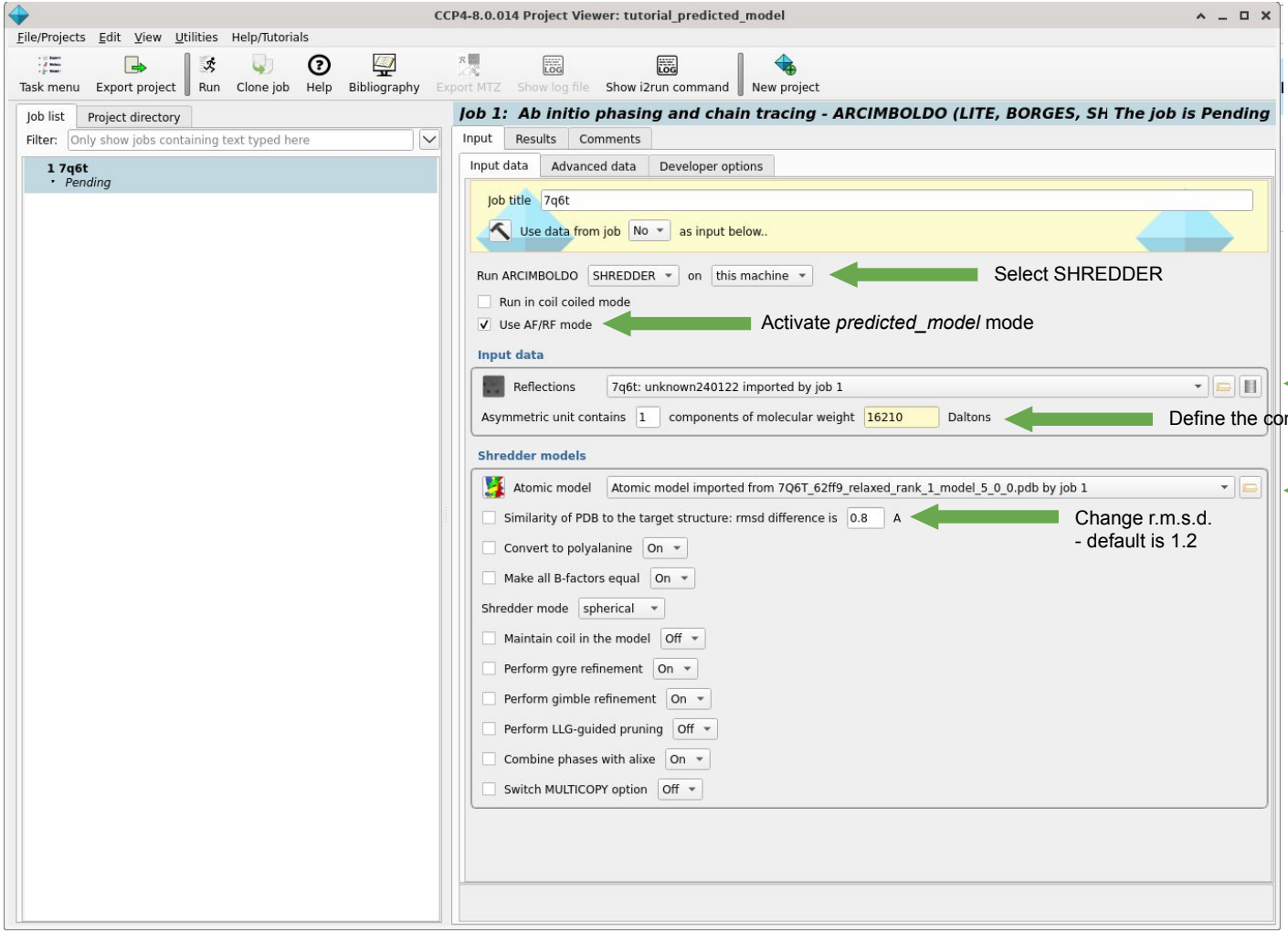
CCP4i2


CCP4-8.0.014 Project Viewer: tutorial_predicted_model
File/Projects Edit View Utilities Help/Tutorials
Task menu
Export project
Run
Clone job
Help
Bibliography
Export MTZ
Show log file
Show i2run command
New project
Job list
Project directory
Filter:
Only show jobs containing text typed here
Filter:
Only show tasks containing text typed here
Import merged data, AU contents, alignments or coordinates
Integrate X-ray images
X-ray data reduction and analysis
AlphaFold and RoseTTAFold Utilities
Interactive model preparation - CCP4mg and MrBUMP
Identify MR models with MrBUMP, display and select with CCP4mg
MrParse
Search online PDB and EBI-AFDB databases to find and process search models for use in molecular replacement
Process Predicted Models
Process Predicted Models - automatically process predicted models
Ab initio phasing and chain tracing - ARCIMBOLDO (LITE, BORGES, SHREDDER)
Structure solution from ideal molecular fragments using PHASER and SHELXE
SliceNDice - Auto model processing and MR
Automated processing of predicted or deposited search models and Molecular Replacement
Experimental phasing
Bioinformatics including model preparation for Molecular Replacement
Molecular Replacement
Automated structure solution - MrBUMP
Run a quick MrBUMP job with streamlined settings
Basic Molecular Replacement - PHASER
Simple MR with optional refinement and rebuilding (Phaser)
Expert Mode Molecular Replacement - PHASER
Advanced MR options followed by refinement and rebuilding (Phaser, Refmac5, Coot)
Molecular Replacement and refinement - MOLREP
Molecular replacement (Molrep)
Match model to reference structure
Match symmetry and origin of output model to reference structure (Csymmatch)
Molecular Replacement with unconventional models - AMPLE
This task is for running Molecular Replacement with unconventional models
Sequence Free Molecular Replacement - SIMBAD
This task is for running Molecular Replacement without a sequence
Ab initio phasing and chain tracing - ARCIMBOLDO (LITE, BORGES, SHREDDER)
Structure solution from ideal molecular fragments using PHASER and SHELXE
New job
Cancel



Select SHREDDER

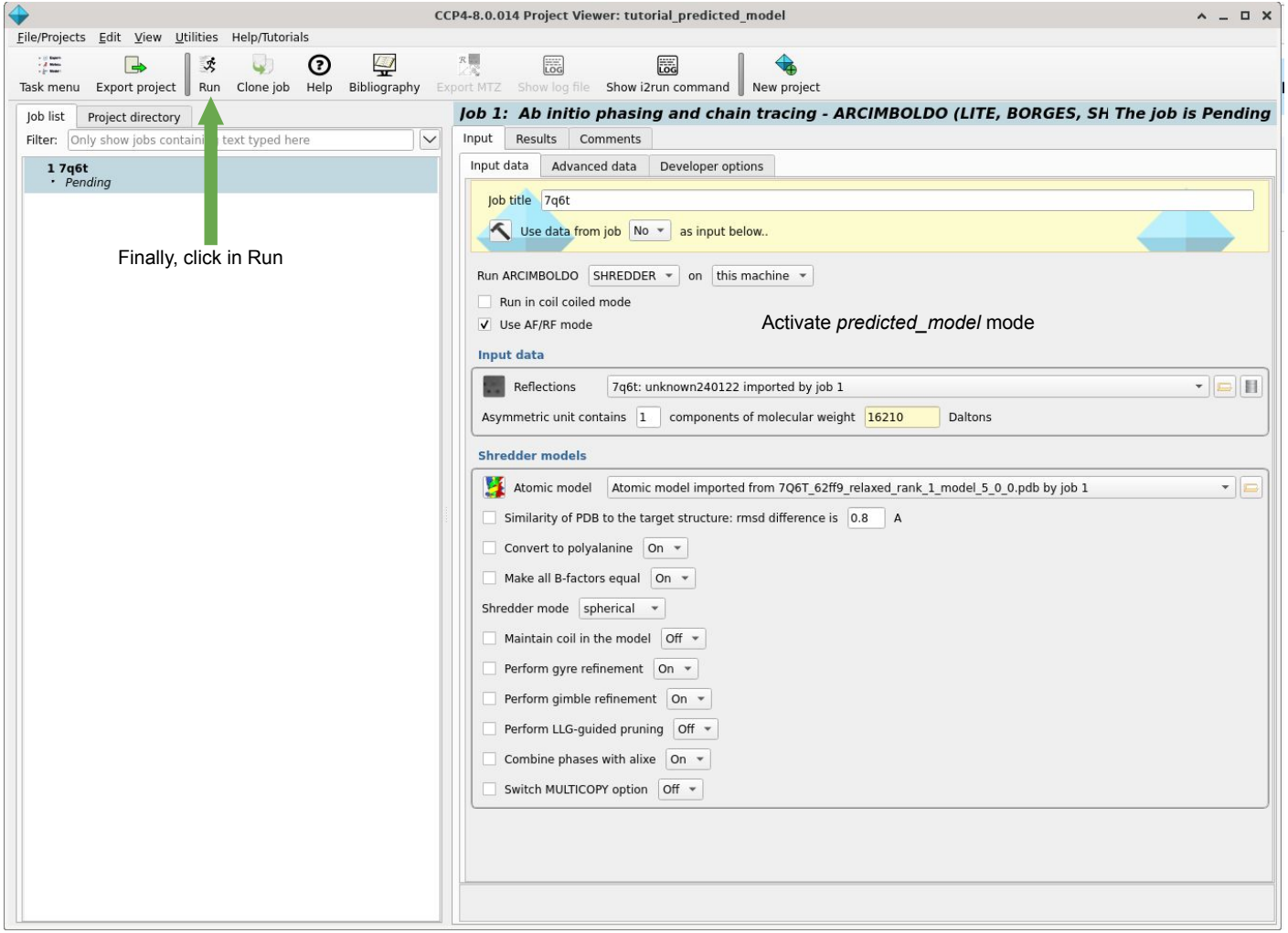
Activate *predicted_model* mode

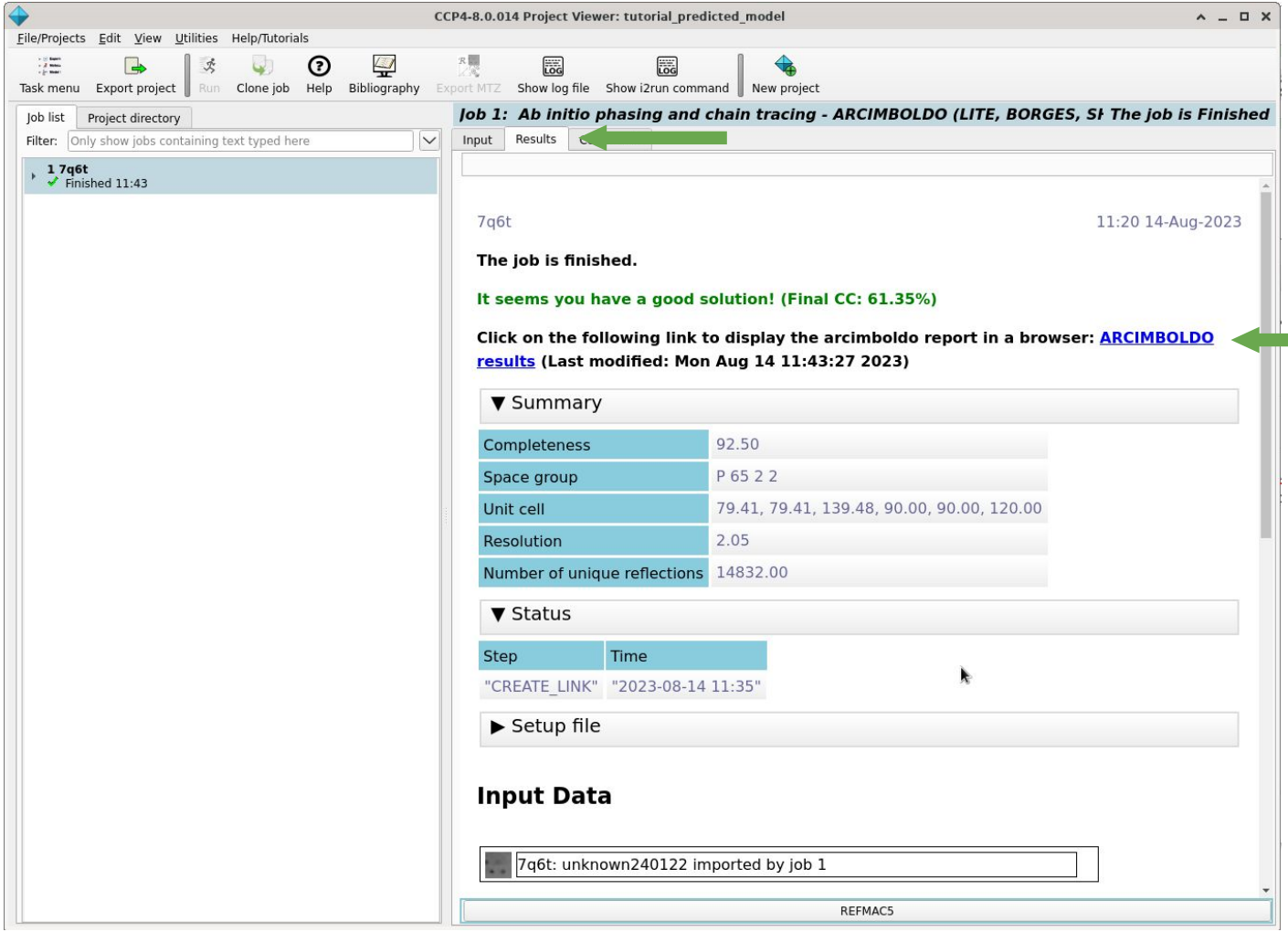
Upload crystallographic data

Define the content of the ASU

Upload predicted model

Change r.m.s.d.
- default is 1.2


CCP4-8.0.014 Project Viewer: tutorial_predicted_model
File/Projects Edit View Utilities Help/Tutorials
Task menu
Export project
Run
Clone job
Help
Bibliography
Export MTZ
Show log file
Show i2run command
New project
Job list
Project directory
Filter:
1 7q6t
Pending
Finally, click in Run
Job 1: Ab initio phasing and chain tracing - ARCIMBOLDO (LITE, BORGES, SH The job is Pending
Input
Results
Comments
Input data
Advanced data
Developer options
Job title 7q6t
Use data from job No as input below..
Run ARCIMBOLDO SHREDDER on this machine
Run in coil coiled mode
Use AF/RF mode
Activate predicted_model mode
Input data
Reflections 7q6t: unknown240122 imported by job 1
Asymmetric unit contains 1 components of molecular weight 16210 Daltons
Shredder models
Atomic model Atomic model imported from 7Q6T_62ff9_relaxed_rank_1_model_5_0_0.pdb by job 1
Similarity of PDB to the target structure: rmsd difference is 0.8 A
Convert to polyalanine On
Make all B-factors equal On
Shredder mode spherical
Maintain coil in the model Off
Perform gyre refinement On
Perform gimble refinement On
Perform LLG-guided pruning Off
Combine phases with alixe On
Switch MULTICOPY option Off


CCP4-8.0.014 Project Viewer: tutorial_predicted_model
File/Projects Edit View Utilities Help/Tutorials
Task menu
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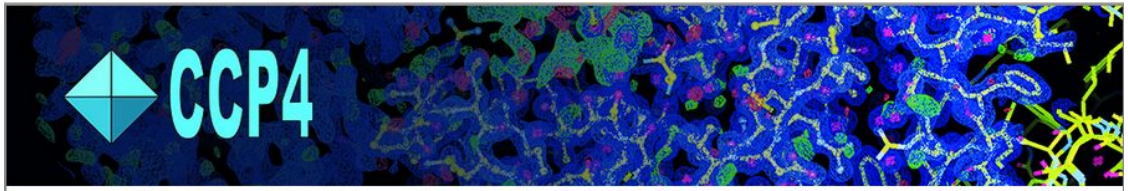
Run
Clone job
Help
Bibliography
Export MTZ
Show log file
Show i2run command
New project
Job list
Project directory
Filter:
Only show jobs containing text typed here
1 7q6t
Finished 11:43
Job 1: Ab initio phasing and chain tracing - ARCIMBOLDO (LITE, BORGES, SH The job is Finished
Input
Results
7q6t
11:20 14-Aug-2023
The job is finished.
It seems you have a good solution! (Final CC: 61.35%)
Click on the following link to display the arcimboldo report in a browser: ARCIMBOLDO results (Last modified: Mon Aug 14 11:43:27 2023)
▼ Summary
Completeness 92.50
Space group P 65 2 2
Unit cell 79.41, 79.41, 139.48, 90.00, 90.00, 120.00
Resolution 2.05
Number of unique reflections 14832.00
▼ Status
Step Time
"CREATE_LINK" "2023-08-14 11:35"
▶ Setup file
Input Data
7q6t: unknown240122 imported by job 1
REFMAC5

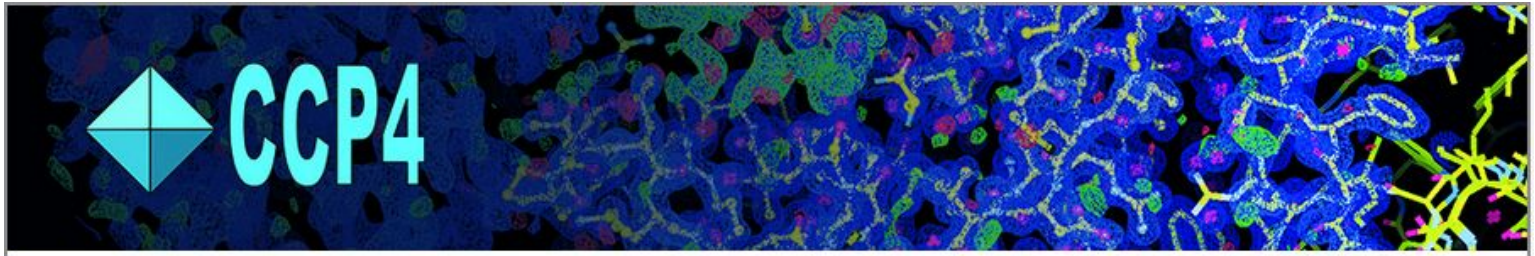
CCP4 online



Programs

Note: *You must have a CCP4 licence to run these programs*.

Balbes	An automated Molecular Replacement (MR) pipeline - Balbes integrates into one system all the components necessary for solving a crystal structure by Molecular Replacement
MrBUMP	An automated Molecular Replacement (MR) pipeline - Given a target sequence and experimental structure factors, it will search for homologous structures, create a set of suitable search models from the template structures, do molecular replacement, and test the solutions with some rounds of restrained refinement. New: MrBUMP now searches the EBI-AFDB AlphaFold database for potential search models in addition to the PDB. This increases the pool of potential search models by 350000 with more to come in the near future.
Zanuda	Space group and crystallographic origin validation
AMPLE	Automated ab initio search model generation for molecular replacement.
SHELX	Automated SHELXC/D/E structure solution pipeline for fast routine experimental phasing. Accepts data in XDS, Scalepack, SHELX hkl or mtz formats and outputs phases and a poly-Ala trace. If a protein sequence is provided, BUCCANEER and REFMAC complete the structure.
CRANK2	Automated structure solution pipeline for experimental phasing using maximum likelihood methods.
MoRDa	MoRDa is a pipeline for molecular replacement protein structure solution based on its own domain database. Models relevant to the target sequence are further adjusted before molecular replacement search.
SIMBAD	Sequence-independent molecular replacement, good for identifying if your crystal contains a contaminant protein. SIMBAD can also do full search of homologous structures in difficult-to-solve novel target cases, but this functionality is not yet available through CCP4-Online.
ARCIMBOLDO	Crystallographic Ab Initio protein solution below atomic resolution



ARCIMBOLDO

CLICK HERE TO START A NEW ARCIMBOLDO RUN

The table below shows your current ARCIMBOLDO runs - the results will be stored on the server for at least 30 days

id	Job Title	Delete/Stop	Date	Status	View Results

CCP4 STFC Rutherford Appleton Laboratory, Harwell Campus
Didcot Oxon OX11 0FA
Tel:(+44) 1235 567726 | Fax: +44 (+44) 1235 567720 | Email: ccp4@ccp4.ac.uk

New ARCIMBOLDO Run

ARCIMBOLDO combines fragment search with PHASER and density modification and autotracing with SHELXE, at resolutions of 2.5 Å or better (4 Å for coiled-coil mode).

ARCIMBOLDO_LITE uses single models, typically polyalanine helices;
ARCIMBOLDO_BORGES uses precomputed libraries of local folds;
ARCIMBOLDO_SHREDDER uses fragments from a distant homolog or predicted models.

Data description

run ARCIMBOLDO:	SHREDDER ← Select SHREDDER
Job title (optional):	7q6t
Input data (.mtz):	Browse… 7q6t.mtz ← Upload crystallographic data
Input type:	amplitudes
Column labels:	SIGF FP F SIGFP
Target Sequence:	
Asymmetric unit description:	**Molecular weight:** 16210 (please give either this or the target sequence) ← Define the content of the ASU
	Number of components: 1

ARCIMBOLDO SHREDDER

Model:	Browse… 7Q6T_62ff9_relaxed_rank_1_model_5_0_0.pdb	r.m.s.d.: 0.8 A
Convert to polyalanine (optional):		
Make all B-factors equal (optional):		
Alphafold or RoseTTaFold model:	True	
Shredder mode:	spherical	
	Fragment size (optional):	
	Maintain coil in the model (optional):	
	Perform gyre refinement (optional):	
	Perform gimble refinement (optional):	
	Perform LLG-guided pruning (optional):	
	Combine phases with alixe (optional):	

Upload predicted model

Activate *predicted_model* mode

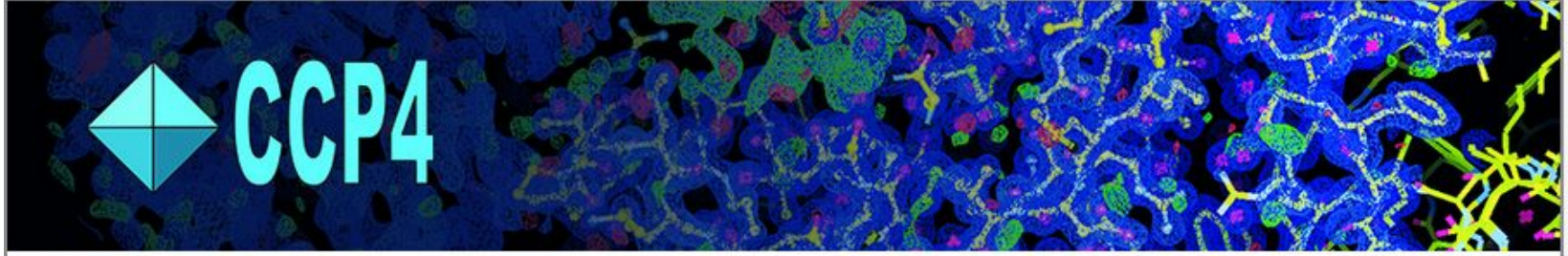
Change r.m.s.d. - default is 1.2

Advanced options

Add keyword-value

Submit | Validate | Restart

Click first in validate, then in submit



ARCIMBOLDO

CLICK HERE TO START A NEW ARCIMBOLDO RUN

The table below shows your current ARCIMBOLDO runs - the results will be stored on the server for at least 30 days

id	Job Title	Delete/Stop	Date	Status	View Results
2609199041	7q6t	stop	14 Aug 2023 [10:03]	starting process	results

CCP4 STFC Rutherford Appleton Laboratory, Harwell Campus
Didcot Oxon OX11 0FA
Tel:(+44) 1235 567726 | Fax: +44 (+44) 1235 567720 | Email: ccp4@ccp4.ac.uk

ARCIMBOLDO

PROCESS **2609199041** IS STARTING

Your results should appear below when the job has started:

Reload Page 

ARCIMBOLDO

PROCESS **2609199041** IS RUNNING

[stop process]

ARCIMBOLDO-SHREDDER

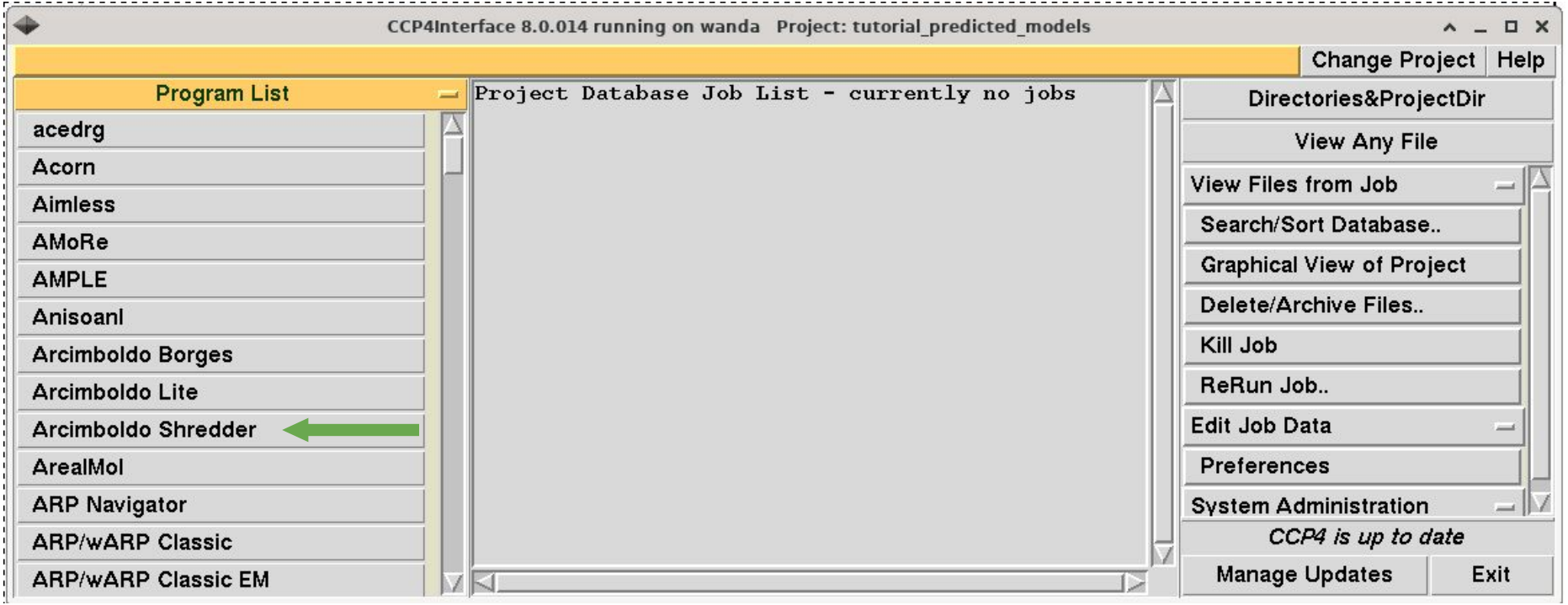
Summary

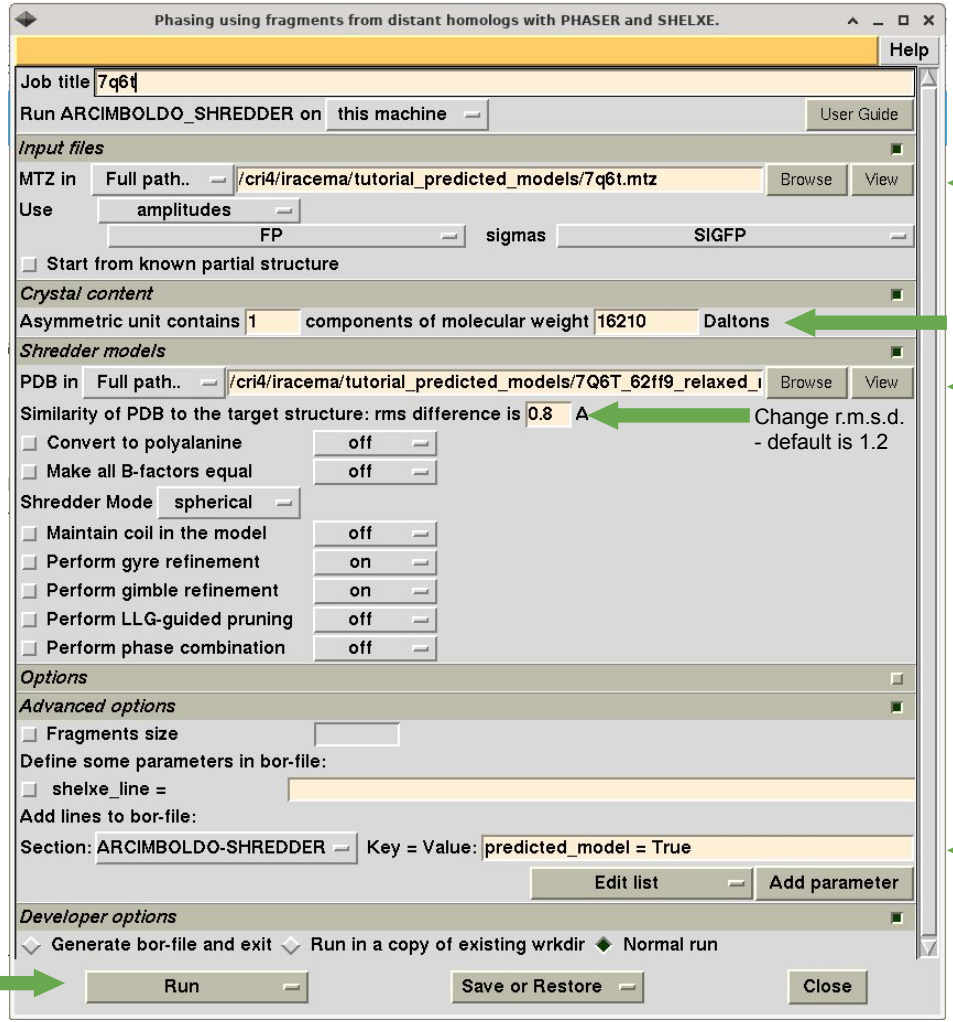
NAME: 7q6t
SPACEGROUP: P 65 2 2
CELL DIMENSIONS: 79.41, 79.41, 139.48, 90.00, 90.00, 120.00
RESOLUTION: 2.05
NUMBER OF UNIQUE REFLECTIONS: 14832.00

Click here to follow the progress with the ARCIMBOLDO_BORGES 

Instruction file

CCP4i


CCP4Interface 8.0.014 running on wanda Project: tutorial_predicted_models
Change Project
Help
Program List
acedrg
Acorn
Aimless
AMoRe
AMPLE
Anisoanl
Arcimboldo Borges
Arcimboldo Lite
Arcimboldo Shredder
ArealMol
ARP Navigator
ARP/wARP Classic
ARP/wARP Classic EM
Project Database Job List - currently no jobs
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
System Administration
CCP4 is up to date
Manage Updates
Exit



Upload crystallographic data

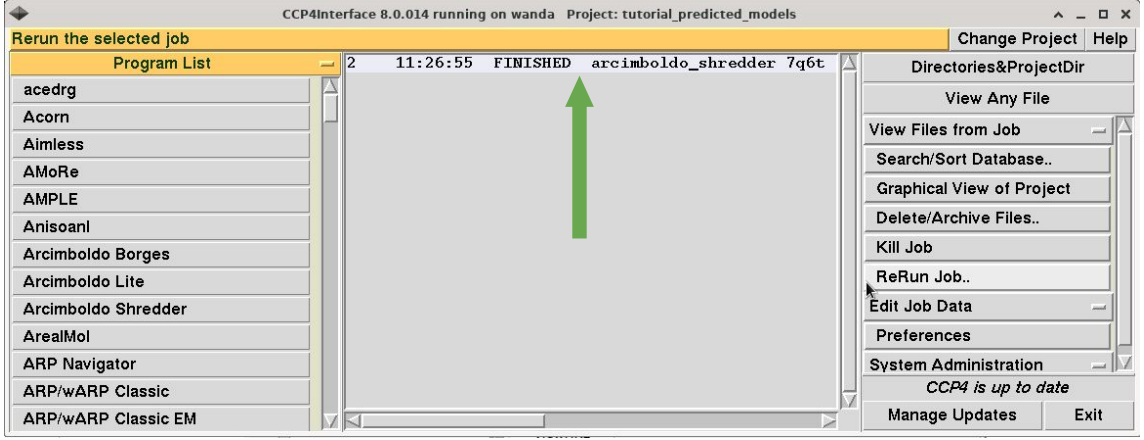
Define the content of the ASU

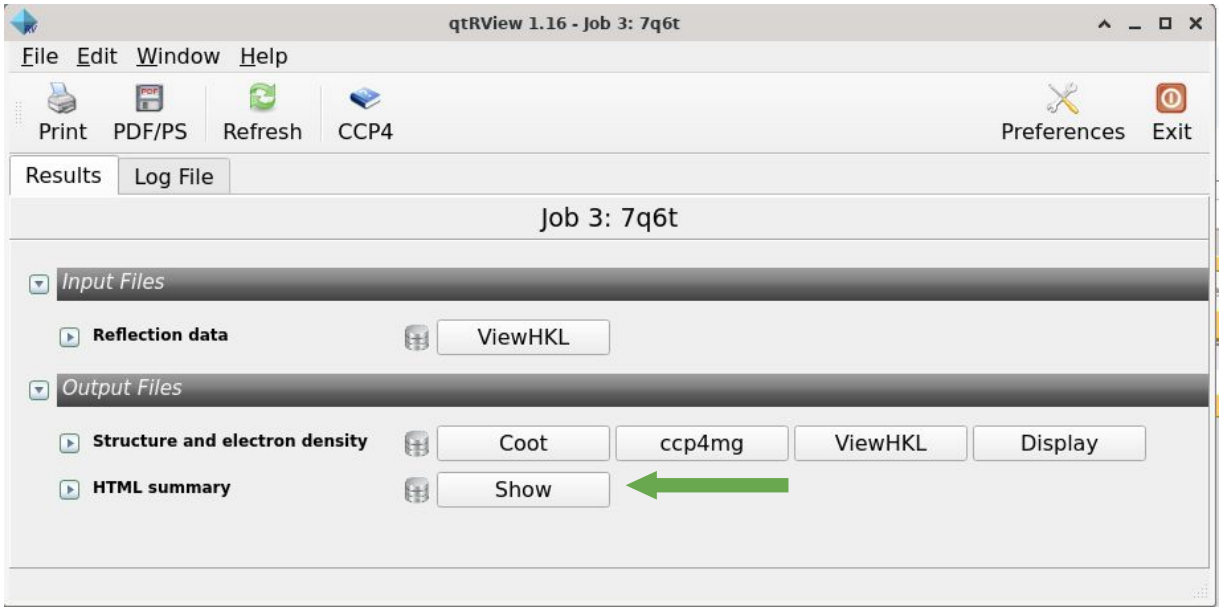
Upload predicted model

Change r.m.s.d.
- default is 1.2

Activate *predicted_model* mode

Finally, click in Run


CCP4Interface 8.0.014 running on wanda Project: tutorial_predicted_models
Rerun the selected job
Change Project
Help
Program List
acedrg
Acorn
Aimless
AMoRe
AMPLE
Anisoanl
Arcimboldo Borges
Arcimboldo Lite
Arcimboldo Shredder
ArealMol
ARP Navigator
ARP/wARP Classic
ARP/wARP Classic EM
2 11:26:55 FINISHED arcimboldo_shredder 7q6t
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
System Administration
CCP4 is up to date
Manage Updates
Exit


qtRView 1.16 - Job 3: 7q6t
File Edit Window Help
Print
PDF/PS
Refresh
CCP4
Preferences
Exit
Results
Log File
Job 3: 7q6t
Input Files
Reflection data
ViewHKL
Output Files
Structure and electron density
Coot
ccp4mg
ViewHKL
Display
HTML summary
Show