

PReSTO @ Arrhenius-CPU

First testing

native.script: update <https://www.nsc.liu.se/support/presto/MX-PReSTO/BioMax/>

DIALS sometimes terminate with:

omptbx error: deadlock in using lock variable

```
Terminal - x_marmo@n940:~
File Edit View Terminal Tabs Help

x_marmo@tetralith3:proj/xray/users/x_marmo/targets/biomax/raw_test x_marmo@n940:~

top - 14:16:25 up 2:56, 0 users, load average: 0.00, 0.01, 0.78
Tasks: 434 total, 1 running, 432 sleeping, 0 stopped, 1 zombie
%Cpu(s): 0.0 us, 0.0 sy, 0.0 ni, 99.9 id, 0.0 wa, 0.0 hi, 0.0 si, 0.0 st
MiB Mem : 95346.2 total, 91584.7 free, 4044.9 used, 384.2 buff/cache
MiB Swap: 1953.0 total, 1953.0 free, 0.0 used, 91301.3 avail Mem

  PID USER      PR  NI   VIRT   RES   SHR  S  %CPU  %MEM    TIME+  COMMAND
 68883 x_marmo   20    0  796636 282624 61296 S   1.0   0.3   0:21.70 python
 68803 x_marmo   20    0  223388  4572   3416 S   0.0   0.0   0:00.01 slurm_script
 68855 x_marmo   20    0  826460 283060 74060 S   0.0   0.3   0:03.64 python
 68890 x_marmo   20    0  2831656 287720 60724 S   0.0   0.3   0:00.28 python
 68891 x_marmo   20    0  1062184 284584 60660 S   0.0   0.3   0:00.20 python
 68892 x_marmo   20    0  1062184 284584 60660 S   0.0   0.3   0:00.33 python
 68893 x_marmo   20    0  2372904 293724 60724 S   0.0   0.3   0:00.26 python
 68894 x_marmo   20    0  1979688 312040 60724 S   0.0   0.3   0:00.24 python
 68895 x_marmo   20    0  1062184 284596 60664 S   0.0   0.3   0:00.23 python
 68896 x_marmo   20    0  1062184 284592 60660 S   0.0   0.3   0:00.35 python
 68897 x_marmo   20    0  1586472 293492 60724 S   0.0   0.3   0:00.19 python
 68898 x_marmo   20    0  1062184 284592 60660 S   0.0   0.3   0:00.17 python
 68899 x_marmo   20    0  1062184 284592 60656 S   0.0   0.3   0:00.26 python
 68900 x_marmo   20    0  2897192 320360 60724 S   0.0   0.3   0:00.58 python
 68901 x_marmo   20    0  1586472 319936 60724 S   0.0   0.3   0:00.63 python
 68903 x_marmo   20    0  2438440 318348 60724 S   0.0   0.3   0:00.27 python
 68904 x_marmo   20    0  1455400 287248 60660 S   0.0   0.3   0:00.23 python
 68905 x_marmo   20    0  2700584 320388 60724 S   0.0   0.3   0:00.43 python
 70570 x_marmo   20    0  224008  5512   3688 S   0.0   0.0   0:00.02 bash
 70632 x_marmo   20    0  226084  4800   3672 R   0.0   0.0   0:00.04 top
```

These four lines resolve the issue but are there better options?

```
dials="\
module use /software/presto/e/karho/modules/all
ml DIALS/3.26.0-PReSTO-karho
export OMP_NUM_THREADS=1
export OPENBLAS_NUM_THREADS=1
export MKL_NUM_THREADS=1
export NUMEXPR_NUM_THREADS=1
cd $outdir/dials
xia2 \
    pipeline=dials failover=true \
    image=$indir:$3:$4 \
    multiprocessing.mode=serial \
    multiprocessing.njob=1 \
    multiprocessing.nproc=128
```

```
lsbatch -N1 --exclusive --ntasks-per-node=128 -A naiss2026-3-674-cpu -t 01:00:00 -J DIALS -o "$outdir/dials.out" --wrap="$dials"
```

	Cosmos time (s)	Cosmos cores	Arrhenius time (s)	Arrhenius cores	SpeedUp	Ideal
XDSAPP	302	48	121	256	2,5	5,3
DIALS	505	48	221	128 ¹	2,3	2,7
autoPROC	2660	48	607	256	4,4	5,3

¹With 256 cores DIALS did NOT crash at Arrhenius, but runtime was 230 seconds
 2 Å dataset from BioMAX with 3600 frames used as test data

Does NOT work

```
dials="\nmodule use /software/presto/e/karho/modules/all\nml DIALS/3.26.0-PreSTO-karho\nexport OMP_NUM_THREADS=2\nexport OPENBLAS_NUM_THREADS=1\nexport MKL_NUM_THREADS=1\nexport NUMEXPR_NUM_THREADS=1\ncd $outdir/dials\nxia2 \n    pipeline=dials failover=true \n    image=$indir:$3:$4 \n    multiprocessing.mode=serial \n    multiprocessing.njob=1 \n    multiprocessing.nproc=64\n\n# autoproc bails out if its outdir basename exists; don't make it\n# mkdir "$outdir/xdsapp"\nmkdir "$outdir/dials"\n\nsbatch -N1 --exclusive --ntasks=64 --cpus-per-task=2 -A naiss2026-3-674-cpu -t 01:00:00 -J DIALS -o "$outdir/dials.out" --wrap="$dials"
```

mochma@n291:~

x

mochma@arrhenius3:~

top - 14:22:44 up 11 days, 19:53, 0 users, load average: 0.00, 0.81, 23.53

Tasks: 3163 total, 1 running, 3162 sleeping, 0 stopped, 0 zombie

%Cpu(s): 0.0 us, 0.0 sy, 0.0 ni,100.0 id, 0.0 wa, 0.0 hi, 0.0 si, 0.0 st

MiB Mem : 773509.8 total, 762846.2 free, 12228.7 used, 1177.6 buff/cache

MiB Swap: 2048.0 total, 2048.0 free, 0.0 used. 761281.0 avail Mem

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
2390085	mochma	20	0	229356	7936	3592	R	0.7	0.0	0:00.12	top
2389353	mochma	20	0	790076	289396	60472	S	0.3	0.0	0:03.32	python
2387918	mochma	20	0	223452	4596	3384	S	0.0	0.0	0:00.00	slurm_script
2389329	mochma	20	0	808040	283004	73436	S	0.0	0.0	0:03.74	python
2389360	mochma	20	0	928528	272908	6152	S	0.0	0.0	0:00.02	python
2389361	mochma	20	0	928528	272924	6152	S	0.0	0.0	0:00.02	python
2389362	mochma	20	0	928528	237500	6152	S	0.0	0.0	0:00.01	python
2389363	mochma	20	0	928528	272912	6152	S	0.0	0.0	0:00.02	python
2389364	mochma	20	0	928528	272912	6152	S	0.0	0.0	0:00.02	python
2389365	mochma	20	0	928528	272912	6152	S	0.0	0.0	0:00.02	python
2389366	mochma	20	0	928528	237508	6152	S	0.0	0.0	0:00.00	python
2389367	mochma	20	0	928528	237508	6152	S	0.0	0.0	0:00.00	python
2389371	mochma	20	0	928528	237508	6152	S	0.0	0.0	0:00.01	python
2389373	mochma	20	0	928528	272920	6156	S	0.0	0.0	0:00.03	python
2389376	mochma	20	0	928528	237512	6156	S	0.0	0.0	0:00.01	python
2389379	mochma	20	0	928528	272916	6156	S	0.0	0.0	0:00.02	python
2389380	mochma	20	0	928528	272916	6156	S	0.0	0.0	0:00.02	python
2389382	mochma	20	0	928528	237508	6156	S	0.0	0.0	0:00.01	python
2389383	mochma	20	0	928528	272916	6156	S	0.0	0.0	0:00.03	python
2389388	mochma	20	0	928528	272916	6156	S	0.0	0.0	0:00.02	python
2389389	mochma	20	0	928528	272916	6156	S	0.0	0.0	0:00.02	python
2389392	mochma	20	0	928528	272916	6156	S	0.0	0.0	0:00.02	python
2389394	mochma	20	0	928528	272916	6156	S	0.0	0.0	0:00.03	python
2389397	mochma	20	0	928528	272916	6156	S	0.0	0.0	0:00.02	python
2389401	mochma	20	0	928528	272964	6204	S	0.0	0.0	0:00.02	python
2389402	mochma	20	0	928528	272964	6204	S	0.0	0.0	0:00.02	python
2389403	mochma	20	0	928528	272964	6204	S	0.0	0.0	0:00.02	python
2389406	mochma	20	0	928528	272964	6204	S	0.0	0.0	0:00.02	python
2389407	mochma	20	0	928528	272964	6204	S	0.0	0.0	0:00.02	python
2389408	mochma	20	0	928528	272964	6204	S	0.0	0.0	0:00.02	python
2389412	mochma	20	0	928528	237552	6200	S	0.0	0.0	0:00.01	python
2389418	mochma	20	0	928528	272968	6204	S	0.0	0.0	0:00.03	python
2389420	mochma	20	0	928528	272968	6204	S	0.0	0.0	0:00.02	python

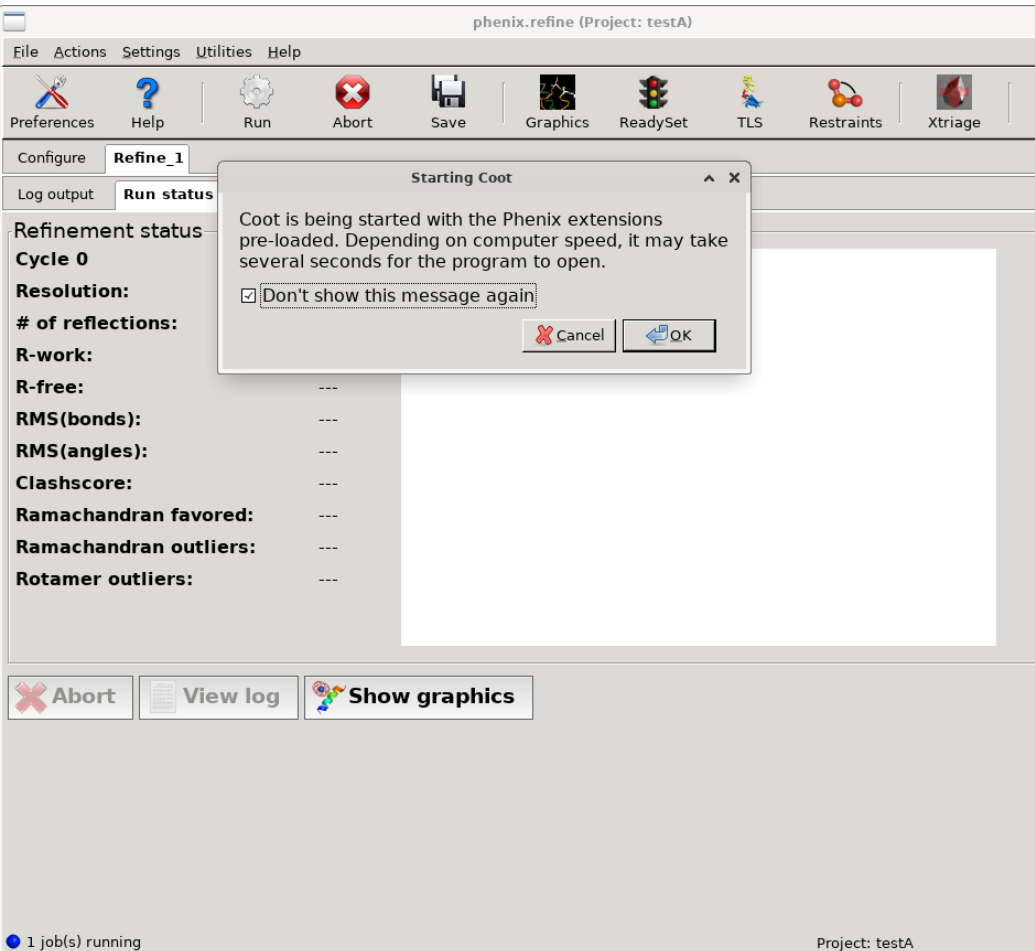
Phenix at login node - not OK

It looks ok a sbatch job is submitted but the directories are empty

```
[mochma@arrhenius3 phenix]$ pwd
/nobackup/proj/disk/xray/personal/mochma/testA/phenix
[mochma@arrhenius3 phenix]$ ls Refine_*
Refine_1:
Refine_2:
Refine_3:
testA_refine_003.cif  testA_refine_003.geo      testA_refine_003.kin  testA_refine_003.mtz
testA_refine_003.eff  testA_refine_003_info.txt testA_refine_003.log  testA_refine_003.pdb
[mochma@arrhenius3 phenix]$
```

...and something happens...

```
[mochma@arrhenius3 phenix]$ squeue -u mochma
  JOBID PARTITION   NAME     USER ST       TIME  NODES NODELIST(REASON)
  2545790      cpu phenix_4  mochma PD        0:00      1 (Resources)
[mochma@arrhenius3 phenix]$ squeue -u mochma
  JOBID PARTITION   NAME     USER ST       TIME  NODES NODELIST(REASON)
[mochma@arrhenius3 phenix]$ sacct -j 2545790
JobID      JobName  Partition  Account    AllocCPUS      State  ExitCode
-----
2545790    phenix_41+  cpu  naiss2026+      256  COMPLETED      0:0
2545790.bat+  batch      naiss2026+      256  COMPLETED      0:0
2545790.ext+  extern      naiss2026+      256  COMPLETED      0:0
2545790.0    libtbx.py+  naiss2026+      256  FAILED          1:0
[mochma@arrhenius3 phenix]$
```



/software/presto/e/karho/software/Phenix/2.0-5936-foss-2023a/bin/phenix

Phenix at compute node - ok but a time waste...

COOT cannot be run at compute node
- perhaps intentional?
Error message? *vglrun is not available*

“Run locally” is working at compute node and job finishes ok!

The screenshot shows the phenix.refine GUI with the 'Run' menu open and 'Run locally' highlighted. Below the GUI, a terminal window displays system statistics:

```
top - 14:54:04 up 13 days, 7:00, 0 users, load average: 3.20, 0.85, 1.06
Tasks: 3098 total, 11 running, 3087 sleeping, 0 stopped, 0 zombie
%Cpu(s): 3.8 us, 0.3 sy, 0.0 ni, 95.9 id, 0.0 wa, 0.0 hi, 0.0 si, 0.0 st
MiB Mem : 773509.7 total, 759969.9 free, 15236.5 used, 914.4 buff/cache
MiB Swap: 2048.0 total, 2048.0 free, 0.0 used, 758273.2 avail Mem
```

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
842157	mochma	20	0	1254864	361828	5708	R	69.3	0.0	0:02.10	python
842163	mochma	20	0	1254864	361828	5708	R	69.3	0.0	0:02.10	python
842165	mochma	20	0	1254864	361828	5708	R	69.3	0.0	0:02.10	python
842158	mochma	20	0	1254864	361828	5708	R	69.0	0.0	0:02.09	python
842159	mochma	20	0	1254864	361828	5708	R	69.0	0.0	0:02.09	python
842160	mochma	20	0	1254864	361832	5712	R	69.0	0.0	0:02.09	python
842161	mochma	20	0	1254864	361828	5708	R	69.0	0.0	0:02.09	python
842162	mochma	20	0	1254864	361828	5708	R	69.0	0.0	0:02.09	python
842164	mochma	20	0	1254864	361828	5708	R	69.0	0.0	0:02.09	python
842166	mochma	20	0	0	0	0	R	69.0	0.0	0:02.09	python
840543	mochma	20	0	1254864	373020	16900	S	14.5	0.0	0:37.84	python
841891	mochma	20	0	229296	7848	3568	R	1.0	0.0	0:00.09	top
840490	mochma	20	0	1234584	333224	95272	S	0.3	0.0	0:09.66	python
838323	mochma	20	0	224724	6320	3756	S	0.0	0.0	0:00.02	bash
841789	mochma	20	0	223908	5528	3748	S	0.0	0.0	0:00.01	bash
842172	mochma	20	0	1254864	357944	1824	S	0.0	0.0	0:00.00	python

The screenshot shows the phenix.refine GUI with the 'Results' tab selected. The 'Output files' section lists several files, and the 'Open in Coot' button is highlighted. The 'Refinement statistics' section shows a warning about R-free increasing during refinement.

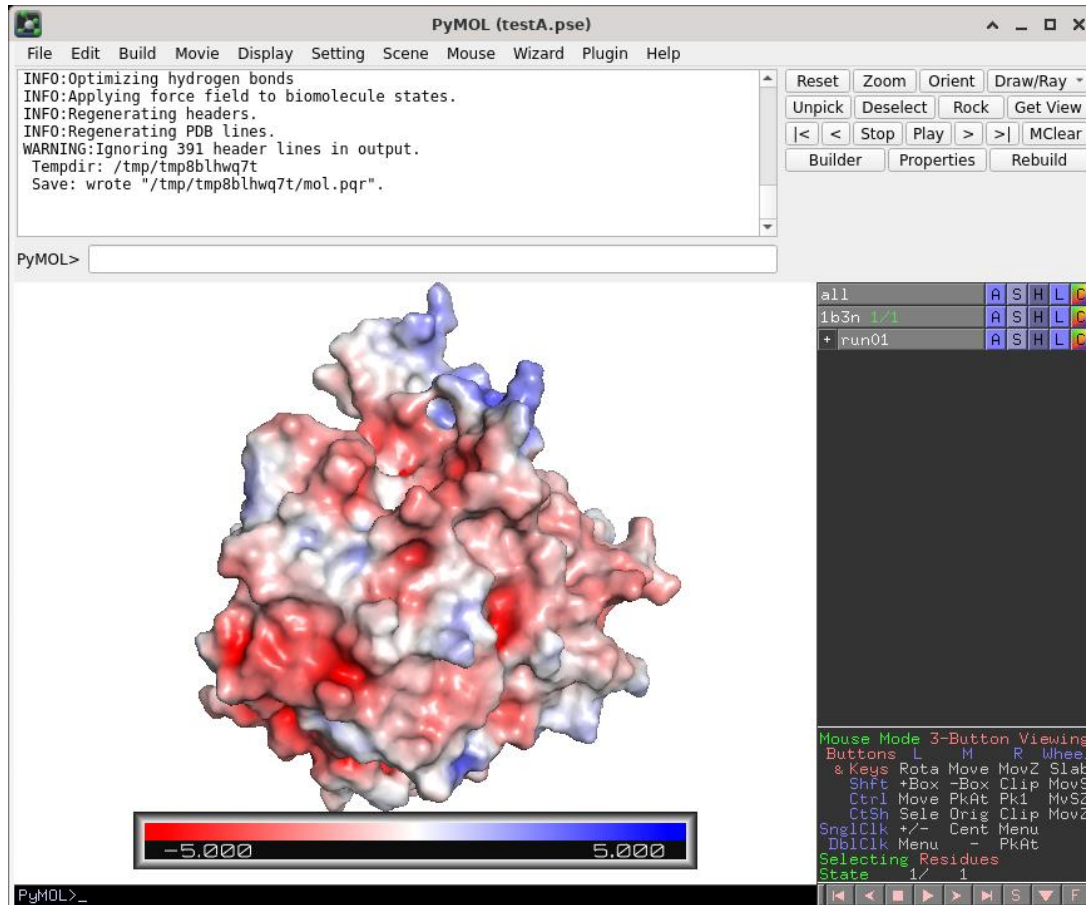
File name	Contents
testA_refine_003.eff	Effective parameters for t...
testA_refine_003.mtz	Map coefficients for Coot
testA_refine_003.pdb	Refined model
testA_refine_003.log	phenix.refine log file
testA_refine_003.geo	Geometry restraints before...

	Starting	Final
R-work	0.2576	0.2887
R-free	0.3185	0.3497

WARNING: R-free increased during refinement; the selected strategy may not be appropriate.

PyMOL OK!

APBS is ok!



High resolution images no problem



Projects Edit View Utilities Help/Tutorials

Export project Run Clone job Help Bibliography Export MTZ Show log file Show i2run command New project

Project directory

Only show jobs containing text typed here

2 COOT

Running 15:46

1 Servalcat

Finished 15:46

R1work=0.1656 R1free=0.2307 (CClwork)=0.8922 (CClfree)=0.7541

Ccp4i2 is ok

Job 2: Model building - COOT 0.9

The job is Running

Input Results Comments

Input data

Job title COOT

Key bindings

Use Bernhard a

Coordinates

Show list

Model fro

Electron dens

Show list

Density n

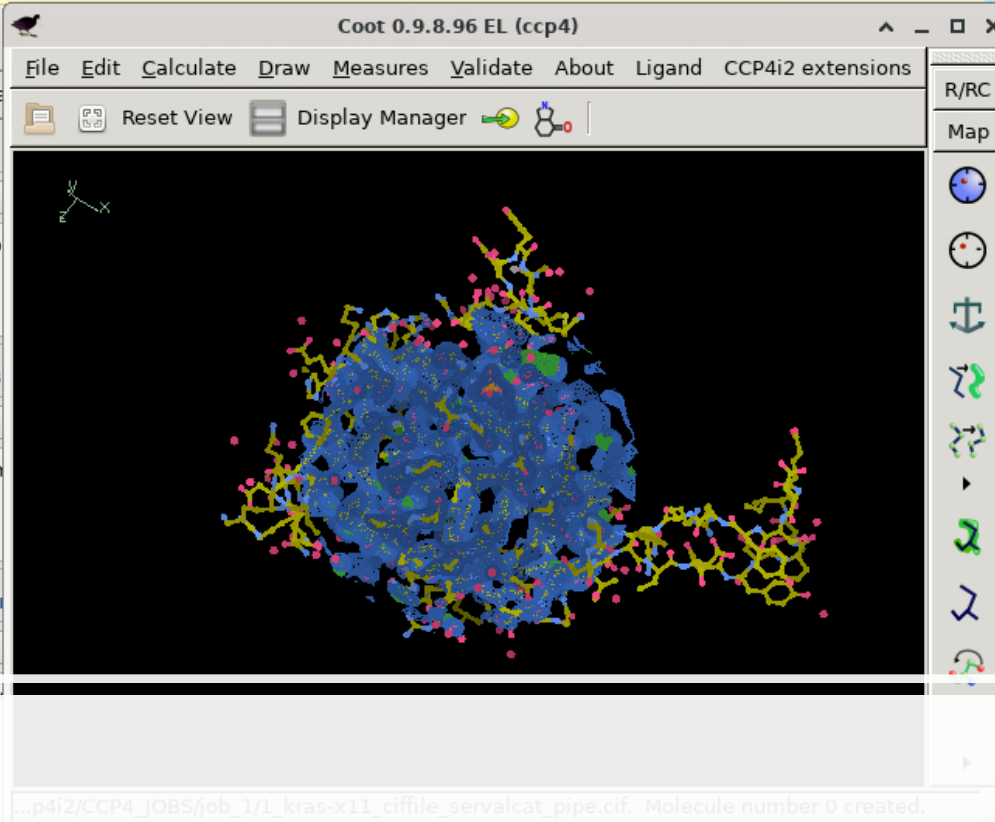
Difference de

Show list

Differen

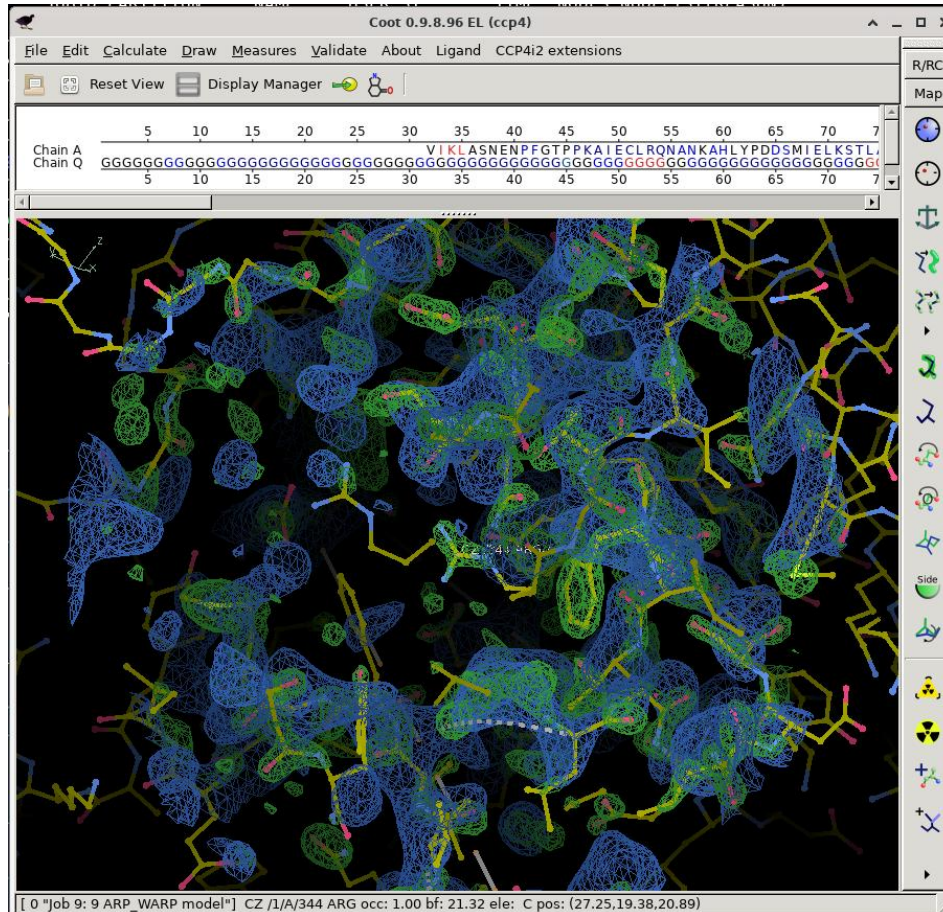
Anomalous di

Show list

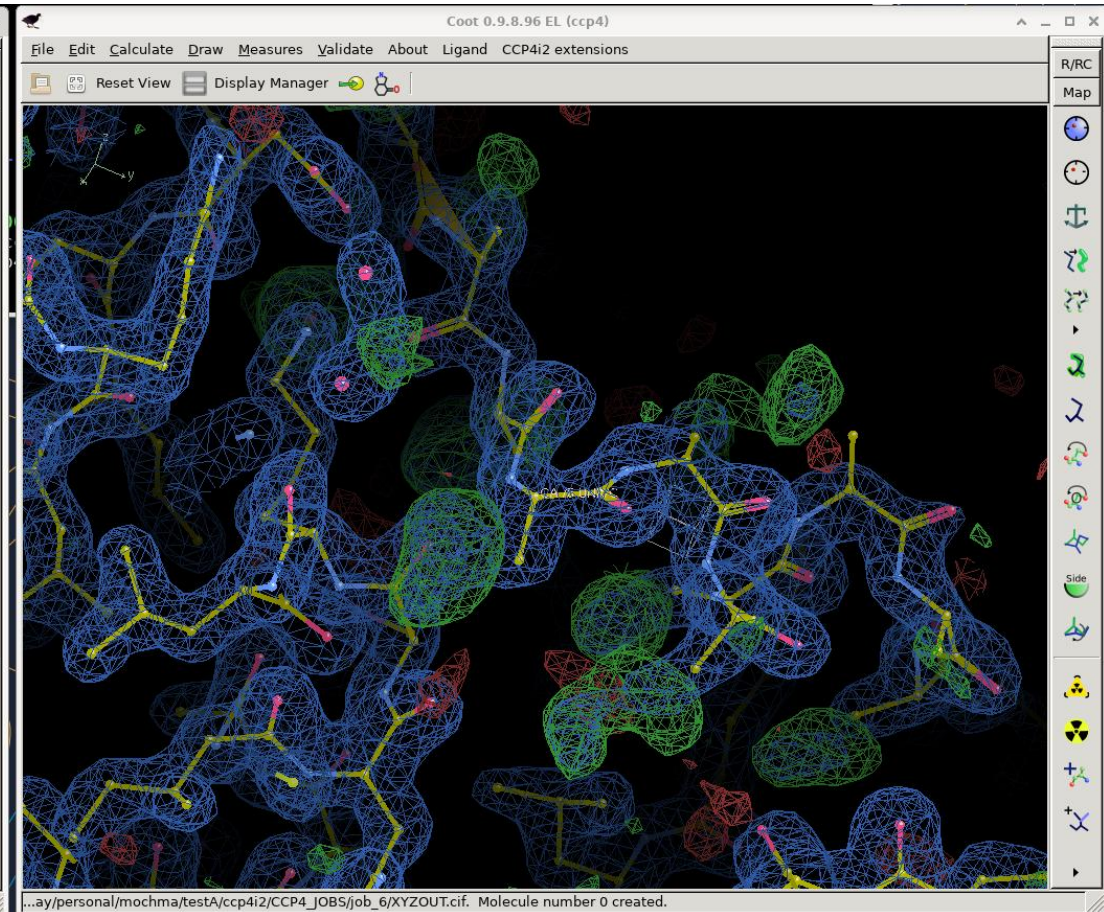


...p4i2/CCP4_JOBS/job_1/1_kras-x11_ciffile_servalcat_pipe.cif. Molecule number 0 created.

Compare arpWarp vs ModelCraft

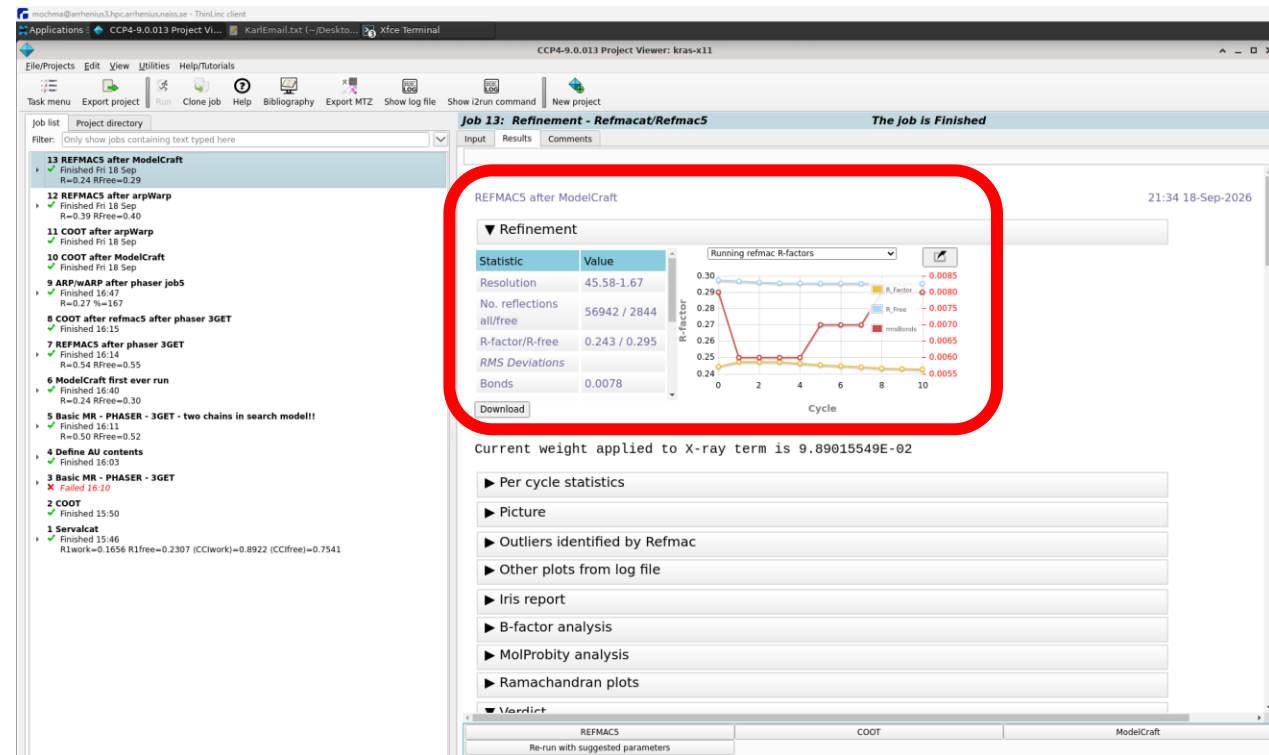
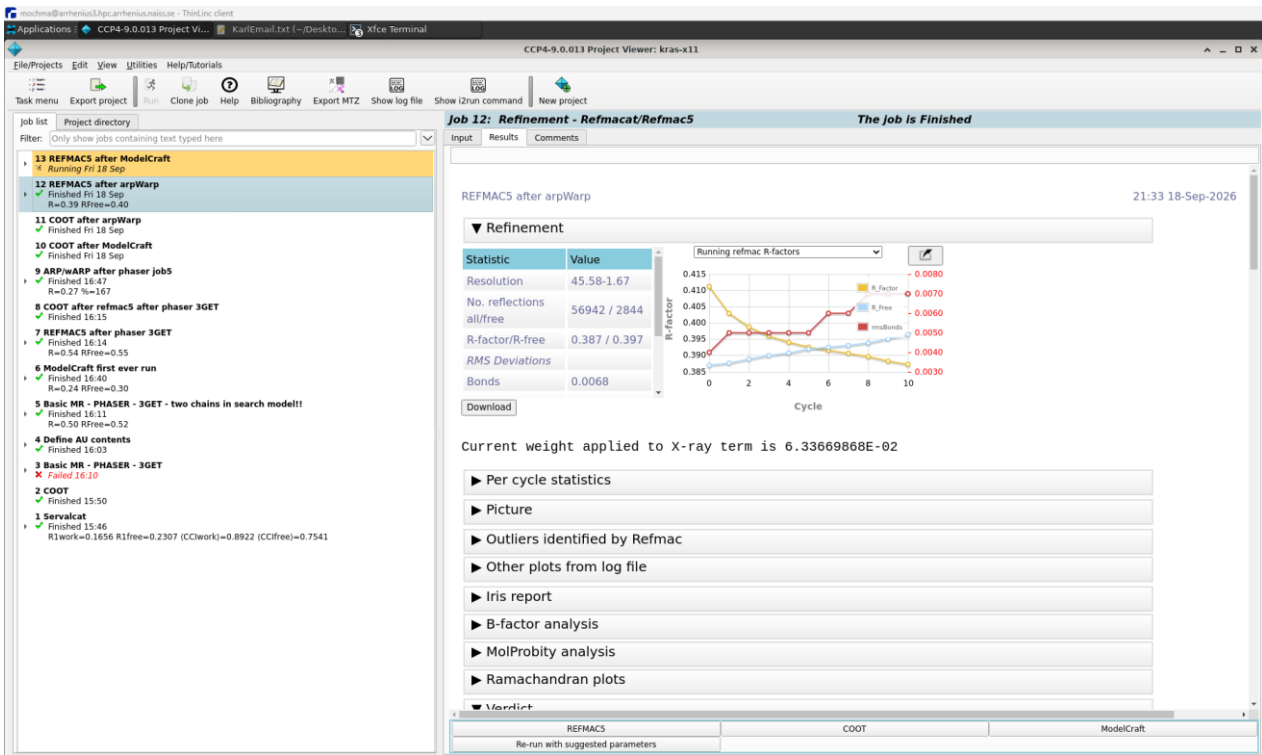


arpWarp

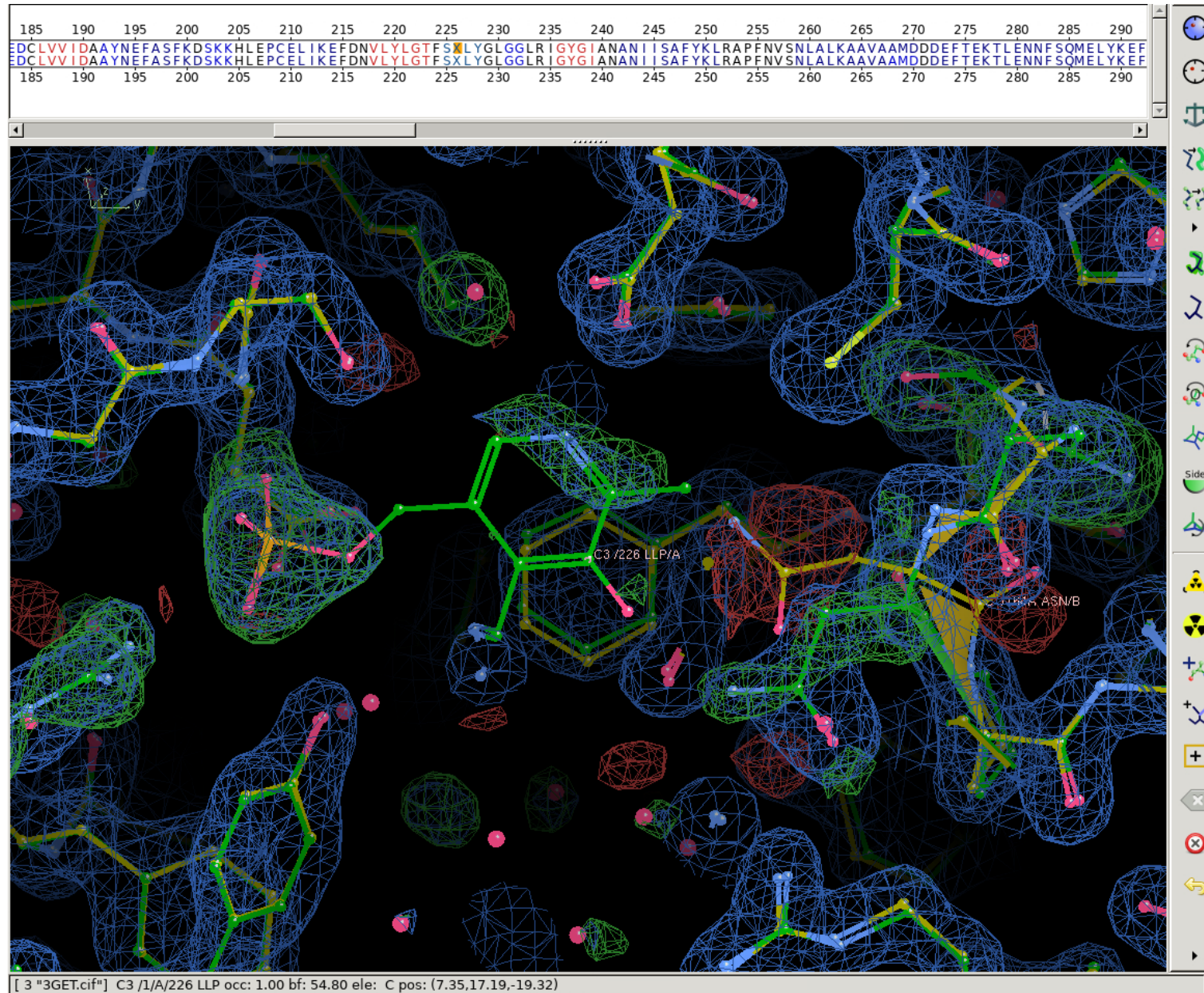


ModelCraft

ModelCraft lower (better) R-values than arpWarp after refmac5



ModelCraft autoBuild vs deposit 3GET



Very impressive results from ModelCraft
since completely “unaware” of PLP ligand!

One minor error in Pro162-Pro166 stretch
close to PLP...

ModelCraft in yellow and 3GET in green.

14 COOT after ModelCraft AND refmac5

* Running Fri 18 Sep

13 REFMAC5 after ModelCraft

✓ Finished Fri 18 Sep
R=0.24 RFree=0.29

12 REFMAC5 after arpWarp

✓ Finished Fri 18 Sep
R=0.39 RFree=0.40

11 COOT after arpWarp

✓ Finished Fri 18 Sep

10 COOT after ModelCraft

✓ Finished Fri 18 Sep

9 ARP/wARP after phaser job5

✓ Finished 16:47
R=0.27 % = 167

8 COOT after refmac5 after phaser 3GET

✓ Finished 16:15

7 REFMAC5 after phaser 3GET

✓ Finished 16:14
R=0.54 RFree=0.55

6 ModelCraft first ever run

✓ Finished 16:40
R=0.24 RFree=0.30

5 Basic MR - PHASER - 3GET - two chains in search model!!

✓ Finished 16:11
R=0.50 RFree=0.52

4 Define AU contents

✓ Finished 16:03

3 Basic MR - PHASER - 3GET

✗ Failed 16:10

2 COOT

✓ Finished 15:50

1 Servalcat

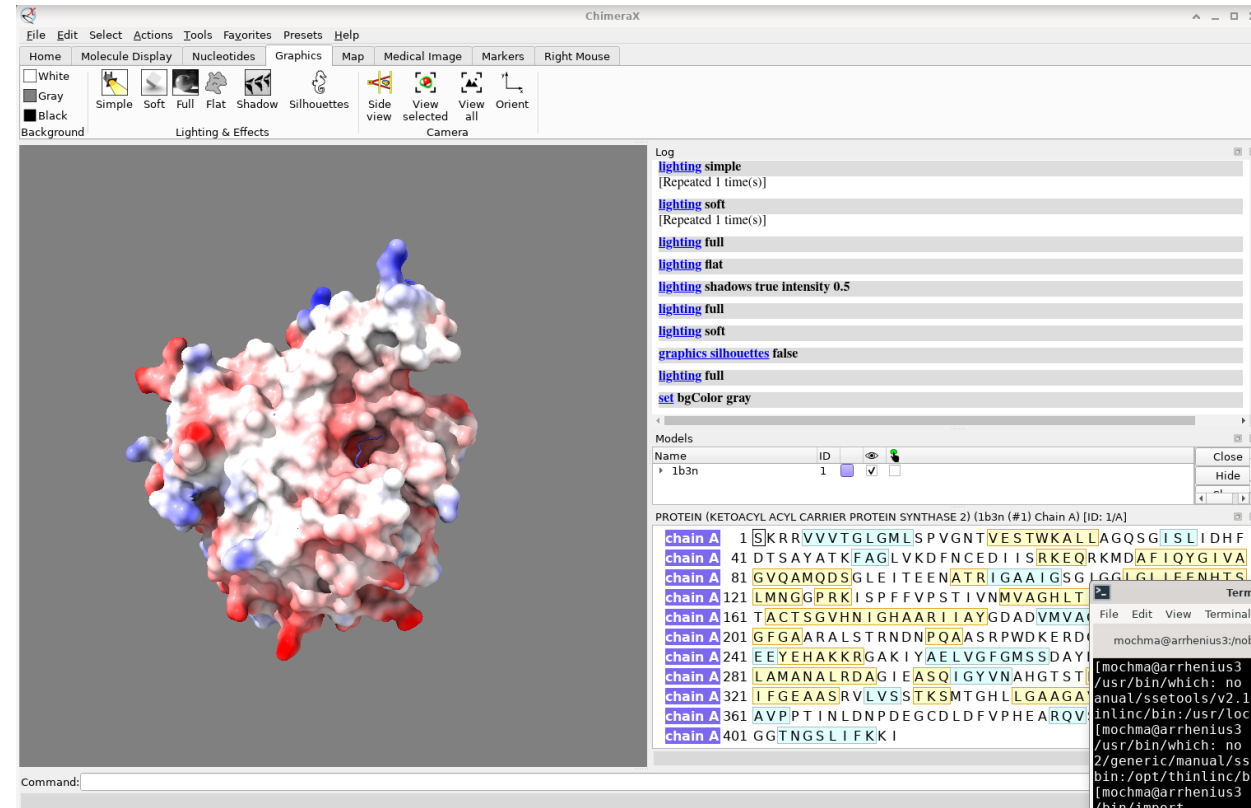
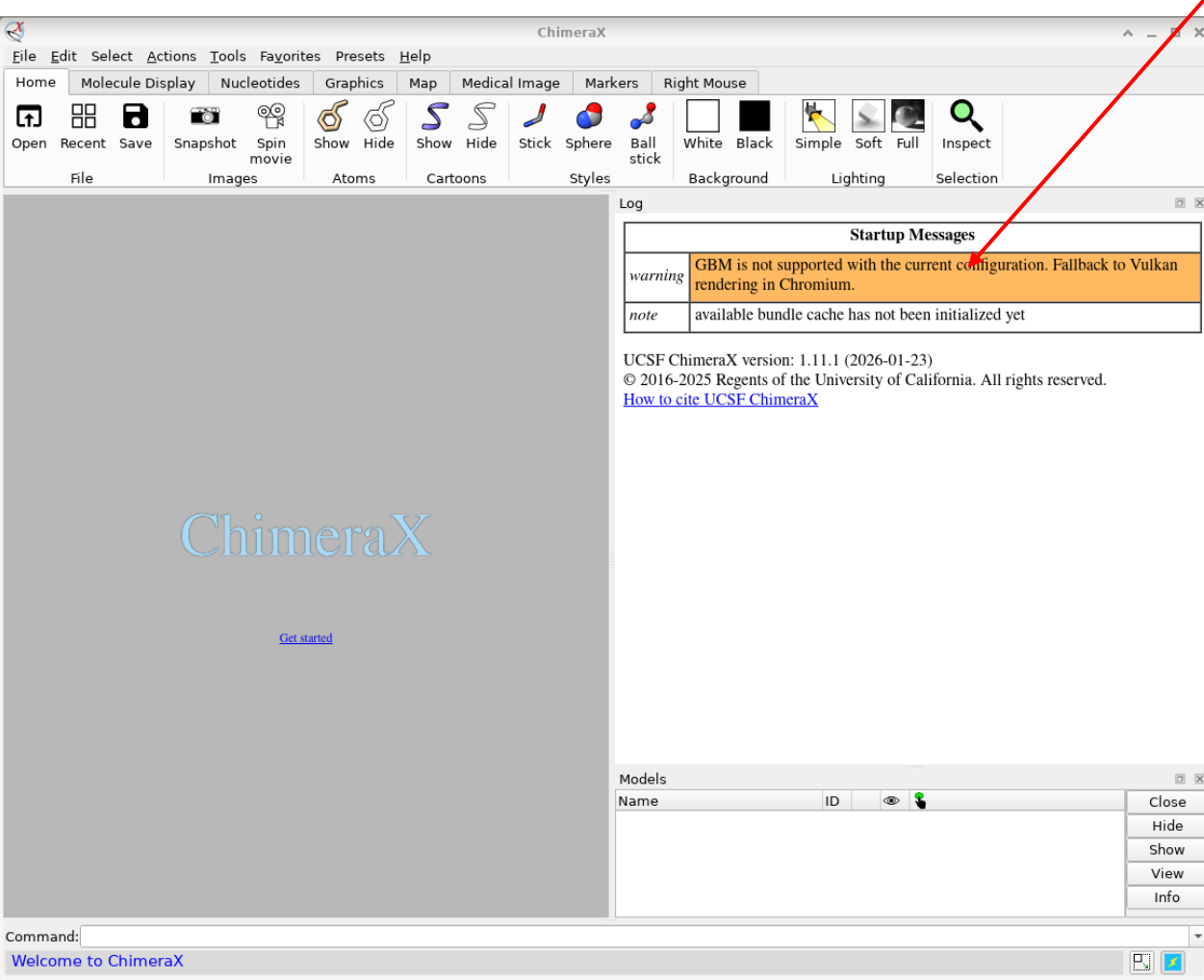
✓ Finished 15:46
R1work=0.1656 R1free=0.2307 (CC1work)=0.8922 (CC1free)=0.7541

ChimeraX

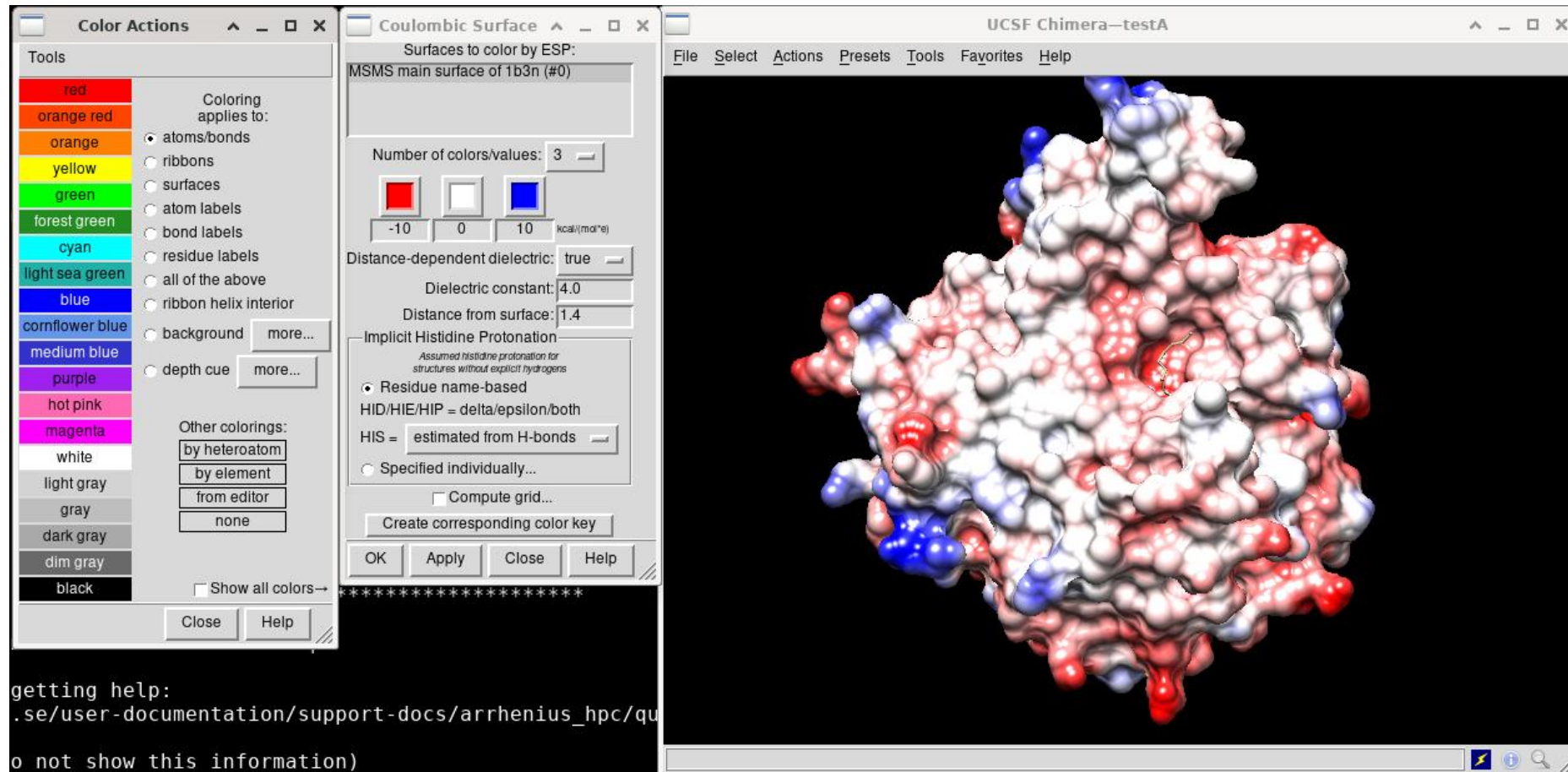
Do two export commands prior to giving the start “chimerax” command

- ✓ `export QTWEBENGINE_DISABLE_SANDBOX=1`
- ✓ `export QTWEBENGINE_CHROMIUM_FLAGS="--no-sandbox --disable-gpu`

ChimeraX start with warning but behave normally



Chimera is ok

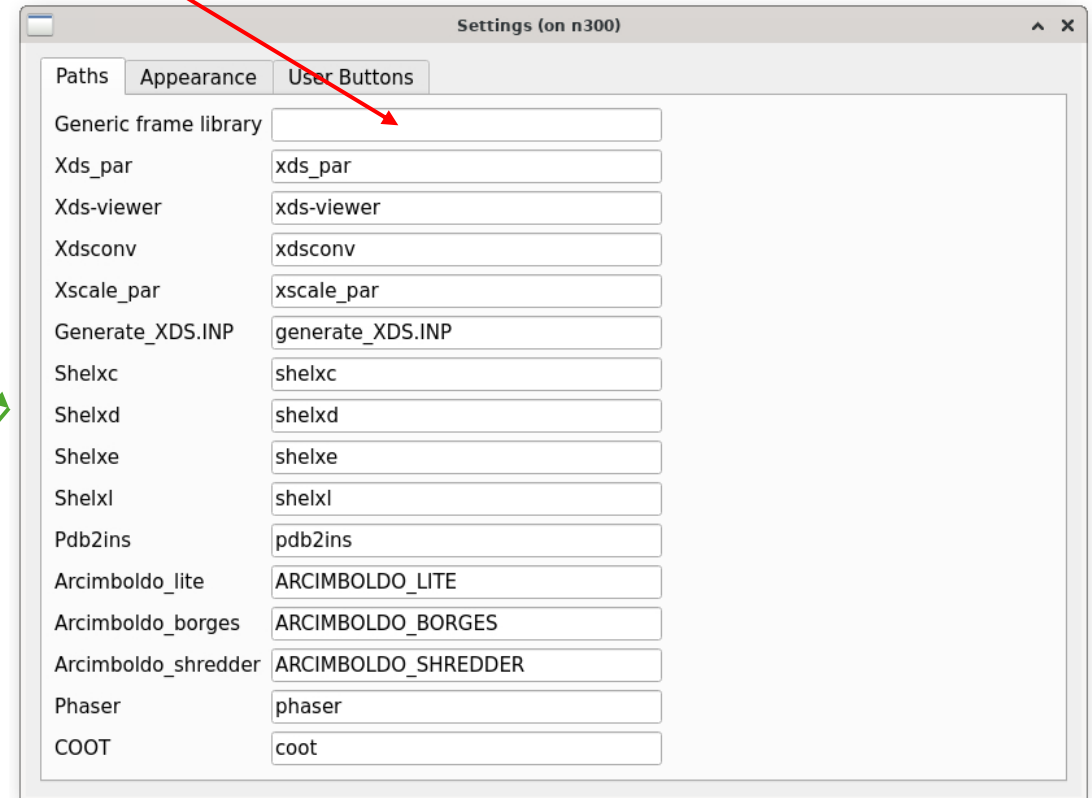
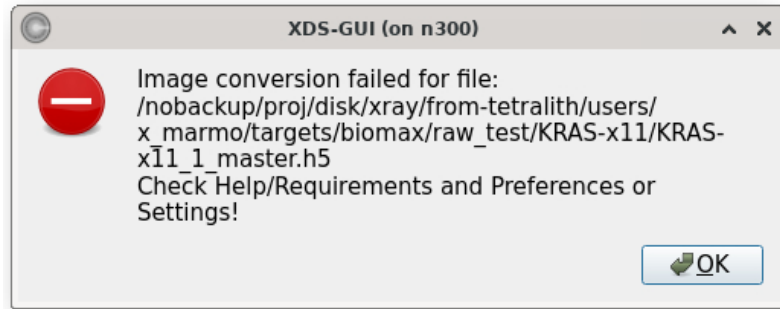


XDSGUI is ok but...

User should add PATH to Durin plugin into
Settings - Generic frame library
so that individual frames can be displayed in XDSGUI

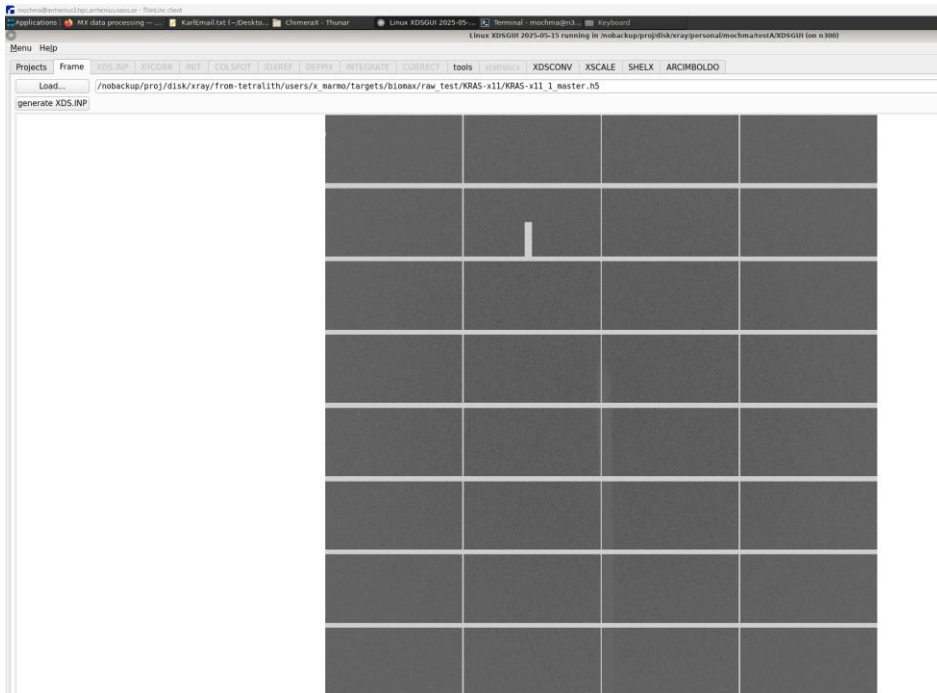
Add Durin plugin to Settings - Generic frame library

`/software/presto/e/karho/software/Durin/2023.10-foss-2023a/lib/durin-plugin.so`



1.

2.

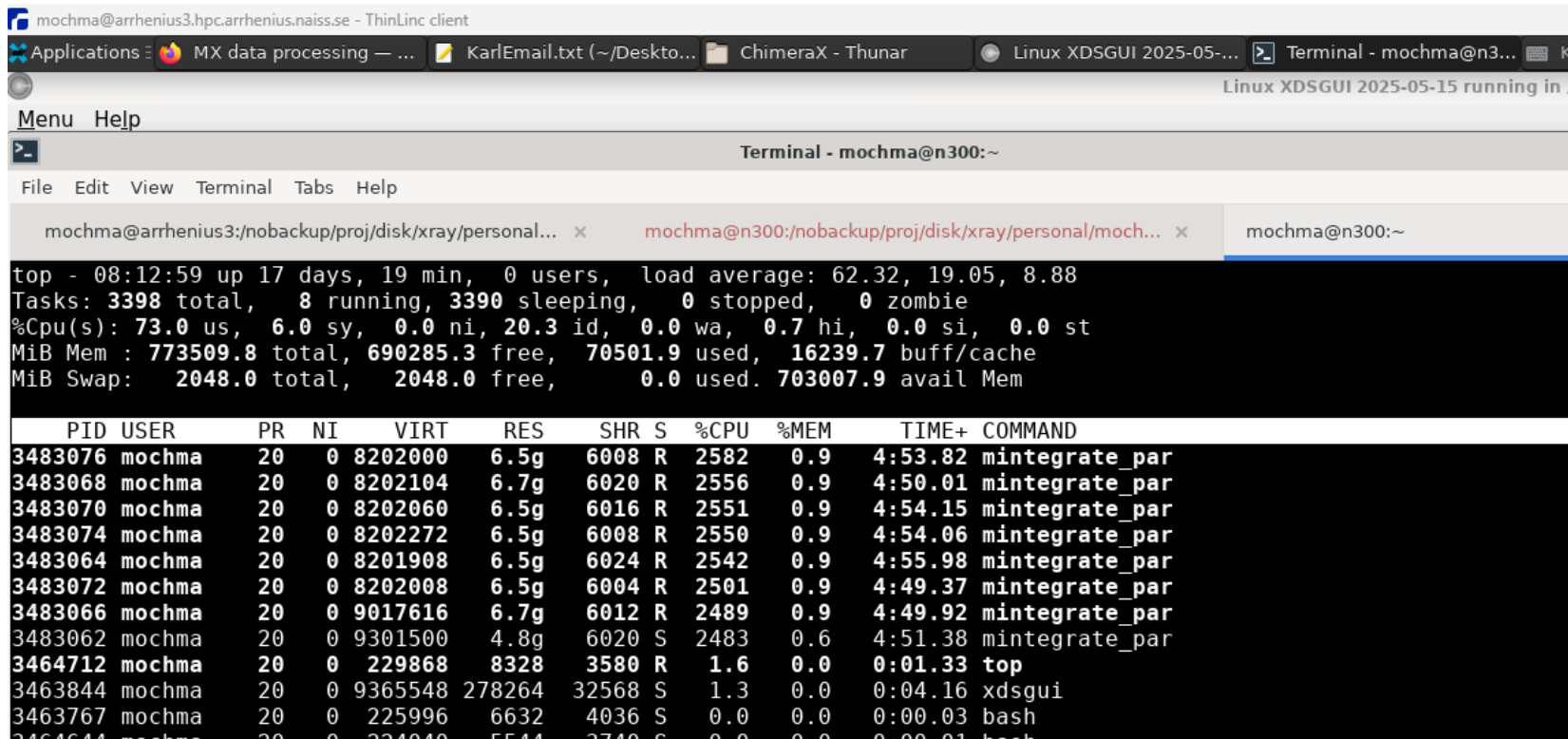


After adding the Durin PATH individual frames are displayed

Add JOBS, PROCESSORS and Durin path to XDS.INP

```
MAXIMUM_NUMBER_OF_JOBS= 8  
MAXIMUM_NUMBER_OF_PROCESSORS= 32  
LIB=/software/presto/e/karho/software/Durin/2023.10-foss-2023a/lib/durin-plugin.so
```

Add three lines into XDS.INP
before “Run XDS”



The screenshot shows a Linux terminal window with the following content:

```
mochma@arrhenius3.hpc.arrhenius.naiss.se - ThinLinc client  
Applications | MX data processing — ... | KarlEmail.txt (~/.Deskto... | ChimeraX - Thunar | Linux XDSGUI 2025-05-... | Terminal - mochma@n300:~ | Ke...  
Linux XDSGUI 2025-05-15 running in /r  
Menu Help  
Terminal - mochma@n300:~  
File Edit View Terminal Tabs Help  
mochma@arrhenius3:/nobackup/proj/disk/xray/personal... x mochma@n300:/nobackup/proj/disk/xray/personal/moch... x mochma@n300:~  
top - 08:12:59 up 17 days, 19 min, 0 users, load average: 62.32, 19.05, 8.88  
Tasks: 3398 total, 8 running, 3390 sleeping, 0 stopped, 0 zombie  
%Cpu(s): 73.0 us, 6.0 sy, 0.0 ni, 20.3 id, 0.0 wa, 0.7 hi, 0.0 si, 0.0 st  
MiB Mem : 773509.8 total, 690285.3 free, 70501.9 used, 16239.7 buff/cache  
MiB Swap: 2048.0 total, 2048.0 free, 0.0 used, 703007.9 avail Mem  


| PID     | USER   | PR | NI | VIRT    | RES    | SHR   | S | %CPU | %MEM | TIME+   | COMMAND        |
|---------|--------|----|----|---------|--------|-------|---|------|------|---------|----------------|
| 3483076 | mochma | 20 | 0  | 8202000 | 6.5g   | 6008  | R | 2582 | 0.9  | 4:53.82 | mintegrate_par |
| 3483068 | mochma | 20 | 0  | 8202104 | 6.7g   | 6020  | R | 2556 | 0.9  | 4:50.01 | mintegrate_par |
| 3483070 | mochma | 20 | 0  | 8202060 | 6.5g   | 6016  | R | 2551 | 0.9  | 4:54.15 | mintegrate_par |
| 3483074 | mochma | 20 | 0  | 8202272 | 6.5g   | 6008  | R | 2550 | 0.9  | 4:54.06 | mintegrate_par |
| 3483064 | mochma | 20 | 0  | 8201908 | 6.5g   | 6024  | R | 2542 | 0.9  | 4:55.98 | mintegrate_par |
| 3483072 | mochma | 20 | 0  | 8202008 | 6.5g   | 6004  | R | 2501 | 0.9  | 4:49.37 | mintegrate_par |
| 3483066 | mochma | 20 | 0  | 9017616 | 6.7g   | 6012  | R | 2489 | 0.9  | 4:49.92 | mintegrate_par |
| 3483062 | mochma | 20 | 0  | 9301500 | 4.8g   | 6020  | S | 2483 | 0.6  | 4:51.38 | mintegrate_par |
| 3464712 | mochma | 20 | 0  | 229868  | 8328   | 3580  | R | 1.6  | 0.0  | 0:01.33 | top            |
| 3463844 | mochma | 20 | 0  | 9365548 | 278264 | 32568 | S | 1.3  | 0.0  | 0:04.16 | xdsgui         |
| 3463767 | mochma | 20 | 0  | 225996  | 6632   | 4036  | S | 0.0  | 0.0  | 0:00.03 | bash           |
| 3464644 | mochma | 20 | 0  | 224040  | 5544   | 2740  | S | 0.0  | 0.0  | 0:00.01 | bash           |


```

CrystFEL is ok

Perhaps run a bit slower than expected but not sure...many sleeping processes

Index all frames

Job/output name:

Indexing

Batch system:

Integration

Submit job to partition:

Advanced indexing

Send notifications to:

Stream contents

Charge resource use to:

Cluster/batch system

Required node features:

Notes

Job time limit (minutes):

Reservation:

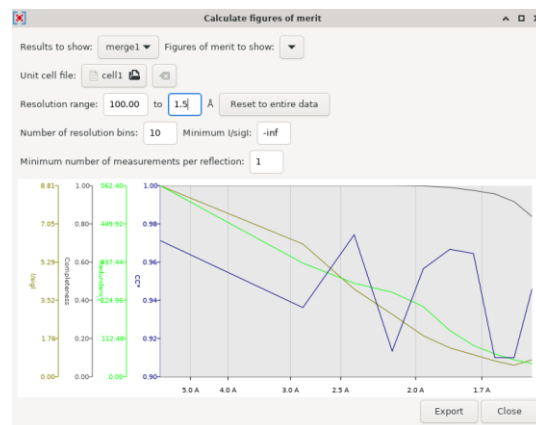
Quality of service:

☒ Request exclusive use of compute node(s)

Split job into blocks of frames

Cancel Run

Settings suitable



Index all frames

Job/output name:

Indexing

Integration

Advanced indexing

Stream contents

Cluster/batch system

Notes

Unit cell file:

Select indexing methods and prior information

Method Prior unit cell Prior lattice type

☒ MOSFLM ☐ ☐

☒ XDS ☐ ☐

☒ XGINDIALF ☐ ☐

☒ PinkIndeeer ☐ ☐

☒ TakeTwo ☐ ☐

☒ ASDP ☐ ☐

☒ Felix ☐ ☐

☒ Small cell ☐ ☐

☒ Rbids (GPU) ☐ ☐

☐ Attempt to find multiple lattices per frame

☒ Refine the indexing solution

☐ Retry indexing if unsuccessful

☒ Check indexing solutions match peaks

☒ Check indexing solutions against reference cell

Unit cell tolerances

☐ Skip frames with fewer than peaks

Cancel Run

Terminal - mochma@n346~

```

top - 09:12:01 up 2 days, 5:55, 0 users, load average: 5351.63, 2260.01, 895.92
Tasks: 3455 total, 61 running, 3394 sleeping, 0 stopped, 0 zombie
%Cpu(s): 65.4 us, 1.0 sy, 0.0 ni, 32.9 id, 0.0 wa, 0.7 hi, 0.1 si, 0.0 st
MiB Mem : 773509.8 total, 682859.1 free, 81149.0 used, 12772.4 buff/cache
MiB Swap: 2048.0 total, 2048.0 free, 0.0 used, 692360.8 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR   S  %CPU  MEM     TIME+  COMMAND
228056 mochma   20   0   16.7g  278876   8292  R   1239  0.0   5:18.91 indexama
228292 mochma   20   0   16.7g  276632   8284  R   1084  0.0   3:09.77 indexama
228834 mochma   20   0   16.7g  273640   8320  R   1061  0.0   3:03.80 indexama
228833 mochma   20   0   16.7g  23752   8304  S   637.7  0.0   6:58.77 indexama
228104 mochma   20   0   16.7g  232828   8188  S   541.8  0.0   4:21.88 indexama
228157 mochma   20   0   16.7g  276108   8264  S   386.9  0.0   2:23.69 indexama
227999 mochma   20   0   16.7g  277904   8304  R   369.0  0.0   2:07.45 indexama
228139 mochma   20   0   16.7g  279824   8304  S   289.2  0.0   2:04.04 indexama
228077 mochma   20   0   16.7g  240636   8156  S   286.3  0.0   1:44.74 indexama
228883 mochma   20   0   16.7g  275636   8232  S   269.3  0.0   1:57.68 indexama
228110 mochma   20   0   16.7g  241160   8300  S   222.2  0.0   2:26.08 indexama
228140 mochma   20   0   16.7g  233620   8316  R   204.6  0.0   2:01.52 indexama
228203 mochma   20   0   16.7g  278516   8156  S   187.9  0.0   2:14.36 indexama
227964 mochma   20   0   16.7g  248608   8260  S   177.5  0.0   3:02.16 indexama
228148 mochma   20   0   16.7g  283132   8320  S   177.1  0.0   4:01.45 indexama
228188 mochma   20   0   16.7g  279420   8212  S   173.2  0.0   2:44.20 indexama
228071 mochma   20   0   16.7g  276496   8264  S   172.9  0.0   2:58.34 indexama
227963 mochma   20   0   16.7g  249788   8304  R   165.0  0.0   1:57.97 indexama
228019 mochma   20   0   16.7g  273824   8312  S   164.7  0.0   1:30.09 indexama
228016 mochma   20   0   16.7g  276712   8322  S   163.4  0.0   2:45.13 indexama
228079 mochma   20   0   16.7g  277236   8292  S   147.7  0.0   3:09.44 indexama
227971 mochma   20   0   16.7g  276532   8212  S   142.5  0.0   1:17.02 indexama
228044 mochma   20   0   16.7g  277208   8308  S   141.8  0.0   2:44.88 indexama
228111 mochma   20   0   16.7g  283264   8300  S   140.2  0.0   2:38.59 indexama
228060 mochma   20   0   16.7g  232808   8268  S   136.9  0.0   1:36.64 indexama
228052 mochma   20   0   16.7g  241080   8300  S   135.6  0.0   1:44.76 indexama
228018 mochma   20   0   16.7g  275800   8292  R   132.7  0.0   1:26.04 indexama
228180 mochma   20   0   16.7g  277316   8184  R   132.4  0.0   1:20.94 indexama
228062 mochma   20   0   16.7g  278692   8288  R   132.0  0.0   1:35.21 indexama
228011 mochma   20   0   16.7g  241020   8276  S   122.9  0.0   2:25.69 indexama
228068 mochma   20   0   16.7g  241712   8216  S   121.2  0.0   3:15.72 indexama
228173 mochma   20   0   16.7g  280136   8328  S   115.7  0.0   2:11.80 indexama
228123 mochma   20   0   16.7g  233404   8196  R   114.4  0.0   2:01.39 indexama
228031 mochma   20   0   16.7g  277904   8316  S   114.1  0.0   1:21.76 indexama
228200 mochma   20   0   16.7g  276132   8284  S   114.1  0.0   3:38.91 indexama
227990 mochma   20   0   16.7g  256112   8240  R   113.1  0.0   1:39.36 indexama
227978 mochma   20   0   16.7g  241052   8160  S   112.7  0.0   2:28.30 indexama
227995 mochma   20   0   16.7g  250672   8304  R   112.1  0.0   2:39.10 indexama
228136 mochma   20   0   16.7g  278548   8180  S   111.4  0.0   1:52.42 indexama
228135 mochma   20   0   16.7g  276244   8200  R   109.8  0.0   1:37.94 indexama
228010 mochma   20   0   16.7g  241206   8236  S   102.9  0.0   2:16.05 indexama
227976 mochma   20   0   16.7g  275856   8212  S   102.6  0.0   1:37.32 indexama
228015 mochma   20   0   16.7g  278176   8240  S   101.6  0.0   1:39.11 indexama
228167 mochma   20   0   16.7g  241372   8272  S   98.7  0.0   1:23.17 indexama
228147 mochma   20   0   16.7g  243220   8256  S   96.4  0.0   2:07.38 indexama
228126 mochma   20   0   16.7g  278592   8300  R   96.1  0.0   2:24.32 indexama
227991 mochma   20   0   16.7g  233332   8272  D   93.5  0.0   1:43.86 indexama
228026 mochma   20   0   16.7g  276140   8316  S   91.5  0.0   1:44.28 indexama
228101 mochma   20   0   16.7g  278840   8288  S   90.5  0.0   1:54.34 indexama
228088 mochma   20   0   16.7g  276456   8168  S   90.2  0.0   1:31.80 indexama
228154 mochma   20   0   16.7g  279844   8212  S   89.5  0.0   2:00.42 indexama
228051 mochma   20   0   16.8g  251804   8300  R   88.9  0.0   3:32.48 indexama
228050 mochma   20   0   16.7g  278652   8212  R   87.3  0.0   1:21.26 indexama

```

CrystFEL run perhaps a bit slower than expected...many sleeping processes...

Merge

Job/output name: Input:

Merging

Model:

Cluster/batch system

Symmetry:

Notes

☒ Scale intensities ☐ Debye-Waller scaling ☐ Post-refinement

Number of scaling/post-refinement cycles:

Polarisation:

☐ Reject bad patterns according to $\Delta CC\%$

☐ Detector saturation cutoff:

Minimum number of measurements per merged reflection:

☐ Split datasets after merging

☒ Write partiality model diagnostics

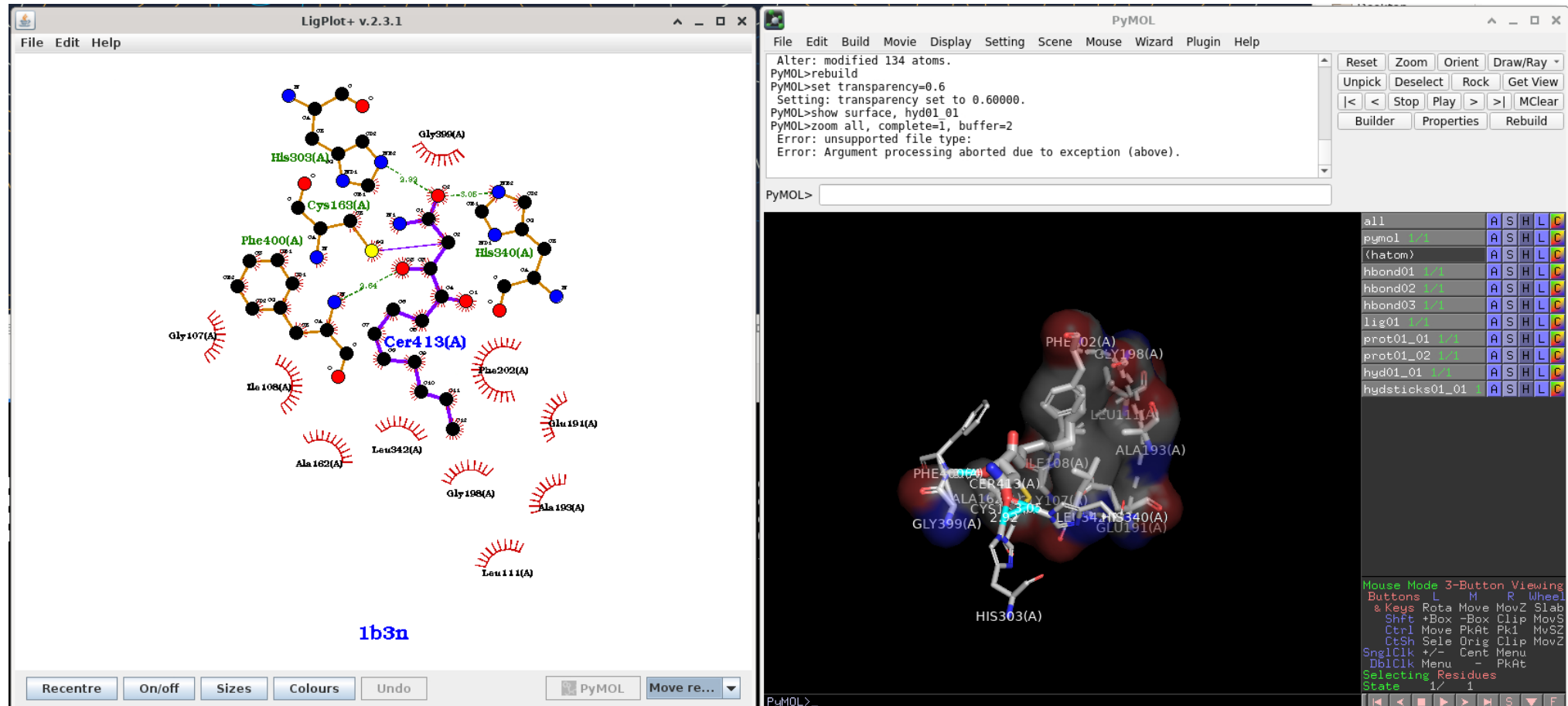
☐ Require minimum estimated pattern resolution Å

☐ Exclude measurements more than nm² above resolution limit

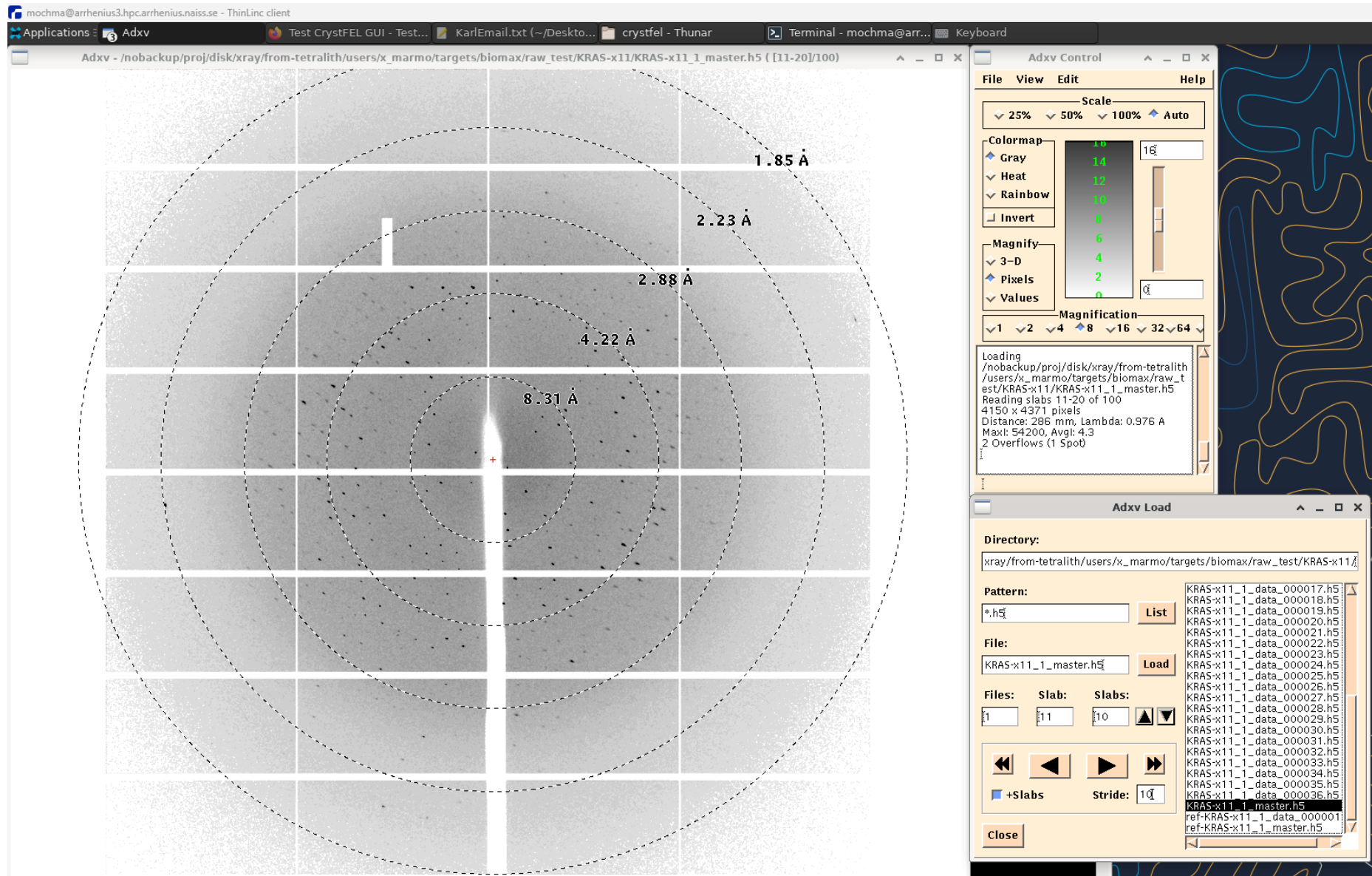
☐ Refine indexing assignments

Cancel Run

LigPlot is OK



adxv is OK



BUSTER and SHARP is OK

Just had to fetch a new BUSTER and SHARP licences to
/nobackup/proj/disk/xray/from-tetralith/software/buster
/nobackup/proj/disk/xray/from-tetralith/software/sharp

SHELXD (part of autoSHARP) use 235 (of 256) cores

```
Terminal - mochma@n298:~
File Edit View Terminal Tabs Help
mochma@n298:~ x mochma@arrhenius3:/nobackup/proj/disk/xray/perso... x mochma@arrhenius3:/nobackup/proj/disk/xray/from-t
top - 11:07:32 up 22 days, 17:14, 0 users, load average: 152.84, 115.07, 97.77
Tasks: 3300 total, 2 running, 3298 sleeping, 0 stopped, 0 zombie
%Cpu(s): 91.2 us, 3.5 sy, 0.0 ni, 3.4 id, 0.0 wa, 1.9 hi, 0.1 si, 0.0 st
MiB Mem : 773509.8 total, 737345.4 free, 37149.6 used, 2337.7 buff/cache
MiB Swap: 2048.0 total, 2048.0 free, 0.0 used. 736360.1 avail Mem

  PID USER      PR  NI   VIRT   RES   SHR S  %CPU  %MEM    TIME+  COMMAND
2198211 mochma    20   0   24.4g   20.2g  1432 R 23503   2.7 174:52.06 shelxd
2201066 mochma    20   0  230932   8168   3592 R   0.7   0.0   0:00.33 top
2176967 mochma    20   0   18172  16240   3140 S   0.3   0.0   0:05.29 shelx.sh
2140723 mochma    20   0  223416   4552   3388 S   0.0   0.0   0:00.00 slurm_script
2142099 mochma    20   0  226856   7112   3616 S   0.0   0.0   0:00.03 run_autoSHARP.s
2142100 mochma    20   0  221192   2368   2064 S   0.0   0.0   0:00.00 tee
2142413 mochma    20   0  229108   9308   3600 S   0.0   0.0   0:00.26 detect.sh
2198209 mochma    20   0    6192   4368   3160 S   0.0   0.0   0:00.00 shelxd_3_16.sh
2200376 mochma    20   0  225876   6508   4028 S   0.0   0.0   0:00.04 bash
2203791 mochma    20   0    2872   1916   1588 S   0.0   0.0   0:00.00 sleep
```

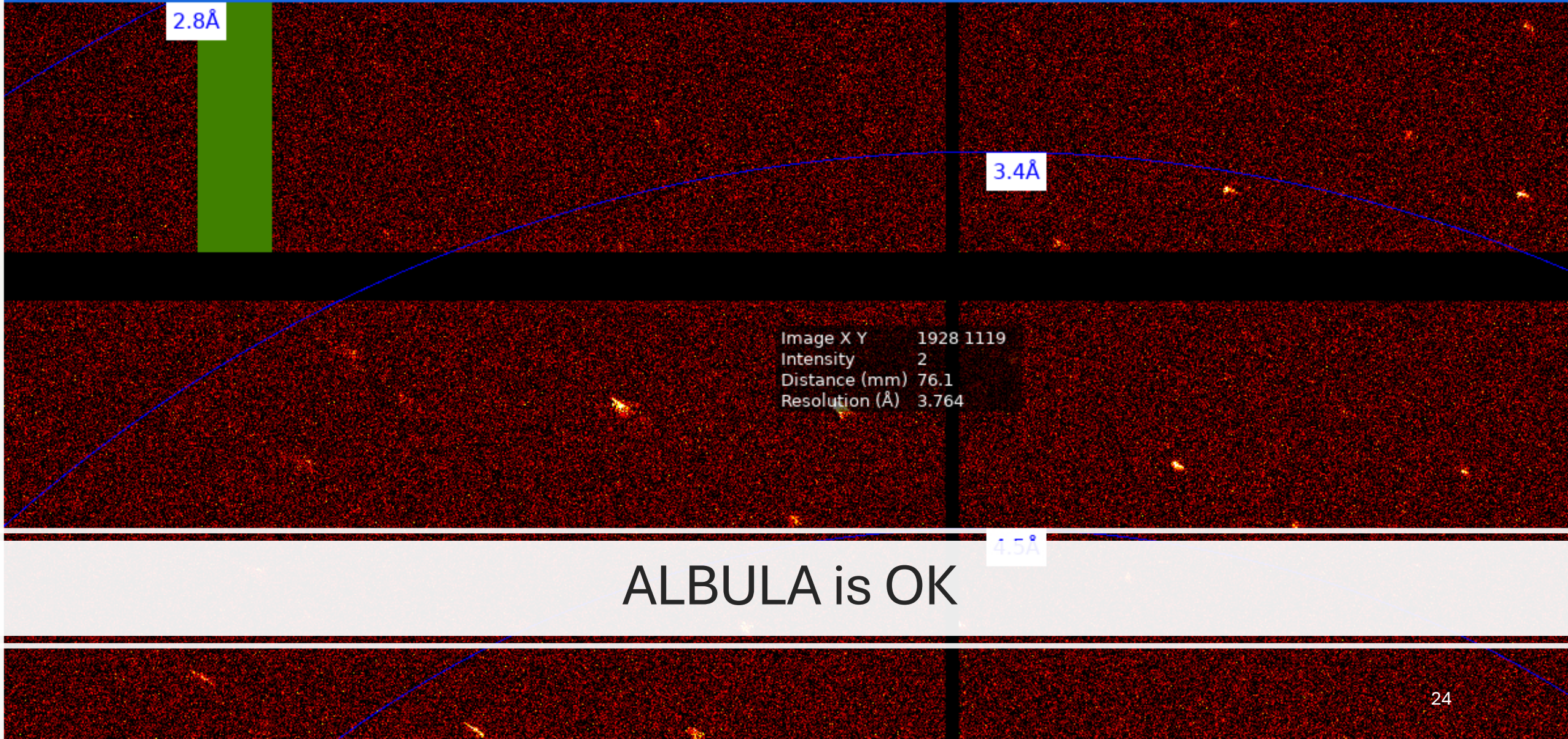
File Synchronize Auto Load Help

DECTRIS

New Window Open Save As Export

Keys Tools

1 ◀ ▶ ⏸ ⏪ ⏩ /nobackup/proj/disk/xray/from-tetralith/users/x_marmo/targets/biomax/raw_test/KRAS-x11/KRAS-x11_1_master.h5 # 1/3600 ×



Hkl2map at interactive node

hkl2map GUI is ok at interactive node!

COOT cannot be launched from hkl2map GUI, likely because COOT cannot be started at all on a compute node

hkl2map at compute node OK

ThinLinc client window showing hkl2map Version 0.4.e-beta interface.

Project name: 3get

SHELXC dmin [Å] / Isigl: 1.67 / 0.3 | 1.67 / 0.3 00:00:00

SHELXD CFbest: 53.0% CCmax: 33.3% Try: 10000 / 10000 00:00:15

Fa in : 3get_fa.hkl Browse

Ins in : 3get_fa.ins Browse

Find 10 heavy atoms of type Se . Use data from 999 to 2.2 Å resolution.

Allow sites on special positions? yes no

Limit number of tries to 10000 .

PDB out : 3get_fa.pdb Browse

more options view graphics Run SHELXD

SHELXE

Current status of data preparation, substructure solution and phasing :

SHELXC / SHELXD / SHELXE original / SHELXE inverted

Try 9986, CPU**, CC All/Weak 23.3 / 11.5, CFOM 34.7, best 53.0, PATFOM 8.05

Try 9987, CPU**, CC All/Weak 9.2 / 1.7, CFOM 10.9, best 53.0, PATFOM 2.85

Try 9988, CPU**, CC All/Weak 7.7 / 2.1, CFOM 9.8, best 53.0, PATFOM 2.17

Try 9989, CPU18, CC All/Weak 33.1 / 19.4, CFOM 52.6, best 53.0, PATFOM 11.24

Try 9990, CPU20, CC All/Weak 32.1 / 18.4, CFOM 50.5, best 53.0, PATFOM 11.37

Try 9991, CPU**, CC All/Weak 9.1 / 3.7, CFOM 12.8, best 53.0, PATFOM 1.65

Try 9992, CPU85, CC All/Weak 33.0 / 19.3, CFOM 52.4, best 53.0, PATFOM 11.22

Try 9993, CPU 7, CC All/Weak 33.0 / 19.4, CFOM 52.4, best 53.0, PATFOM 11.12

Try 9994, CPU56, CC All/Weak 33.1 / 19.4, CFOM 52.6, best 53.0, PATFOM 11.18

Try 9995, CPU**, CC All/Weak 10.0 / 3.7, CFOM 13.7, best 53.0, PATFOM 3.00

Try 9996, CPU 9, CC All/Weak 9.2 / 3.8, CFOM 13.1, best 53.0, PATFOM 2.83

Try 9997, CPU76, CC All/Weak 33.1 / 19.4, CFOM 52.6, best 53.0, PATFOM 11.23

Try 9998, CPU26, CC All/Weak 9.1 / 3.3, CFOM 12.4, best 53.0, PATFOM 3.21

Try 9999, CPU65, CC All/Weak 33.1 / 19.4, CFOM 52.6, best 53.0, PATFOM 11.18

Try 10000, CPU**, CC All/Weak 33.1 / 19.4, CFOM 52.6, best 53.0, PATFOM 11.35

+ 3get_fa finished at 10:44:39 Elapsed time: 15.60 secs +

Waiting

hkl2map Version 0.4.e-beta - SHELXD statistics

File Display Appearance

- Histogram CCall -

Quantity

CCall

Terminal - mochma@n300:~

top - 10:44:36 up 18 days, 2:50, 0 users, load average: 63.89, 40.80, 73.51

Tasks: 3133 total, 2 running, 3121 sleeping, 0 stopped, 10 zombie

%Cpu(s): 96.1 us, 1.1 sy, 0.0 ni, 1.3 id, 0.0 wa, 1.5 hi, 0.0 si, 0.0 st

MiB Mem : 773509.8 total, 751989.7 free, 23419.9 used, 508.5 buff/cache

MiB Swap: 2048.0 total, 2048.0 free, 0.0 used, 750089.9 avail Mem

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
3519902	mochma	20	0	10.8g	8.6g	1440	R	24764	1.1	54:35.65	shelxd
3519004	mochma	20	0	302596	79732	5220	I	38.6	0.0	0:23.76	wish
3519895	mochma	20	0	229272	7856	3604	R	0.7	0.0	0:00.59	top
3518192	mochma	20	0	226028	6788	4036	S	0.0	0.0	0:00.02	bash
3519015	mochma	20	0	0	0	0	Z	0.0	0.0	0:00.00	shelxc
3519016	mochma	20	0	0	0	0	Z	0.0	0.0	0:00.01	grep
3519017	mochma	20	0	0	0	0	Z	0.0	0.0	0:00.04	shelxd
3519018	mochma	20	0	0	0	0	Z	0.0	0.0	0:00.01	grep
3519019	mochma	20	0	0	0	0	Z	0.0	0.0	0:00.00	shelxd

SHELXD was done with 10000 tries before I did the screen dump using 247 cores (256 available)

COOT not started from hkl2map GUI

hkl2map Version 0.4.e-beta

Project name: 3get

SHELXC dmin [Å] / |sig|: 1.67 / 0.3 | 1.67 / 0.3 00:00:00

SHELXD CFbest: 53.0% CMax: 33.3% Try: 10000 / 10000 00:00:15

SHELXE Nres: 396 / [635] CC: 20.8% Cst: 0.415 0.484 Cycle: 20 - 20 / 20 00:04:50

Native in: 3get.hkl Browse

Fa in: 3get_fa.hkl Browse

SHELXD out: 3get_fa.res Browse

Phase structure based on given sites and modify the electron density for 20 cycles.

Use fractional solvent content of 0.5 Estimate the solvent content

Native data do include heavy atoms.

Extend diffraction data to A [native data extend to 1.67 Å].

Run 3 cycles of autotracing with initial search for secondary structure.

Interrupt calculations for incorrect enantiomorph after 4 cycles.

Invert heavy atom substructure for phasing? try both enantiomorphs

Phases ori: 3get_m20_s0.5_e.phs run coot Browse

Phases inv: 3get_m20_s0.5_e_i.phs run coot Browse

more options view graphics Run SHELXE

Current status of data preparation, substructure solution and phasing:

SHELXC / SHELXD / SHELXE original / SHELXE inverted

CPU times required in seconds

0.3	- Setup, data input and phasing
10.9	- FFTs and peak-searches
28.6	- Sphere of influence
0.6	- Rest of density modification
103.6	- Alpha-helix search
74.9	- Tripeptide search
47.9	- Chain tracing
0.0	- NCS analysis
22.3	- B-value refinement for trace
0.2	- Rest of tracing
0.0	- Comparison with known structure
0.0	- Side-chain tracing

+ SHELXE finished at 10:51:02 Total time: 289.33 secs +

Waiting

hkl2map Version 0.4.e-beta - SHELXE statistics

File Display Appearance

- Contrast vs. Cycle -

Contrast

Cycle

original
inverted

Psdlo-free CC
47.20%
56.47%

#res [max-pdb]
192 [215]
396 [396]

CC(trace,nat)
8.87
20.78

```
[mochma@n300 hkl2map]$ which coot
/software/presto/e/karho/software/CCP4/9.0.013-foss-2023a-SHELX-ARP-8.0/bin/coot
[mochma@n300 hkl2map]$ coot
vglrun is not available
[mochma@n300 hkl2map]$
```

3519895	mochma	20	0	229272	7856	3604	R	0.7	0.0	0:04
3518192	mochma	20	0	226028	6788	4036	S	0.0	0.0	0:00
3519015	mochma	20	0	0	0	0	Z	0.0	0.0	0:00
3519016	mochma	20	0	0	0	0	Z	0.0	0.0	0:00
3519017	mochma	20	0	0	0	0	Z	0.0	0.0	0:00
3519018	mochma	20	0	0	0	0	Z	0.0	0.0	0:00
3519019	mochma	20	0	0	0	0	Z	0.0	0.0	0:00
3519020	mochma	20	0	0	0	0	Z	0.0	0.0	0:00

COOT did not start at Compute node

Running COOT on a 256-core compute Node is perhaps a waist of compute time...However a quick check is always useful

COOT does not start at Arrhenius compute node so has nothing with hkl2map to do.