XChem
Drop-in Session

15th July 2024

Filesystem and cluster migration

- GPFS02 file system decommissioned due to age and lack of support

- All MX beamlines, including XChem, migrated to GPFS04 file system

- Migration necessitated transition to Wilson cluster and SLURM job scheduler
  - Required significant backend updates to XCE

- Unscheduled power outage during shutdown delayed filesystem migration and testing/debugging of XCE updates
  - Migration complete and all live data should be accessible
  - Serious failure of GPFS02 system
  - No known data loss – please report if data not available on filesystem or DataGateway (icat)

- Updated XCE now available and XChem user manuals updated
  - Please report any issues to XChem team as normal

Running jobs on Wilson cluster with SLURM

- *"source /dls/science/groups/i04-1/software/XChem/xchempaths.sh"*

- Launching a job on the Wilson cluster requires your password

- Default token time 1 hour – may need to re-enter password or restart XCE to launch jobs ("error 7000")

- To check the status of jobs on the cluster, type into terminal:
  - *"ssh wilson"* – connect to the Wilson Cluster
  - *"sacct"* – display jobs
  - *"scancel <jobid>"* – cancel a job
  - *"watch sq.sh -u <yourfedid> -nf"* – watch jobs
  - *"sbatch <script>"* – submit batch job

SLURM Authentication ×

Password:

Cancel   OK

```
Every 2.0s: sq.sh -u ill13029 -nf

ill13029's queue

No jobs running.

No jobs pending.

Previous 10 jobs (last fortnight):

JobID    'Job Name'   #N #C  Start Time    Run Time  Status
9363997  'xce_buster'  1 1c  Jul 1st 08:38  40m 20s  Completed
9368556  'xce_buster'  1 1c  Jul 1st 12:58  36m 21s  Completed
9370433  'xce_buster'  1 1c  Jul 1st 13:50  33m 4s   Completed
9372944  'xce_buster'  1 1c  Jul 1st 14:55  24m 30s  Completed
```
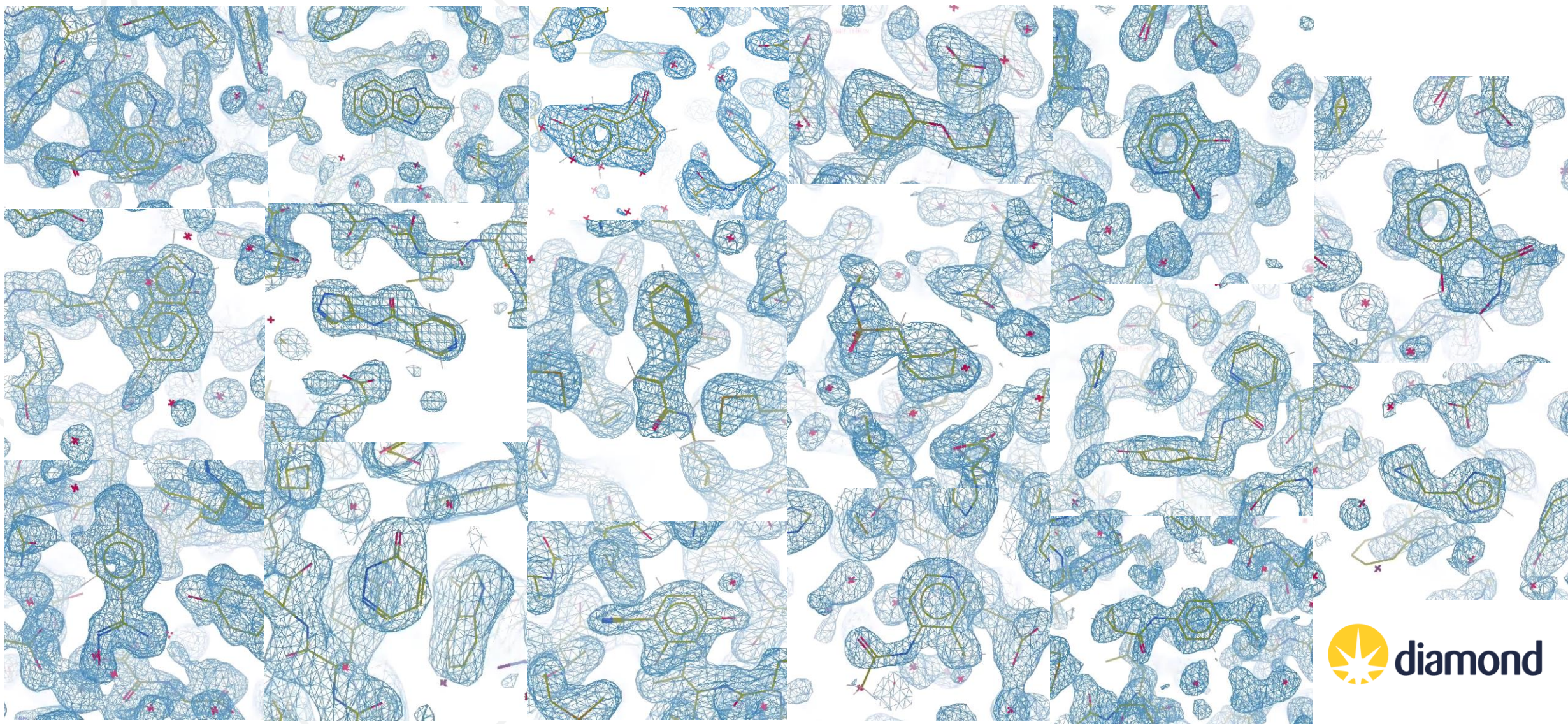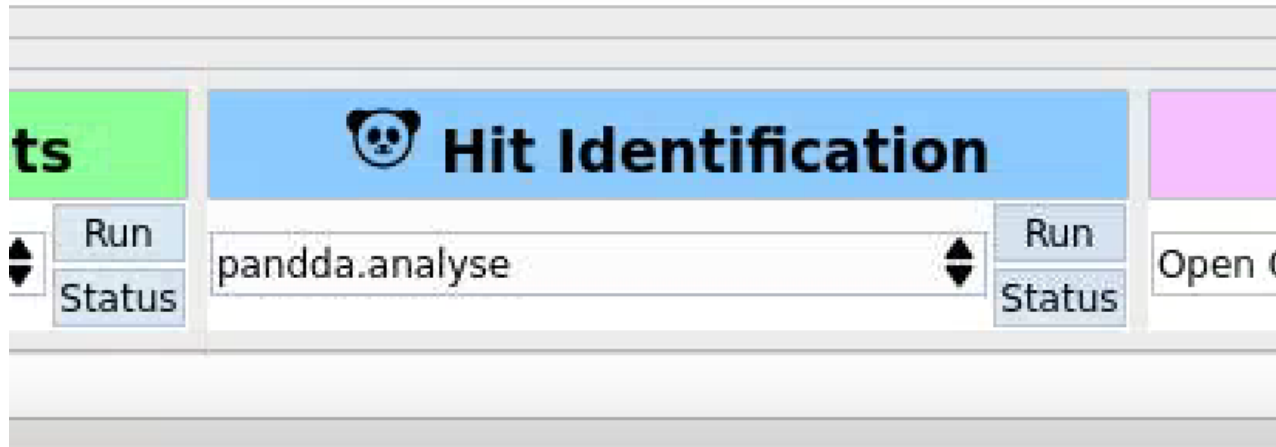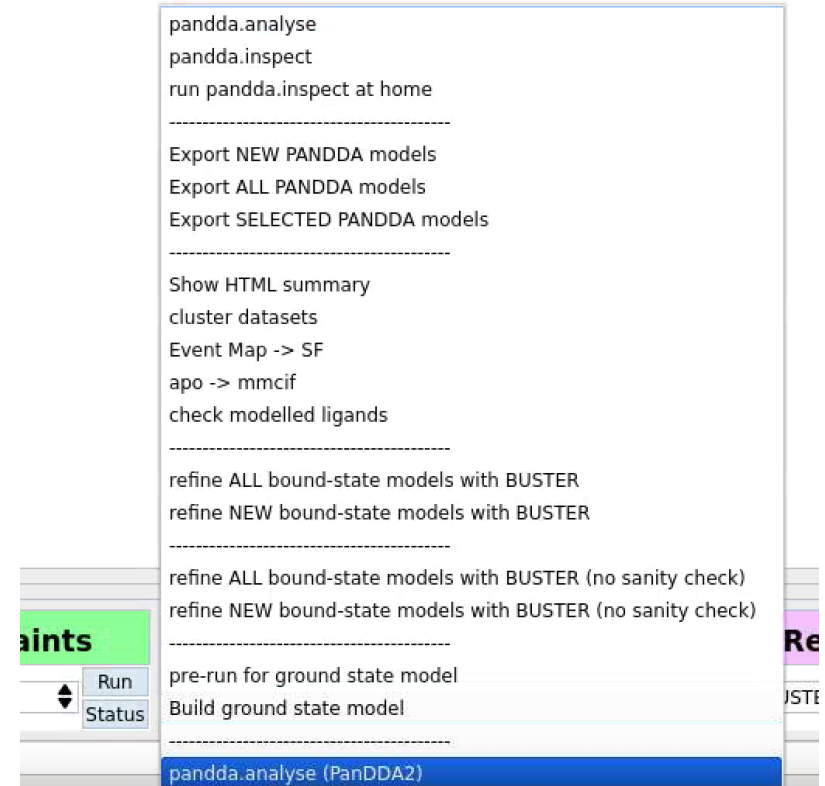
PanDDA 2 discovers new hits

Convincing models in every studied system with over 15 systems studied in detail

PanDDA 2 can now be accessed via XCE

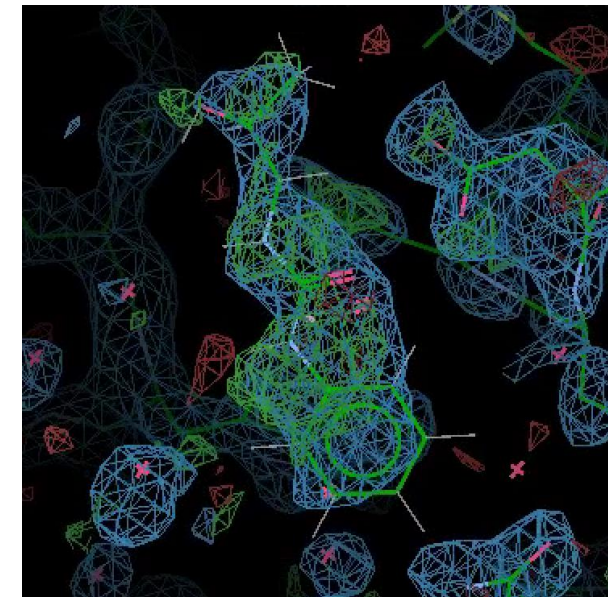The process is otherwise the same as PanDDA 1

Changes to PanDDA.inspect

Expect more events but they are better ranked within sites

Autobuilt models will be present in some events

Autobuilt models may be spurious and should be deleted if so
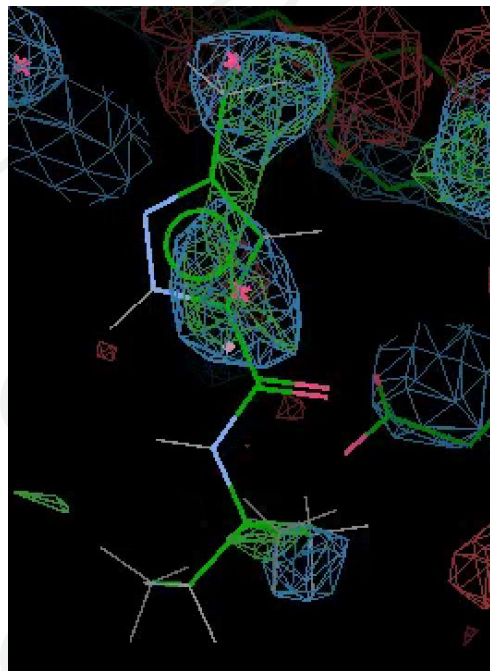
Z-blob peak now contains a score from 0.0 to 1.0, with higher being more ligand-binding-event-like

Overall Inspection Event/Site Progress:			
Event	1	of	1083
Site	0	of	29

1 - BDC	0.18
Z-blob Peak	0.9
Z-blob Size	247

pandda.analyse PanDDA2 - Useful tricks

PanDDA 2 accepts several keyword arguments that may be useful:

To Run Subsets Of Data

`--dataset_range="100-200"`

`--only_datasets="BAZ2BA-x102,BAZ2BA-x097"`

To Filter Poor Quality Data

`--high_res_lower_limit=3.0`

`--max_rfree=0.3`

PanDDA2 Documentation

grid spacing (default=0.5)

0.5

keyword arguments (pandda2 only)

Questions?