

Beamline Data Processing @ LS-CAT, Sector 21

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LS-CAT

- Macromolecular X-ray Sciences Beamlines
- 8 Member Institution & extras
- Currently 3 Experimental end stations
 - 1 fully tunable
 - 2 fixed energy @ 12.7KeV
 - CATS Sample changing robots



Current Operations

- RemoteAccess – Main application for remote data collection at LS-CAT
 - Indexing and Strategy via Labelit and Best
 - Use 2 frames
 - Auto Processing
 - Upon completion of a dataset Xia2 is launched
 - We were running AutoProc at various intervals
 - Tarball download of dataset
 - Rsync data



Indexing and Strategy Setup

LS-CAT Remote Access
https://ls-cat.org/lsrcat.html#

Data View Video Feeds MD2 Rsync Fullscreen Logoff About

ESAF: 97284 Powers Image: /Powers_2_2_09/CJ-49.001 Info Res 13.64Å

Current Status
Directory Browser

Search: Clear

- ▼ f
- ▼ Powers_1_2_02
 - ▼ CJ-49
 - CJ-49.S.001
 - CJ-49.S.002
 - CJ-49.S.003
 - CJ-49.S.004
 - CJ-49.S.005
 - CJ-49.S.006
 - ▶ cJuneoaxlwt_F11cj33-1
 - ▶ Powers_1_1_05
 - ▶ Powers_2_1_04
 - ▶ Powers_1_2_04
 - ▶ Powers_1_1_01
 - ▶ Powers_1_3_01
 - ▼ Powers_1_2_03
 - ▼ CJ-49
 - CJ-49.S.001
 - CJ-49.S.002
 - ▼ Powers_1_1_06
 - ▼ Powers_2_2_09
 - ▼ CJ-49
 - CJ-49.S.001
 - CJ-49.S.002
 - CJ-49.S.003
 - CJ-49.S.004
 - CJ-49.S.005
 - CJ-49.S.006
 - CJ-49.S.007
 - CJ-49.S.008
 - CJ-49.001
 - CJ-49.002
 - CJ-49.003
 - CJ-49.004
 - CJ-49.005
 - CJ-49.006
 - CJ-49.007
 - CJ-49.008
 - CJ-49.009
 - CJ-49.010
 - CJ-49.011
 - CJ-49.012
 - CJ-49.013
 - CJ-49.014
 - CJ-49.015
 - CJ-49.016
 - CJ-49.017
 - CJ-49.018
 - CJ-49.019



Indexing and Strategy Results

Mosfilm Best Solutions					Parameters					
#	:)	Space Group	RMS	Resolution	File 1	File 2	Mosaicity	Dist	Beam x	Beam y
2	:)	C2	0.037	1.47	CJ-49.001	CJ-49.089	0.90	129.88mm	112.61mm	112.00mm

BEST Strategy					
Start Angle (°)	Distance (mm)	Osc. Angle (°)	Osc. Range	Completeness (%)	Redundancy
174.00	129.1	0.40	211.2	99	4

Labelit Solutions														
#	:)	Metric	System	Fit	Rmsd	Spots	Symbol	a	b	c	alpha	beta	gamma	Vol
1	:)	0.0000	triclinic	dg	0.168	405	aP	35.90	73.45	103.02	69.12	81.50	89.99	250609
2	:)	0.0144	monoclinic	dg	0.080	389	mC	192.50	73.43	35.90	90.00	99.10	90.00	501031

[Reindex](#)



Current Development

- Using Spotfinder via distl apache server
 - Used for rastering/crystal centering via diffraction
 - Used to track data progress
- Reporting data processing statistics
 - Displaying tables
 - Interactive graphs
- Reprocessing/fine tuning data processing
- Brute force/multi scenario indexing

