Automated Crystal Screening at the Advanced Light Source

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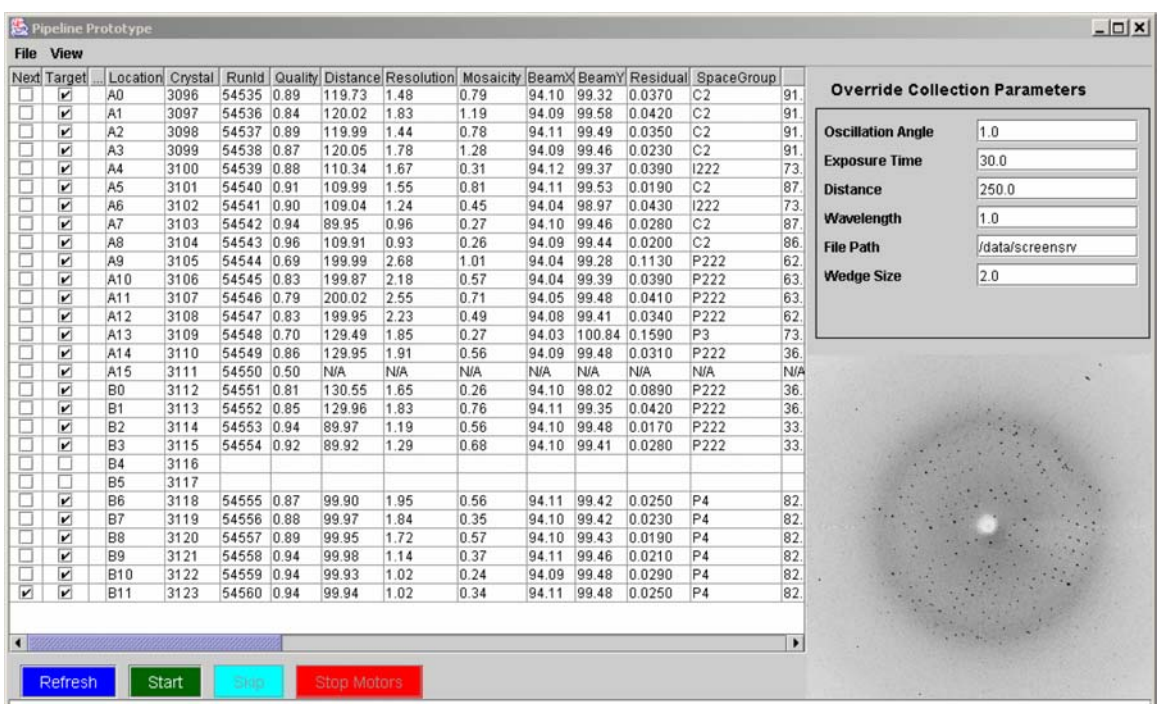
ABSTRACT

We have implemented a macromolecular crystal screening environment at the Advanced Light Source allowing the beamline user to assess the diffraction quality automatically from dozens of samples. This assessment enables the user to collect full datasets on the best crystals from the initial screen. Oscillation images are analyzed in real time to determine the feasibility of autoindexing. Bragg reflections are chosen with the program DISTL (Z. Zhang & A. Deacon, SSRL), and autoindexing is accomplished with the new LABELIT package. Crystals are ranked with a quality score that includes factors such as resolution limit, mosaicity, and residual fit. Plans for the future include a script to determine the optimal data collection strategy for the sample, and automated collection and analysis of full datasets once the strategy is decided upon.

Components of the system include a robotic mounter to repeatedly transfer cryocooled samples to the goniometer, a database to track high volumes of information, a facility to autocenter the crystal loop in the beam, and a graphical user interface (Fig. 1) to orchestrate the entire process. Minimal input is required, as the process is automatically handled using scripted tools. Unattended, the system can screen up to 112 crystals. The prototype is installed on branchlines 5.0.1, 5.0.2, and 5.0.3 of the ALS, and is suitable for either individual users or large-scale structural genomics efforts.



Next	Target	...	Location	Crystal	RunId	Quality	Distance	Resolution	Mosaicity	BeamX	BeamY	Residual	SpaceGroup	
☐	☑		A0	3096	54535	0.89	119.73	1.48	0.79	94.10	99.32	0.0370	C2	91.
☐	☑		A1	3097	54536	0.84	120.02	1.83	1.19	94.09	99.58	0.0420	C2	91.
☐	☑		A2	3098	54537	0.89	119.99	1.44	0.78	94.11	99.49	0.0350	C2	91.
☐	☑		A3	3099	54538	0.87	120.05	1.78	1.28	94.09	99.46	0.0230	C2	91.
☐	☑		A4	3100	54539	0.88	110.34	1.67	0.31	94.12	99.37	0.0390	I222	73.
☐	☑		A5	3101	54540	0.91	109.99	1.55	0.81	94.11	99.53	0.0190	C2	87.
☐	☑		A6	3102	54541	0.90	109.04	1.24	0.45	94.04	98.97	0.0430	I222	73.
☐	☑		A7	3103	54542	0.94	89.95	0.96	0.27	94.10	99.46	0.0280	C2	87.
☐	☑		A8	3104	54543	0.96	109.91	0.93	0.26	94.09	99.44	0.0200	C2	86.
☐	☑		A9	3105	54544	0.69	199.99	2.68	1.01	94.04	99.28	0.1130	P222	62.
☐	☑		A10	3106	54545	0.83	199.87	2.18	0.57	94.04	99.39	0.0390	P222	63.
☐	☑		A11	3107	54546	0.79	200.02	2.55	0.71	94.05	99.48	0.0410	P222	63.
☐	☑		A12	3108	54547	0.83	199.95	2.23	0.49	94.08	99.41	0.0340	P222	62.
☐	☑		A13	3109	54548	0.70	129.49	1.85	0.27	94.03	100.84	0.1590	P3	73.
☐	☑		A14	3110	54549	0.86	129.95	1.91	0.56	94.09	99.48	0.0310	P222	36.
☐	☑		A15	3111	54550	0.50	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
☐	☑		B0	3112	54551	0.81	130.55	1.65	0.26	94.10	98.02	0.0890	P222	36.
☐	☑		B1	3113	54552	0.85	129.96	1.83	0.76	94.11	99.35	0.0420	P222	36.
☐	☑		B2	3114	54553	0.94	89.97	1.19	0.56	94.10	99.48	0.0170	P222	33.
☐	☑		B3	3115	54554	0.92	89.92	1.29	0.68	94.10	99.41	0.0280	P222	33.
☐	☐		B4	3116										
☐	☐		B5	3117										
☐	☑		B6	3118	54555	0.87	99.90	1.95	0.56	94.11	99.42	0.0250	P4	82.
☐	☑		B7	3119	54556	0.88	99.97	1.84	0.35	94.10	99.42	0.0230	P4	82.
☐	☑		B8	3120	54557	0.89	99.95	1.72	0.57	94.10	99.43	0.0190	P4	82.
☐	☑		B9	3121	54558	0.94	99.98	1.14	0.37	94.11	99.46	0.0210	P4	82.
☐	☑		B10	3122	54559	0.94	99.93	1.02	0.24	94.09	99.48	0.0290	P4	82.
☑	☑		B11	3123	54560	0.94	99.94	1.02	0.34	94.11	99.48	0.0250	P4	82.

Fig. 1. Java-based GUI for controling the automated screen.