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designed to increase automounter reliability (also available from Hampton Research as part No. HR4-779).

The gripper is mounted on a pneumatic X–Y–θ stage, which is used to transport samples between the goniometer and the storage Dewar. A vertical Y stage moves the gripper in and out of the Dewar, a 90° rotational θ stage orients the gripper either horizontally or vertically, and a long horizontal X stage moves the gripper between the Dewar and the goniometer mount points.

When they are not mounted on the goniometer for data collection, the samples are maintained in a small cylindrical Dewar (see Fig. 9.2.2.1*b*). A custom cassette or puck (Fig. 9.2.2.1*a*) facilitates automated handling and bulk transport. Up to seven cassettes (112 samples) can be loaded into the sample Dewar. The Dewar is mounted on an R–θ motorized stage, which is used to position the selected sample for access by the gripper. The Dewar can also be positioned such that the gripper will be inserted into an unoccupied space for a precooling action when boiling of liquid nitrogen might endanger the samples. The Dewar is automatically filled directly from the facility's liquid-nitrogen supply system. During normal operations, an insulated and heated cover reduces icing and evaporation of liquid nitrogen. The gripper reaches into the Dewar through a small heated hole in the cover. The sample cassettes are moved in or out of the Dewar through a small access port in the cover.

The Robosync web site (http://smb.slac.stanford.edu/robosync/), maintained by the SSRL Structural Molecular Biology Group, features a list of biological crystallography beamlines with automated crystal mounting systems.

Important for the efficient and productive use of robotic crystal mounters is their integration into the beamline control system (McPhillips *et al.*, 2002; Snell *et al.*, 2004). The different motions of the automounter can typically be actuated from a software interface, either individually or through scripts which run a sequence of actions. The development of more fully automated capabilities requires the integration of the automounter and beamline control system with the data collection and analysis software. To this end, software has been developed that provides a framework for indexing integration and symmetry determination, along with suggested strategies for data collection (González *et al.*, 2008). When coupled with bright synchrotron beamlines and automounters, the underlying requirements for building fully automated and optimized data collection are mostly in place. The development of intelligent automated control (through *e.g.* artificial-intelligence approaches) should permit fully automated data-collection facilities to collect optimized data from a wide range of structural projects in the most efficient and cost-effective way and with minimal human intervention prior to the scientific analysis of the structures obtained.

9.2.3. Conclusion

In summary, the development of automounters over the past decade has been driven by the demands of greater access to synchrotron resources, the need for high-throughput data collection from projects that require numerous structures (*e.g.* structure-based drug-design and structural genomics programmes) and the demonstrated improvement in data quality for more challenging projects (such as large complexes and membrane proteins) that require the screening of numerous crystals in order to select those with the best diffraction characteristics. A number of different designs have been implemented at synchrotron sources worldwide, to the significant advantage of the structural biology community.

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References

Cipriani, F., Felisaz, F., Launer, L., Aksoy, J.-S., Caserotto, H., Cusack, S., Dallery, M., di-Chiaro, F., Guijarro, M., Huet, J., Larsen, S., Lentini, M., McCarthy, J., McSweeney, S., Ravelli, R., Renier, M., Taffut, C., Thompson, A., Leonard, G. A. & Walsh, M. A. (2006). *Automation of sample mounting for macromolecular crystallography. Acta Cryst.* D**62**, 1251–1259.

Cohen, A. E., Ellis, P. J., Miller, M. D., Deacon, A. M. & Phizackerley, R. P. (2002). *An automated system to mount cryo-cooled protein crystals on a synchrotron beamline, using compact sample cassettes and a small-scale robot. J. Appl. Cryst.* **35**, 720–726.

Cork, C., O'Neill, J., Taylor, J. & Earnest, T. (2006). *Advanced beamline automation for biological crystallography experiments. Acta Cryst.* D**62**, 852–858.

González, A., Moorhead, P., McPhillips, S. E., Song, J., Sharp, K., Taylor, J. R., Adams, P. D., Sauter, N. K. & Soltis, S. M. (2008). *Web-Ice: integrated data collection and analysis for macromolecular crystallography. J. Appl. Cryst.* **41**, 176–184.

McPhillips, T. M., McPhillips, S. E., Chiu, H.-J., Cohen, A. E., Deacon, A. M., Ellis, P. J., Garman, E., Gonzalez, A., Sauter, N. K., Phizackerley, R. P., Soltis, S. M. & Kuhn, P. (2002). *Blu-Ice and the Distributed Control System: software for data acquisition and instrument control at macromolecular crystallography beamlines. J. Synchrotron Rad.* **9**, 401–406.

Muchmore, S. W., Olson, J., Jones, R., Pan, J., Blum, M., Greer, J., Merrick, S. M., Magdalinos, P. & Nienaber, V. L. (2000). *Automated crystal mounting and data collection for protein crystallography. Structure*, **8**, R243–R246.

Snell, G., Nordmeyer, R., Cornell, E., Meigs, G., Cork, C., Yegian, D., Jaklevic, J., Jin, J., Stevens, R. C. & Earnest, T. (2004). *Automatic sample mounting and alignment system for biological crystallography at a synchrotron source. Structure*, **12**, 536–545.

Ueno, G., Kanda, H., Hirose, R., Ida, K., Kumasaka, T. & Yamamoto, M. (2006). *RIKEN structural genomics beamlines at the SPring-8; high throughput protein crystallography with automated beamline operation. J. Struct. Funct. Genom.* **7**, 15–22.

Wakatsuki, S. & Earnest, T. N. (2000). *The impact of synchrotron radiation in protein crystallography. Synchrotron Radiat. News*, **13**, 4–8.