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LARGE FORMAT IP SCANNER WITH MULTI-READING HEADS FOR AUTOMATED PROTEIN CRYSTALLOGRAPHY USING SR

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IP is one of the most powerful detectors for collecting diffraction data in the sense that it has a wide detection area, high sensitivity, large dynamic range, high accuracy, and reasonable pixel size. In spite of such excellent features, a high-speed automatic data collection device that has enough speed to maximize use of SR X-rays is very difficult to make, due to the slow digitization speed of the IP. We have solved this difficulty by using a fully cylindrical IP cassette (radius = 400 mm, width = 450 mm) where several diffraction images can be recorded and be read by five IP reading heads. This devise called Galaxy has been developed and installed at BL6C in the PF. Net digitization time is 5 min and 2.5 min for pixel size being 100fÊm and 200fÊm, respectively. This is enough speed for a PF bending magnet beamline. This means, that when 2.88 Å resolution data using 1.0 Å x-rays are collected, a digitized speed for a diffraction image is 16.6sec for 100fÊm pixel size, because in this condition, 18 images can be recorded in an IP cassette. Additionally, the maximum resolution is 0.58° for 1.0 Å x-rays.

Two examples follow;(1) sample crystal is Insulin, collected up to 1.0 Å collection range ; f¢f=63°, completeness=0.83, average redundancy= 1.42 and R-merge is 4.79%, (2) Citidine; data up to 0.7Å were recorded only 4 sheets using Weissenberg mode, with 80° on each sheet, completeness = 0.58, redundancy = 4.49 and R-merge = 3.2%.

Keywords: IMAGING PLATE, PROTEIN CRYSTALLOGRAPHY, AUTOMATIC DIFFRACTION INTENSITY DATA COLLECTION SYSTEM

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ADVANCES IN X-RAY CONVERSION TECHNOLOGY FOR CCD DETECTORS

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CCD-based detectors have become a key tool for x-ray crystallography, both at synchrotron beam lines and in the home laboratory. However, the performance of CCD-based detectors is fundamentally limited by the characteristics of the phosphor screens used to convert the incident x-ray flux to visible light. In particular, the spatial resolution of the detector is limited by photon scattering in the polycrystalline phosphor matrix. Also, the active areas which can be achieved are limited by the quantum efficiency of the phosphor. Here we describe a fundamentally new technology for the detection of x-ray quanta: the Quantum Resonance Converter (QRC). QRC technology allows quantum efficiencies several times higher than conventional phosphor screens and also eliminates the PSF degradation due to scattering. We describe the operation of these novel devices and report on their first experimental tests.

Keywords: CCD DETECTOR SCINTILLATOR

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STRUCTURES OF A Y-FAMILY POLYMERASE IN ACTIVE TERNARY COMPLEXES: A MECHANISM FOR ERROR-PRONE AND LESION-BYPASS REPLICATION

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Sulfolobus solfataricus P2 DNA polymerase IV (Dpo4) is a member of the newly classified Y-family of DNA polymerases. The Y-family polymerases are best characterized by their low-fidelity synthesis on undamaged DNA templates and propensity to traverse normally replication-blocking lesions. Crystal structures of Dpo4 in ternary complexes with DNA and an incoming nucleotide, either correct or incorrect, have been solved at 1.7 Å and 2.1 Å resolution, respectively. Despite a conserved active site and a hand-like configuration similar to all known polymerases, Dpo4 has relatively small finger and thumb domains and an extra C-terminal domain. The small finger domain makes limited and nonspecific contacts with the replicating base pair thus relaxing base selection. The extra C-terminal domain binds the DNA major groove and assist thumb domain to hold DNA. Dpo4 is also captured in the crystal accommodating two template bases in the active site, suggesting a possible mechanism for bypassing thymine dimers.

Keywords: DNA POLYMERASE ERROR PRONE REPLICATION TRANSLESION SYTHESIS

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CRYSTAL STRUCTURE OF EXONUCLEASE RECJ BOUND TO MANGANESE ION

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RecJ is a 5-prime to 3-prime exonuclease specific for ssDNA and is involved in homologous recombination, base excision repair, and mismatch repair. RecJ is also known to be a key enzyme for recombination-dependent replication. RecJ has five characteristic motifs in its sequence; the proteins having these motifs are ubiquitous in archaea, prokaryotes, and higher eukaryotes and they form a large family of the predicted phosphoesterases (DHH family). But the structure of neither RecJ protein nor the homologue in the DHH family was available. We crystallized RecJ from *Thermus thermophilus* HB8 bound to manganese ion essential for its activity and determined its crystal structure by SAD method. RecJ has a novel fold, in which two domains are interconnected with a long helix to form a central groove. This groove is composed of conserved residues and positively charged, which may be involved in DNA binding. The width of the groove is too narrow (11 Å) to bind to double-stranded DNA (20 Å width), indicating the specificity for ssDNA. Manganese is coordinated by amino acid residues in the motifs characteristic to the DHH family. The structure of RecJ suggested the putative catalytic residues for its nuclease reaction. Mutation of these residues resulted in the loss or severe reduction of the nuclease activity. Based on these results, we proposed the mechanism of the nuclease reaction by RecJ.

Keywords: DNA REPAIR EXONUCLEASE DHH FAMILY