

## **W0364**

**Data Truncation and Water Building Parameters for Optimal Refinement.** Annie Heroux, Alexei Soares, Edgar Weckert, Robert Sweet, Biology, Bldg 463, Brookhaven National Laboratory, Upton, NY 11973.

Triplet phases recorded from insulin crystals were used to investigate the effects that truncation of the x-ray data had on the subsequent refinement of the structure. We found that overly conservative data truncation generates undesirable water molecules that the triple phases showed to be spurious. The triplet phases were not used at any point in the refinement, and consequently are a validation tool similar to the Rfree. However, the Rfree was insensitive to these data truncation effects, and we speculate that the spurious water molecules arise from Fourier series termination ripples in the electron density. We also examined the impact of other user-selectable parameters on water building and refinement.