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The Effects of Energy and Crystal Composition on the Radiation Dose Absorbed by Macromolecular Crystals. Elspeth F. Garman¹, James W. Murray¹, Raimond B.G. Ravelli²,
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Radiation damage restricts the useful lifetime for macromolecular crystals in the X-ray beam, even at cryogenic temperatures. With the development of structural genomics pipelines, it will be essential to incorporate projected crystal lifetime information into the automated data collection software routines. As a step towards this goal, a computer program, RADDPOSE, is presented which is designed for use by crystallographers in optimising the amount of data that can be obtained from a particular crystal. The program uses the composition of the crystal and buffer constituents, as well as the beam energy, flux and dimensions, to compute the absorption coefficients and hence the time taken to reach a given absorbed dose.

Example cases will be discussed along with the implications for anomalous data collection.