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Computational Removal of Radiation-induced Changes. Zbyszek Otwinowski Dominika Borek Marcin Cymborowski Wladek Minor, Biochemistry, UT Southwestern Medical Center at Dallas, 5323 Harry Hines Blvd, Dallas, TX 75390-8816 USA.

The dominant characteristics of radiation-induced changes, described either in real or reciprocal space, can vary between experiments. Real-space characteristics are important for the chemical interpretation of a crystal structure and could potentially also be used for phasing. On the other hand, the reciprocal-space characteristics consist of resolution-dependent decay combined with each reflection having an independent, continuous change of the structure factor with dose. Prior to an experiment, the magnitude and character of these changes cannot be accurately predicted. However, for the purpose of data analysis, a particular model of radiation damage must be assumed in order to avoid adding an unreasonable number of parameters. This procedure is additionally complicated by the fact that the magnitude of phasing signals and error estimators are unknown.

We present a number of examples showing which particular model of radiation damage in reciprocal space is most suitable for individual cases. Often, making the right choice has a dramatic impact on the structure solution process.