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Supporting information for article:

The potential benefits of using higher X-ray energies for macromolecular crystallography

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Monte Carlo simulations

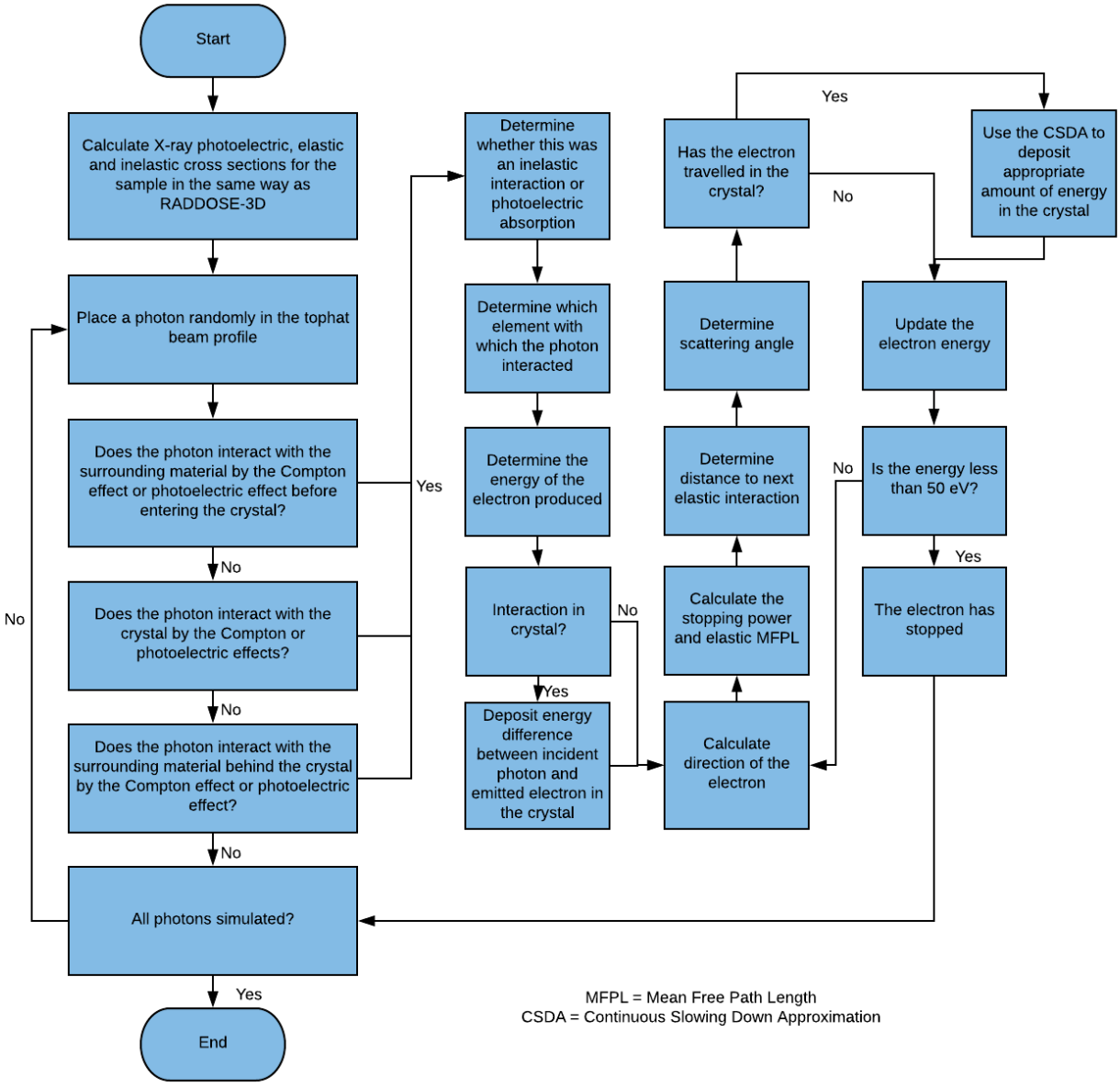

Figure S1 Description of the architecture of the code used to perform the Monte Carlo simulations for this study.

In the Monte Carlo simulations, the surrounding material was modelled as pure water and the crystal composition was similar to insulin but with the S and Zn atoms removed. 10 million and 50 million photons were simulated for energies below and above 18 keV respectively. The photons were tracked one at a time and placed randomly in the *x* and *y* beam profile at a *z* position that is in front of the crystal by the maximum photoelectron range calculated using the continuous slowing down approximation (CSDA). Electron stopping powers are calculated using the same method as the ESTAR database (Berger *et al.*, 2005). The distance s travelled by an X-ray before an interaction is calculated using the following equation (Joy, 1995):

$$s = -\alpha \ln(RND)$$

where RND is a random number between 0 and 1 and α is the average distance a photon will travel before being inelastically scattered or absorbed.

If the initial interaction was by the Compton effect, the scattering angle θ of the photon is chosen randomly and the energy lost by the photon and given to the resulting free electron (E_{comp}) is calculated using the following equation:

$$E_{comp} = \frac{E_{inc}^2(1-cos\theta)}{mc^2(1+\frac{E_{inc}(1-cos\theta)}{mc^2})}$$

Where *m* is the rest mass of an electron and *c* is the velocity of light. The momentum is conserved so the recoil angle ϕ of the electron is:

$$tan\varphi = \frac{(\tan\left(\frac{\theta}{2}\right))^{-1}}{1+\frac{E_{inc}}{mc^2}}$$

If the initial interaction is by the photoelectric effect, the energy of the photoelectron is equal to the energy of the incident photon minus the electron shell binding energy. The initial direction of the photoelectron is biased to be preferentially emitted in the same direction as the polarisation vector of the synchrotron beam (Cooper & Zare, 1968), which is approximately 75% in the horizontal direction (Rybicki & Lightman, 1979; Koch *et al.*, 1983). An angle θ between the polarization vector and the direction of the ejected electron is chosen weighted by the differential emission cross section of the photoelectron $d\sigma/d\Omega$, which follows the equation:

$$d\sigma/_{d\Omega} = \left(\frac{\sigma_{total}}{4\pi}\right)[1+\beta P_2(cos\theta)]$$

Where $P_2(cos\theta) = 0.5(3cos^2\theta - 1)$, σ_{total} is the total cross section, and β is an asymmetry parameter. The asymmetry parameter varies between -1 and 2 depending on the element and the electron shell from which the photoelectron is emitted. For photoelectrons emitted from K shells, θ is always equal to 2. If the photoelectron is not from a K shell, θ will vary but in the simulations it is assumed to be 0 so the photoelectron will be emitted in a random direction.

The Compton recoil electrons and photoelectrons are tracked using Monte Carlo simulations. Total elastic cross sections and elastic differential cross sections were calculated using the ELSEPA database

(Salvat *et al.*, 2005). If the electron crosses a boundary between the surrounding material and the crystal or undergoes an elastic scattering event, the energy the electron has lost since the last event is calculated using the continuous slowing down approximation (CSDA) and if the electron travelled in the crystal, the energy it lost is deposited in the crystal. The stopping power and elastic cross sections are updated for the new electron energy and, if a boundary between crystal and surrounding was crossed, for the new material. Secondary electrons produced from electron inelastic interactions were not tracked in these simulations.

Supplementary references

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