Crystallographic Data to Model relationship Equation:

Data is all of the measured diffraction, indexed by h, k, ℓ.
Amplitude is proportional to the square root of the measured intensity for each of the h, k, ℓ data points.

Model is the coordinates of all atoms.

Compare the calculated amplitudes with the measured amplitudes ...

$$\vec{F} = |F_{hk\ell}| \cdot e^{i\phi_{hk\ell}} = \sum_{n}^{N} O_n \cdot f_{n,\theta} \cdot e^{-B_n (\sin\theta / \lambda)^2} \cdot e^{i\, 2\pi(hx_n + ky_n + \ell z_n)}$$

Amplitude • phase ...calculated from the model.

Amplitude • phase

λ	:	wavelength of radiation
$\theta_{hk\ell}$	:	angle of incident beam to the measured h, k, ℓ indexed data measurement.
h, k, ℓ	:	integer index numbers of a particular measured diffracted ray.
$\lvert F_{hk\ell} \rvert$	:	amplitude of the $hk\ell^{th}$ diffracted ray, proportional to the square root of the measured intensity.
$\phi_{hk\ell}$	:	the phase of the $hk\ell^{th}$ diffracted ray
B_n	:	B-factor of the $n^{th\ atom}$ (uncertainty factor)
$f_{n,\theta_{hk\ell}}$	:	individual atomic scattering factor of the n^{th} atom as a function of $\theta_{hk\ell}$
x_n, y_n, z_n	:	coordinates of the n^{th} atom
N	:	total number of atoms in the repeating unit of the crystal
O_n	:	occupancy of the n^{th} atom,