

On the relationship between cumulative correlation coefficients and the quality of crystallographic data sets

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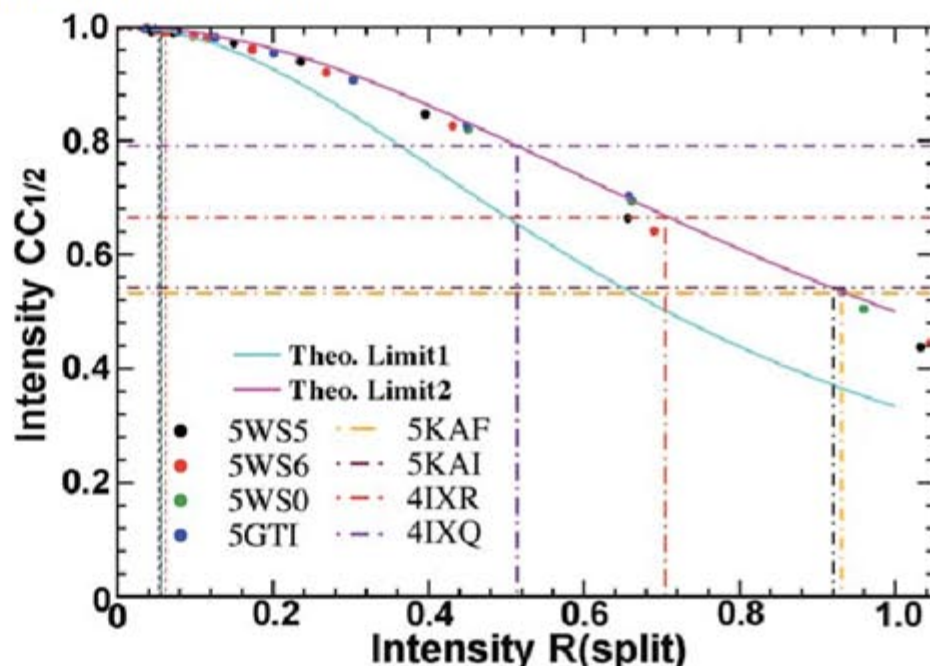
Protein Sci. (2017)

in press DOI: [10.1002/pro.3314](https://doi.org/10.1002/pro.3314)

Theoretical limit:

$$CC_{1/2} = \frac{1}{1 + aR_{diff}^2},$$

$1 < a < 2$ depends only on the symmetry-related multiplicity



CC1/2 and R(diff) values have been computed for four XFEL experimental data sets for PSII (5WS5, black spheres; 5WS6, red; 5WS0, green; 5GTI, blue) as a function of resolution. follow the magenta curve, as do their cumulative CC1/2 values.