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

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\textit{Protein Sci.} (2017)
in press DOI: 10.1002/pro.3314

Theoretical limit:

\[ CC_{1/2} = \frac{1}{1 + \alpha R_{\text{diff}}^2}, \]

1 < \( \alpha \) < 2 depends only on the symmetry-related multiplicity

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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.