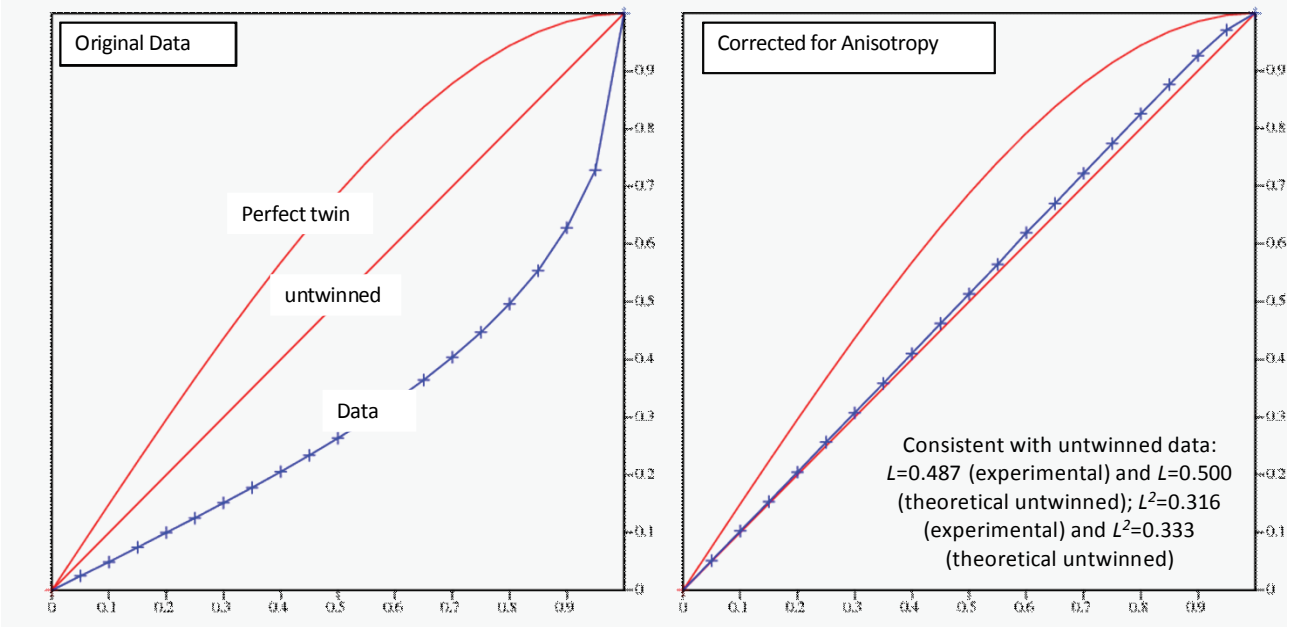
Supplemental Information:

Table 1: Crystallization and Cryo-preservations conditions used for WT SOD1cys. Red indicates the condition that yielded the current structure.

Protein	Crystallization Buffer	Cryo Condition	Number of Crystals
WT SOD1 (co-crystals)	0.1 M MES, pH 6.25 20 % PEG 3350	20 % glycerol/HEPES	4
WT SOD1 (co-crystals)	0.1 M MES, pH 6.25 20 % PEG 3350	20 % glycerol/MES	8
WT SOD1 (co-crystals)	20 % PEG 2000 0.1 M imidazole, pH 8.0 0.2 M calcium acetate	2.4 M sodium malonate, pH 6.8	5
WT SOD1 (co-crystal)	0.1 M HEPES, pH 7.3 20% PEG 3350	2.4 M sodium malonate, pH 6.8	4
WT SOD1 (soaked)	0.1 M MES, pH 6.25 20 % PEG 3350	20 % glycerol/MES	4
WT SOD1 (soaked)	0.1 M MES, pH 6.25 20 % PEG 3350	30 % glycerol/HEPES	2
WT SOD1 (soaked)	0.1 M MES, pH 6.25 20 % PEG 3350	30 % ethylene glycol	2
WT SOD1 (soaked)	0.1 M MES, pH 6.25 20 % PEG 3350	2.4 M sodium malonate, pH 6.8	10
WT SOD1 (soaked)	10 mM Tris, pH 8.0 0.1 M sodium chloride 2.4 M ammonium acetate	20% glycerol	2

Cysteinylation causes local conformational changes that likely affect crystallization of SOD1 thus, the majority of the crystals screened had no cysteinylation present. It is possible that cysteinylation was both labile and lost or that only the non-cysteinylated protein crystallized. The crystallization condition that yielded the cysteinylated SOD1 crystal is one in which SOD1 was cysteinylated prior to crystallization. Another possibility is that if cysteinylation was induced during crystallization (soaked) that some conditions prevent cysteinylation.

Supplemental Figure S1



Supplemental Figure S1: SODcys Data Set is Untwinned. The method of Padilla and Yeates was used to determine the possibility of a twinned data set[1]. The plot on the left was generated using our original data set (blue line) and does not match either the theoretical traces for untwinned (straight red line) or twinned (curved red line) data. The plot on the right is the analysis of our data set corrected for anisotropy, which is consistent with an untwinned data set (straight red line). In addition to the graphical representation, *L* of 0.487 for our data, is in good agreement with the predicted *L* for untwinned data (0.500) as is the L^2 (our data=0.316, an untwinned data set= 0.333, and a twinned data set=0.200).

[1]Padilla, J. E., and Yeates, T. O. (2003) A statistic for local intensity differences: robustness to anisotropy and pseudo-centering and utility for detecting twinning, *Acta Crystallogr D Biol Crystallogr 59*, 1124-1130.