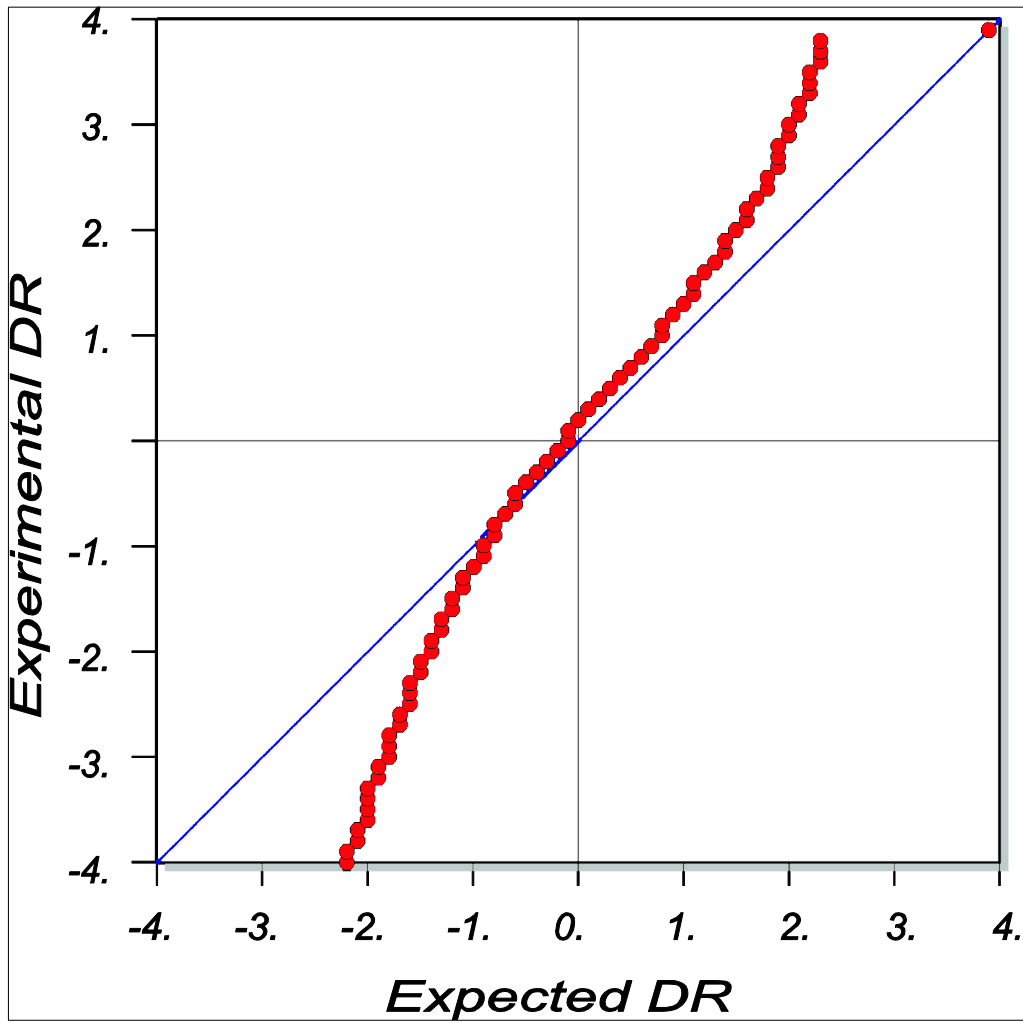
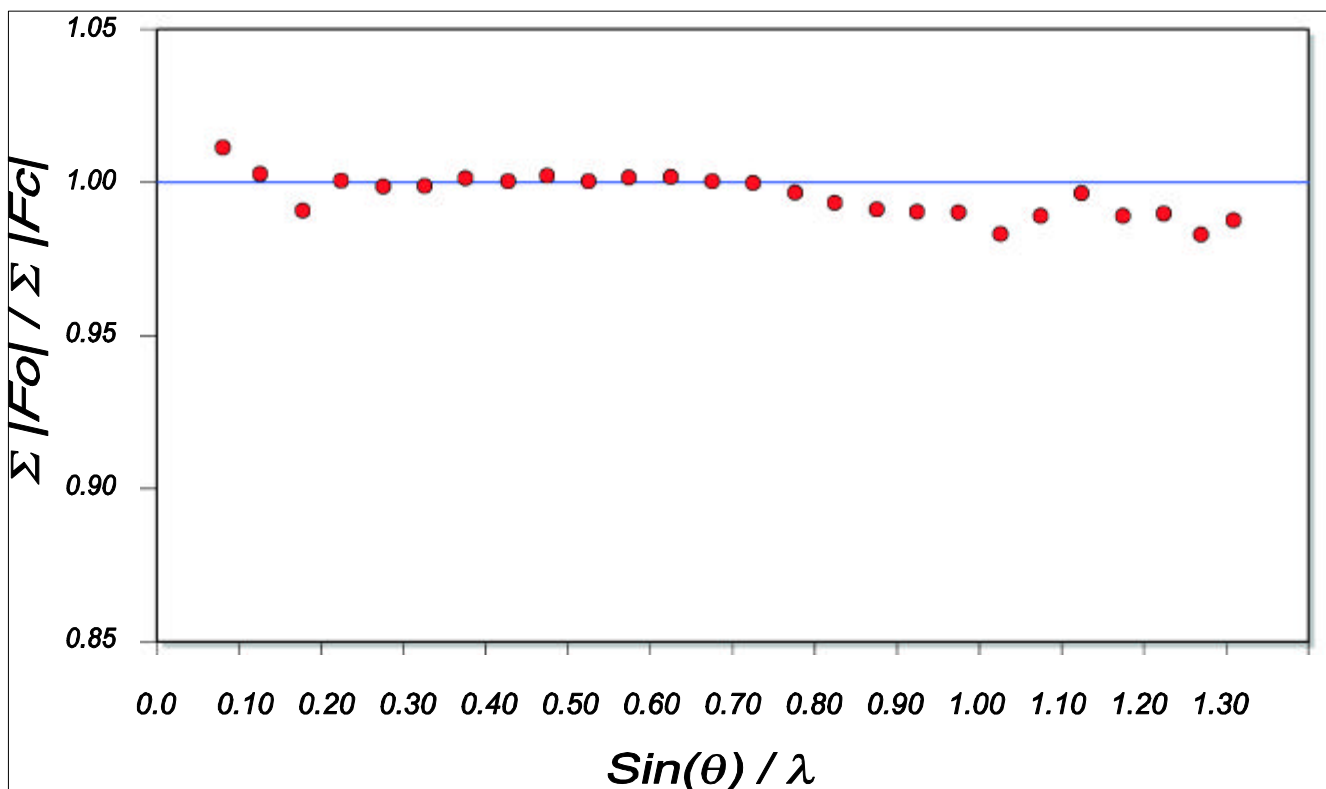


SUPPLEMENTARY MATERIAL

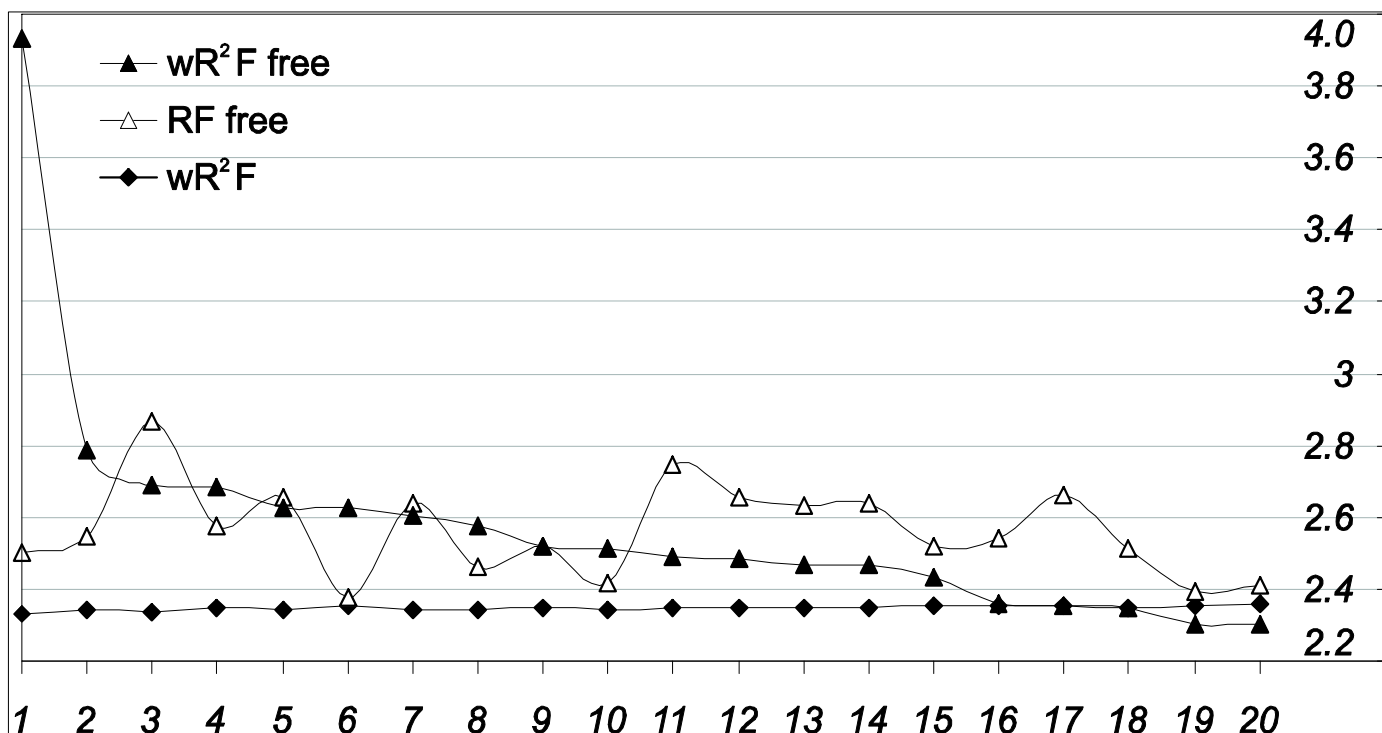
Figure Sup1. Diagram of normal probability plots for 1-nitroindoline after SCA5 refinement.



**Figure Sup2.** Scale factor vs. resolution plots for 1-nitroindoline after SCA5 refinement.

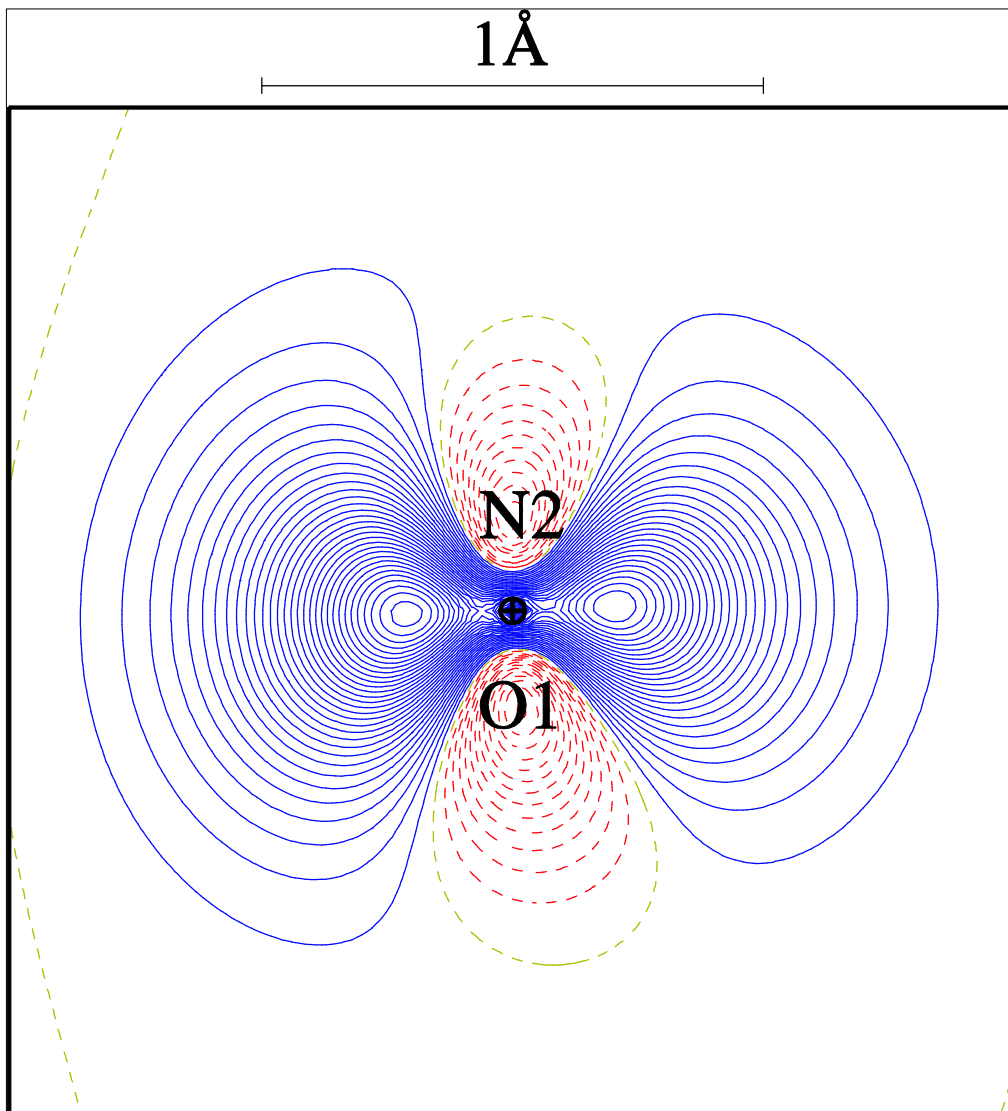


**Figure Sup3.** Distribution of the twenty wR2(F)- free, wR2(F) and R(F)-free factors for the optimal restraints refinement. The distribution was ordered with decreasing wR2(F)- free values.



**Figure Sup4.** Experimental static deformation electron density maps showing the electron lone pairs for the O1 oxygen atom of the nitro group. The views are in the planes containing the oxygen atom and perpendicular to the N2- O1 bond.

(a) without symmetry and chemical equivalence restraints.



(b) with optimally weighted symmetry and chemical equivalence restraints

Contour intervals  $0.05 \text{ \AA}^{-3}$ , solid lines represent positive contours, dashed are negative and yellow dashed are zero.

