

# Chapter 9.10

## WTANAL

P.R. MALLINSON AND K.W. MUIR,  
DEPARTMENT OF CHEMISTRY,  
UNIVERSITY OF GLASGOW,  
GLASGOW G12 8QQ

WTANAL analyses the structure factor file (name.FCF file in LIST 4 format) written by SHELXL and prints various distributions of  $F_{obs}$  and  $w\sigma^2$  as functions of the indices, even/odd combinations of the indices, ranges of  $\sin\theta/\lambda$ , and ranges of  $F_{obs}$ . The weights are first placed on an absolute scale so that  $\Sigma w\sigma^2 = N_{obs} - N_{param}$ . Also, reflections for which  $|F_{obs}| > g * \text{sig}(F_{obs})$  are listed, so the program will ask for the desired value of  $g$ .

The program also requires the file SHELXL.LST for the parameters of the weighting scheme used in refinement. A graphical display is optionally available