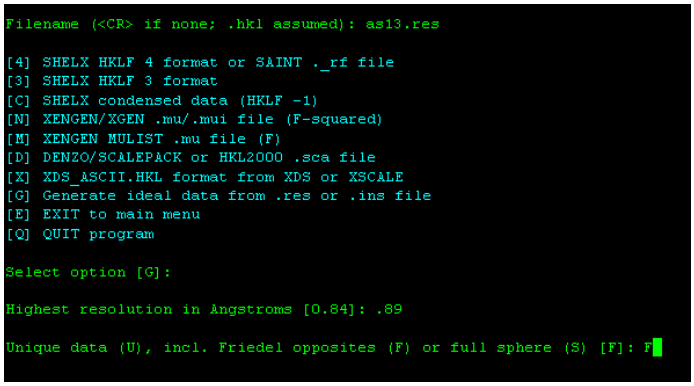
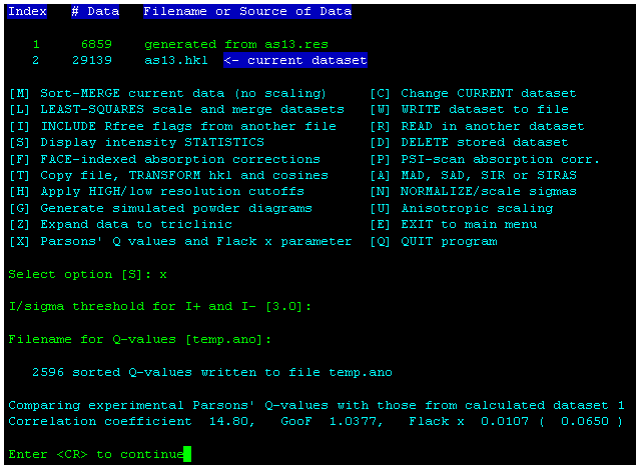
PARSONS' Q Values

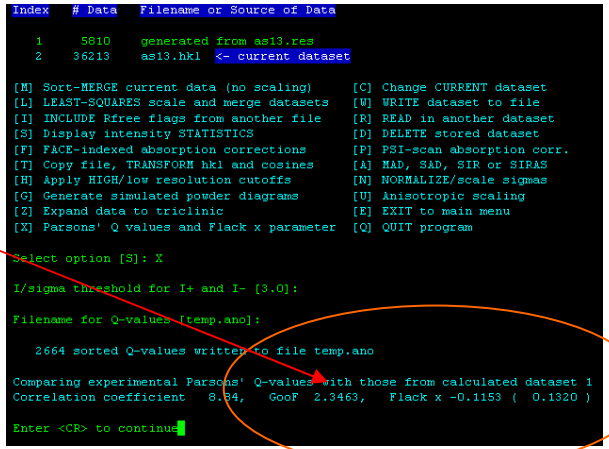
How To run Parsons' Q values for Absolute Configuration Studies (Parsons and Flack, 2004) in XPREP.

1. Refine the structure to the completion.
2. Start XPREP without anything on the command line
3. When prompted enter *your res file*
4. Generate data CONTAINING Friedel opposites with the same resolution as the data set!
5. Follow the usual prompts inputting the space group etc. until you reach the D menu.
6. Read in the experimental data with the R command, follow the prompts back to the D menu
7. Select X and follow the prompts
8. The Goof should be near 1.0 and the Flack parameter and s.u. will be seen in the case shown it is 0.010(65)





Note if the Goof is too large (>1.5) then the g value in SADABS has been set too high. Run SADABS again with a lower value.



PARSONS, S. & FLACK, H. (2004) Precise Absolute-Structure Determination in Light-Atom Crystals. *22nd European Crystallographic Meeting, ECM22.* Budapest, IUCR.