

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)

```
Filename (<CR> if none; .hkl assumed): as13.res

[4] SHELX HKLF 4 format or SAINT .rf file
[3] SHELX HKLF 3 format
[C] SHELX condensed data (HKLF -1)
[M] XENGEN/XGEN .mu/.mui file (F-squared)
[M] XENGEN MULIST .mu file (F)
[D] DENZO/SCALEPACK or HRL2000 .sca file
[X] XDS_ASCII.HKL format from XDS or XSCALE
[G] Generate ideal data from .res or .ins file
[E] EXIT to main menu
[Q] QUIT program

Select option [G]:

Highest resolution in Angstroms [0.84]: .89

Unique data (U), incl. Friedel opposites (F) or full sphere (S) [F]: F
```

```
Index # Data Filename or Source of Data
1 6859 generated from as13.res
2 29139 as13.hkl <- current dataset

[M] Sort-MERGE current data (no scaling) [C] Change CURRENT dataset
[L] LEAST-SQUARES scale and merge datasets [W] WRITE dataset to file
[I] INCLUDE Rfree flags from another file [R] READ in another dataset
[S] Display intensity STATISTICS [D] DELETE stored dataset
[F] FACE-indexed absorption corrections [P] PSI-scan absorption corr.
[T] Copy file, TRANSFORM hkl and cosines [A] MAD, SAD, SIR or SIRAS
[H] Apply HIGH/low resolution cutoffs [N] NORMALIZE/scale sigmas
[G] Generate simulated powder diagrams [U] Anisotropic scaling
[Z] Expand data to triclinic [E] EXIT to main menu
[X] Parsons' Q values and Flack x parameter [Q] QUIT program

Select option [S]: x

I/sigma threshold for I+ and I- [3.0]:

Filename for Q-values [temp.ano]:

2596 sorted Q-values written to file temp.ano

Comparing experimental Parsons' Q-values with those from calculated dataset 1
Correlation coefficient 14.80, Goof 1.0377, Flack x 0.0107 ( 0.0650 )

Enter <CR> to continue
```

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.

```
Index # Data Filename or Source of Data
1 5810 generated from as13.res
2 36213 as13.hkl <- current dataset

[M] Sort-MERGE current data (no scaling) [C] Change CURRENT dataset
[L] LEAST-SQUARES scale and merge datasets [W] WRITE dataset to file
[I] INCLUDE Rfree flags from another file [R] READ in another dataset
[S] Display intensity STATISTICS [D] DELETE stored dataset
[F] FACE-indexed absorption corrections [P] PSI-scan absorption corr.
[T] Copy file, TRANSFORM hkl and cosines [A] MAD, SAD, SIR or SIRAS
[H] Apply HIGH/low resolution cutoffs [N] NORMALIZE/scale sigmas
[G] Generate simulated powder diagrams [U] Anisotropic scaling
[Z] Expand data to triclinic [E] EXIT to main menu
[X] Parsons' Q values and Flack x parameter [Q] QUIT program

Select option [S]: X

I/sigma threshold for I+ and I- [3.0]:

Filename for Q-values [temp.ano]:

2664 sorted Q-values written to file temp.ano

Comparing experimental Parsons' Q-values with those from calculated dataset 1
Correlation coefficient 8.84, Goof 2.3463, Flack x -0.1153 ( 0.1320 )

Enter <CR> to continue
```

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

