

Program EFRESOL

to calculate the effective and optical resolutions of a diffraction data set

References: L.Urzhumtseva, B.P.Klaholz, A.Urzhumtsev, 2013, *Acta Cryst.*, **D69**, 1921-1934;
L.Urzhumtseva, A.Urzhumtsev, 2015, *J.Appl. Cryst.*, **48**, in press

Send suggestions and 'bug' reports to: sacha@igbmc.fr

1. Definitions

- The minimum distance for a given diffraction data set and a given type of scatterers is the shortest distance at which the images of these scatterers are yet seen separately in the Fourier synthesis calculated with these data and with the ideal phases if they were known.
- The effective resolution, $d_{\text{effective}}$, of a data set is equal to the highest resolution of the complete data set such that the minimum distance for point scatterers is the same for both sets. The value of $d_{\text{effective}}$, in comparison with the highest-resolution cut-off d_{high} , shows the loss of resolution due to the missed structure factors. For complete data sets, $d_{\text{effective}} = d_{\text{high}}$.
- The optical resolution, d_{optical} , of a given set of structure factor amplitudes or intensities is the minimum distance for typical atoms (with the typical B-factor value) of the corresponding structure in the non-weighted synthesis calculated with these amplitudes and with the ideal phase values if they were known.
- The value $1.25*d_{\text{optical}}$ shows, by comparison with $d_{\text{effective}}$, the loss of resolution due to the shape of the atoms with the typical B value.

2. The purpose

The program defines the effective resolution of a given set of reflections. This value reflects both the high-resolution data cut-off and the reflections missed in the data set.

For anisotropic data sets both the highest and the lowest resolutions, depending on the direction, are determined. The corresponding directions are also calculated.

The program defines also the minimum and maximum optical resolution for the given values of the amplitudes / intensities.

3. The procedure

Four steps shall be executed consecutively for the full analysis; however, the first step may be sufficient for a number of cases. Three first steps are relatively fast; the fourth step may take a minute or so, depending on the size of the data set and the parameters used. You can execute these steps one by one clicking the corresponding virtual buttons.

Step 1. Calculate the effective resolution along the coordinate axes.

Step 2. Define (assign) the typical B value for the given set of amplitudes / intensities.

Step 3. With the selected B value, calculate the optical resolution along the coordinate axes.

Step 4. Calculate the effective and optical resolutions for all directions (vectors to the grid points on a sphere) and find their mean, extreme values and the rms deviation.

4. Program results and examples

The principal results are obtained in Step 4; they are the minimum and maximum effective and optical resolutions. The anisotropy ratio is also calculated. Corresponding plots can be saved in the png format. The plots for intermediate results from Steps 1-3 are also available and printable. Clicking the left mouse button on the curve points highlights the corresponding resolution value.

The effective and optical resolutions along the coordinate axes are calculated not only with the full data set but also for several subsets where the high-resolution cut-off is lowered in purpose. For severely incomplete data sets, this curve may give an idea of the best resolution cut-off to be applied to obtain the highest effective resolution (see Figure below). The user may define the number of these subsets and the resolution step to calculate them.

When analyzing the effective resolution along all directions, Step 4, its histogram is calculated and shown. This allows getting an idea of the overall geometry of the data set.

As an example, the file `data_IF2_APO_wt.mtz` contains a complete data set at a resolution of 1.95 Å for which the effective resolution `d_effective` coincides with `d_high`. This also shows a size of computational errors, that of order of 0.01 Å. Another file `data_IF2_GDP_pH65.mtz` contains a highly anisotropic data set for which the effect of the high resolution cut-off and incompleteness is well pronounced (see Figure below). These data sets were obtained when working on the IF2 structure (Simonetti *et al.*, 2013, *Acta Cryst.*, **D69**, 925-933).

Note that the completeness statistics (main window) is given only for a reference. It does not take into account systematic extinctions of the particular space group. For details of completeness of the data set and the distribution of missed reflections, use the program FOBSOM (Urzhumtseva & Urzhumtsev, 2011, *J.Appl.Cryst.*, **44**, 865-872).

5. Input data and parameters

The program reads a list of reflections including their indices and amplitudes (or intensities) from a file in MTZ (*.mtz), XDS (*.hkl), HKL2000 (*.sca), CNS (*.hkl), cif (*.cif) formats. For the formats where the unit cell parameters and the space groups are not defined, these parameters shall be defined by the user in the corresponding windows. To choose the particular set of amplitudes/intensities if they are several in the file, and to choose/modify the Laue group if required, double click on your choice.

The typical B-factor value can be assigned manually or chosen from the Wilson plot. The resolution limits for the plot can be modified with the moving pen (click left mouse button).

More technical parameters can be modified by pressing the button 'Parameters'. Please type a new value (or use 'Default values' button to restore those) and confirm the changes by pressing the virtual button "Accept". Otherwise your modifications will not be activated. Parameter modification may require repeating previously executed steps.

6. System requirements

The basic version of the program has been developed for Windows while it runs also under Linux and MacOS; Python versions starting from 2.6 are required. Python library Numpy is required.

The program can be run using either independently installed Python libraries or using Python installed in the frame of other program suites. For example, when PHENIX is installed, one can run the program typing a command

```
phenix.wxpython efresol_n_m.py
```

where 'n_m' is the number of the current version, *e.g.* `efresol_3_1.py`.

Fig. 1. Screen-shots of the *efresol* session with the file data_IF2_GDP_pH65.mtz

