BEST

Version 1.1

27.03.2003

A program for optimising the X-ray data collection from macromolecular crystals

Manual

EMBL Hamburg Outstation

Alexander N. Popov sasha@EMBL-Hamburg.de
Gleb P. Bourenkov gleb@mpghdb.desy.de

Contents

1. Program description

BEST is a program for optimal planning of X-ray data collection from protein crystals using the rotation method. From one, or a few, initial diffraction images, BEST predicts statistical characteristics of a data set for different combinations of data collection parameters, and suggests the most optimal ones. According to the option chosen, the optimal set of parameters predicts a given average signal-noise ratio $\bar{I}/\bar{\sigma}(I)$ at a given resolution either in the shortest time or with the minimum total radiation dose.

Initially, the program estimates the total data collection time (and dose) required in order to achieve $\bar{I}/\bar{\sigma}(I) = 3$, 5 or 10 as a function of resolution. Then, on the basis of the resolution and $\bar{I}/\bar{\sigma}(I)$ requested by the user, the program proposes the plan of data collection. The plan defines the total rotation range, scan speed, rotation range per frame, detector distance and the detector diameter (when applicable). The rotation range per frame and scan speed vary with the rotation angle in a way to make the distribution of $\bar{I}/\bar{\sigma}(I)$ over the reciprocal space as uniform as possible. The program estimates the data statistics (mean intensity, mean sigma, R-merge, distribution of $I/\sigma(I)$ and relative number of overloaded reflections as a function of resolution) for the data that will be collected according to the plan.

In addition, BEST can calculate the optimum plan for a user-defined total rotation range. The data statistics can be predicted for any set of data collection parameters defined by the user, but in this case the rotation range per frame and scan speed are assumed to be constant during data collection.

BEST assumes that the exposed volume of crystal does not vary with the spindle axis position.

In BEST v1.1 no special option for MAD data collection is provided. The detector is considered to have a circular area with the direct beam projecting onto the centre. No detector offsets, linear or 2θ, are supported. The program reads all the parameters that are needed for calculations and partial reflection intensities from the DENZO '. x' file.

2. Measuring initial images

Exposure time

The initial image(s) would usually be measured with a **short** exposure time. The presence of overloaded spots severely biases the predictions. The images that contain no ‘visible’ reflections at the edge of the detector are adequate for BEST. However, in total there should be enough measurable reflections to index the pattern.

The detector distance

BEST will calculate neither plans nor predictions for the resolution extending beyond the limit defined by the detector distance at which the initial image(s) were measured. Thus, the initial image(s) would usually be measured at a relatively **short** distance (see **Overlaps**). BEST is then used to define the resolution of the final data collection at a distance longer than that for the initial frames(s).

Rotation range

Unless the **-s** option is being used, BEST reconstructs the intensities from partials. This works well only when the rotation range is wider then half of the crystal mosaicity. The initial image(s) would usually be measured with a relatively **large** rotation (see **Overlaps**).

Overlaps

Ideally, the reflections should not overlap. If overlaps appear at low resolution, the distance should be increased until they are resolved. High-resolution data collection will not be possible anyway. A small fraction of overlapping reflections at high resolution can be tolerated. If severe overlapping cannot be avoided and the rotation range is wider than half of the mosaicity, several thin frames covering a range of about twice the mosaiciy should be measured and the partials summed (e.g., using SCALEPACK). In this case the **-s** option of BEST should be used.

Number of frames

For triclinic and monoclinic crystals, a minimum of two frames measured at c.a. orthogonal spindle axis positions are always required. For higher symmetries a single frame may be sufficient depending on the number of reflections. If there is not enough input data, BEST will suggest a spindle value at which further frame(s) should be measured. However, the more data that are input the higher the accuracy of predictions. Every plan is supplied with an estimate of the uncertainty in the expected $I/\sigma(I)$ ratio. The necessary amount of the input data can be guided by those estimates.

IMPORTANT: if several frames are used, they must be on the same scale, i.e. they must be measured under identical conditions except for the spindle angle. If the **-s** option is used, the data in the input file must be on the same scale as the input image (e.g. DEFAULT SCALE 1 should be set in SCALEPACK).

Evaluating initial image(s)

The symmetry of the crystal must be known prior to running BEST. The initial image(s) should be indexed and integrated correctly. BEST will issue a warning if it suspects that the indexing is wrong, but it might not necessarily be able to detect misindexing. If more than one frame is used, the indexing must not necessarily be consistent (e.g., turning a trigonal lattice by 60 degrees is permitted, permuting orthorombic axes is not). Reasonable estimates of mosaicity and spot size should be made, according to the processing software you are using. For example, overestimating mosaicity by ten per cent will translate in a signal-to-noise <5% higher then predicted. A proper value for the **air absorption length** should be used (note that the DENZO default =860 corresponds to a wavelength of 1.54 Å).

3. The command line

SYNOPSYS

best -f <detector> -t <time> [-r <n> -3|5|10 -d <n> -p –e <n> -q -h -g -I -l -m <n> -s <file> -o <file>] <image_file> <file1.x> {<file2.x> <?>}

PARAMETERS

-f <detector>

The name of the detector that was used to measure <image_file>. In addition to the type of detector, the name encodes unique properties of each device and/or data format. Use –l option to find out the names available at your installation.

(For EMBL-Hamburg beam-lines: mccd_x11, mccd_x13, mar2300, image2300 etc.)

The detector name can be defined via the shell variable best_default_detector (e.g. setenv best_default_detector myccd in .csh file if you have got only one detector). The parameter –f <detector> can then be omitted on the command line.

-t <time>

The exposure time of initial image in seconds. If dose mode is used for data collection, the preset dose should be specified as well using **–d <dose>** option. For instruments where incident intensity varies in time (e.g., proportional to the storage ring current), the average time that corresponds to your preset dose can be used instead of a true exposure time for the initial image(s).

<image_file>

The name of the image data file. The image is used for evaluating the background scattering level.

<file1.x> {<file2.x> ...}

The name(s) of one or more '.x' files. The crystal cell, orientation, detector distance, wavelength, mosaicity and spot sizes will be taken from the first file in the list. This file must correspond to the input image. All files from the list will be used for reconstructing intensities and scaling, unless **-s** option is specified. BEST assumes that intensities in all the '.x' files are on the same scale, i.e. they are measured at identical conditions except for crystal orientation.

OPTIONS

-h

Print help message and exits the program.

-g

Plots of (a) rotation range necessary to obtain 85, 90, 95 and 99% completeness as a function of starting angle, (b) maximum permitted rotation range per frame as a function of resolution and rotation angle, (c) predicted and experimental mean intensity as a function of resolution (Wilson plot), (d) relative error of mean intensity prediction and relative intensity in the last shell of resolution as a function of rotation angle will be displayed using **plotmtv** program.

-o <file>

The plots (see **-g** option) will be saved in mtv (see **plotmtv**) format file.

-i

Activate interactive input. Ignores **-r -p -3|5|10 -e** options. Default not to activate. The program prints the table of estimated optimal time for data collection as a function of resolution and prompts several options for further calculations (see **Interactive mode**).

-m <number>

If the 'multyread' or 'dezingering' option was used for measuring the image(s), give a number of detector read outs. Default 1.

-l

Print the list of configured detectors (see **-f)** and exits the program.

-s <file>

Reads reflection intensities in HKL '.sca' format file and uses them for the absolute scaling, instead of reconstructing the intensities from partials from '.x' files. Used this option should give more accurate results provided the intensities in a file are on the same scale as on the image.

-r <number>

Desired resolution in Å, default as for the initial image.

-d <number>

Preset counts (dose) of initial image.

-q

Minimise the absorbed dose. Default to minimise total time of data collection

-3|5|10

Aimed $I/\sigma(I)$ at highest resolution, default 3

-e <number>

The maximum number of plan entries, default up to 36

-p

Output data collection plan only.

4. Interactive mode

If an interactive input is activated, BEST prints the table of the estimated optimal time for data collection as a function of resolution and prompts several options for further calculations.

Options

plan <resolution> <I/SigI>

Print the data collection plan for current (shortest or user-defined) total rotation range.

stat

Print statistics correspond the plan.

isigi <number> <number> <number>

Define $I/\sigma(I)$ other then 3, 5 and 10 and repeat prediction.

phi <start> <end >

Change the total rotation range and repeat prediction. By default, BEST proposes to measure the shortest total range with a minimum redundancy. While $I/\sigma(I) \le 10$ (e.g., for "high resolution" data collection) this is the most efficient strategy. Using BEST you may verify that up to an order of magnitude higher dose may be required to obtain the same signal-to-noise ratio in a target resolution shell with a ~4 fold higher redundancy. On the other hand, reaching $I/\sigma(I) >> 10$ (e.g., for anomalous scattering measurements) in many circumstances may only be possible with higher redundancy. Using this option, the redundancy (approximately proportional to the total range) can be adjusted (manually) until the required $I/\sigma(I)$ is reached. The plan generated by BEST over the user-defined range remains optimal.

split <number of plan entries >

The plan consist of entries that differ in scan speed and rotation range per frame. The variation depends on the anisotropy of the diffraction and geometrical limitations of the rotation range per frame. Neighbouring entries differ by least 20% in scan speed and/or 0.1 degree in range. There may be up to 72 entries. Each plan entry would correspond to a "data set" or a "segment" in terms of the data collection programs. Using this option one can enforce a simpler plan (e.g., feasible to input to a data collection GUI) for the costs of beamtime and data quality. In an extreme case of **split 1** the anisotropy is totally ignored and smallest scan interval allowed on the total range is applied over the whole range.

width <width of rot.[dg]>

Change allowable minimum of rotation width (the default is equal to 0.05 degree) and repeat prediction.

constant <resolution> <width of rotation [dg]> <exposure [s]>

Print predicted statistics for data collection with given resolution, constant exposure time and width of rotation. To be used (together with **phi <start> <end>**) to compare the predictions with the results using your old data.

end

end of the program job.

5. Examples (how to run BEST)

1. Single initial image, 10 s expose time, dose 300, Image plate detector (345 mm diameter - mar2300), interactive input, display plots

best -f mar2300 -t 10 -d 300 -i -g test_001.mar2300 test_001.x

2. Nine initial images

best -f mar2300 -t 10 -d 300 -i -g test_001.mar2300 test_00[1-9].x

3. Calculate the plan of data collection at resolution 2.5 Å, $I/\sigma(I)$ ratio=5, maximum number of plan entries = 4, minimisation of the absorbed dose

best -f mar2300 -t 10 -d 300 -q -r 2.5 -5 test_001.mar2300 test_00[1-9].x

4. To run BEST with the '.sca' file

best -f mar2300 -t 10 -d 300 -q -r 2.5 -5 -s test.sca test_001.mar2300 test_001.x

6. Example

Mitochondrial Isomerase, Space group: C2, a=101.2 Å b=79.6Å c=112.9Å beta=115.6°

Beam-line: X31 EMBL-Hamburg, MAR Image Plate detector, wavelength 1.5Å.

The aim was collect data set to a resolution better than 2Å.

12 hours was available for this measurement.

Initial images: Two images separated by rotation on 90^0 with exposure time 5 min (dose=10500), detector diameter 345 mm, detector-crystal distance 150 mm (maximal resolution 1.82Å), $\Delta\varphi$=1°.

Start BEST (with interactive input, display plots)

>> best -f mar2300 -t 300 -d 10500 -i -g ../init_001.mar2300 x/init_00*.x

```
 Program Best /A.Popov & G.Bourenkov/ Version 1.1 27.03.2003
------------------------------------------------------------------------
Relative n.of achievable unique reflections =100.00%
Shortest range for providing the 99% of overal achievable completeness
  for resolution from 12.00 to  7.31
      Phi_start = 10.00  Phi_finish =170.00
  for resolution from 12.00 to  1.82
      Phi_start = 74.00  Phi_finish =211.00
scal=  9.26  B-factor=  18.12 eigenvalues 16.22  17.10  22.03
------------------------------------------------------------------------

          Table (Option: total time is minimal)
          =====================================
(D.C.Time - total data collection time  E.Time - total exposure time)
Phi spliting to take account of anisotropy =   5 degree
Allowable minimum of rotation width = 0.05 degree
Relative Error of estimation for last shell =  4.94%
--------------------------------------------------------------
Phi_start =  74.0  Phi_finish = 211.0
Overall Completeness =  99.1% and  Redundancy =  2.81

                                Ratio (I/Sigma)
                   |<=================================================>|
                   |         3       |         5       |        10       |
 Resolution |      |-----------------|-----------------|-----------------|
    shell   |Compl.|D.C.Time  E.Time |D.C.Time  E.Time |D.C.Time  E.Time |
  [ Angst.] |  %   | h: min   h: min |  h: min   h: min| h: min   h: min |
------------|------|-----------------|-----------------|-----------------|
12.00  7.31 | 92.77|  0:33.2   0: 2.0|  0:34.6   0: 3.4|  0:38.5   0: 7.3|
 7.31  5.73 | 93.55|  0:35.6   0: 4.4|  0:38.7   0: 7.6|  0:47.8   0:16.6|
 5.73  4.87 | 96.15|  0:36.3   0: 3.4|  0:38.7   0: 5.9|  0:45.8   0:12.9|
 4.87  4.31 | 95.38|  0:38.1   0: 3.0|  0:40.3   0: 5.2|  0:46.6   0:11.4|
 4.31  3.90 | 97.12|  0:41.7   0: 3.8|  0:44.5   0: 6.6|  0:52.7   0:14.8|
 3.90  3.59 | 98.17|  0:45.4   0: 5.3|  0:49.3   0: 9.2|  1: 1.3   0:21.2|
 3.59  3.35 | 97.33|  0:49.7   0: 7.4|  0:55.4   0:13.1|  1:13.3   0:31.0|
 3.35  3.15 | 98.13|  0:56.4   0:11.2|  1: 5.4   0:20.2|  1:35.3   0:50.2|
 3.15  2.98 | 98.40|  1: 3.7   0:16.4|  1:17.3   0:29.9|  2: 4.6   1:17.3|
 2.98  2.84 | 98.48|  1:12.9   0:23.9|  1:33.8   0:44.7|  2:50.3   1:57.0|
 2.84  2.71 | 98.97|  1:24.9   0:32.0|  1:53.7   1: 0.8|  3:38.3   2:36.9|
 2.71  2.60 | 99.51|  1:37.0   0:41.9|  2:16.2   1:21.4|  4:37.0   3:27.3|
 2.60  2.50 | 99.11|  1:52.5   0:54.6|  2:47.7   1:47.0|  5:53.4   4:33.0|
 2.50  2.42 | 99.52|  2: 8.2   1: 8.0|  3:16.8   2:11.2|  7:18.3   5:46.5|
 2.42  2.34 | 99.62|  2:24.1   1:16.3|  3:43.6   2:33.6|  8:18.4   6:36.9|
```

All unique reflections can be measured. The total fraction of reflections located in the 'blind region' is equal to 0.

```
 2.34  2.27 |100.00|  2:42.6   1:32.5|  4:20.2   3: 4.0| 10: 4.6   8: 4.7|
 2.27  2.20 |100.00|  3: 6.6   1:53.7|  5: 6.4   3:43.3| 12:18.0   9:54.5|
 2.20  2.14 | 99.62|  3:41.5   2:16.4|  6:11.8   4:37.8| 15: 6.3  12:15.9|
 2.14  2.08 |100.00|  4:15.9   2:44.7|  7:14.6   5:33.9| 18: 4.7  14:50.1|
 2.08  2.03 |100.00|  5:12.0   3:25.5|  8:50.0   6:46.8| 21:55.2  18:12.6|
 2.03  1.99 |100.00|  6:22.2   4:23.3| 10:58.9   8:35.5| 27:26.9  23: 1.3|
 1.99  1.94 |100.00|  7:58.6   5:50.0| 14:18.1  11:35.2| 36:57.0  31:30.9|
 1.94  1.90 |100.00| 10:26.7   7:44.4| 18:43.5  15:18.0| 48:44.9  42:14.1|
 1.90  1.86 |100.00| 12:56.4   9:44.2| 23:29.3  19:25.7| 61:59.5  54:14.8|
 1.86  1.82 |100.00| 16:55.0  12:59.0| 31:26.8  26:20.2| 84:45.9  74:53.9|
-------------------------------------------------------------------------
```

Total time of data collection to achieve I/Sigma=3 at resolution shell 1.86-1.82 Å is equal to 16 hours and 55 min

Total exposure time

We have decided to look how long a data collection will take if I/Sigma is about 2 in highest resolution shell

```
    ->>>Please give instruction (h - help) <<<-
h
```

To get the list of options, print ‘h’

```
plan  <resolution>  <I/Sigma>
======> Plan of data collection to achieve given resolution limit and statistic
             ( I/Sigma in the highest resol.shell has to be 3, 5, or 10)
stat
======>  Print statistics correspond the plan
isigi  <number1> <number2> <number3>
======>  Change I/Sigma values and repeat prediction
phi  <phi_start> <phi_final>
======> Change start Phi and oscillation range and repeat prediction
split <n.of small intervals>
======> Change maximum number of plan entries and repeat prediction
width <width of rot.[dg]>
======> Change allowable minimum of rotation width  and repeat prediction
constant  <resol.> <width of rot.[dg]> <exposure [s]> <detect.diameter>
======> Statistics achieved by collecting data with constant exposure and Delta_Phi
             detect.diameter 345.0  300.0  240.0  180.0
end
======> The end of the program job

    ->>>Please give instruction (h - help) <<<-
isigi 1 2 3
```

Ask BEST to change I/Sigma values

```
          Table (Option: total time is minimal)
          =====================================
(D.C.Time - total data collection time  E.Time - total exposure time)
Phi spliting to take account of anisotropy =   5 degree
Allowable minimum of rotation width = 0.05 degree
Relative Error of estimation for last shell =  2.45%
--------------------------------------------------------------
Phi_start =  74.0  Phi_finish = 211.0
Overall Completeness =  99.1% and  Redundancy =  2.81

                                Ratio (I/Sigma)
                   |<==================================================>|
                   |         1        |         2        |         3        |
 Resolution |      |------------------|------------------|------------------|
    shell   |Compl.|D.C.Time   E.Time |D.C.Time   E.Time |D.C.Time   E.Time |
  [Angst.]  |  %   | h: min    h: min | h: min    h: min| h: min    h: min |
------------|------|------------------|------------------|------------------|
12.00  7.31 | 92.77|  0:31.8   0: 0.6|  0:32.5   0: 1.3|  0:33.2   0: 2.0|
 7.31  5.73 | 93.55|  0:32.6   0: 1.4|  0:34.1   0: 2.9|  0:35.6   0: 4.4|
 5.73  4.87 | 96.15|  0:34.0   0: 1.1|  0:35.1   0: 2.2|  0:36.3   0: 3.4|
 4.87  4.31 | 95.38|  0:36.1   0: 1.0|  0:37.1   0: 2.0|  0:38.1   0: 3.0|
 4.31  3.90 | 97.12|  0:39.1   0: 1.2|  0:40.4   0: 2.5|  0:41.7   0: 3.8|
 3.90  3.59 | 98.17|  0:41.8   0: 1.7|  0:43.6   0: 3.4|  0:45.4   0: 5.3|
```

```
 3.59  3.35 | 97.33|  0:44.6   0: 2.3|  0:47.1   0: 4.8|  0:49.7   0: 7.4|
 3.35  3.15 | 98.13|  0:48.7   0: 3.5|  0:52.4   0: 7.2|  0:56.4   0:11.2|
 3.15  2.98 | 98.40|  0:52.3   0: 5.0|  0:57.7   0:10.4|  1: 3.7   0:16.4|
 2.98  2.84 | 98.48|  0:56.2   0: 7.1|  1: 4.1   0:15.1|  1:12.9   0:23.9|
 2.84  2.71 | 98.97|  1: 2.4   0: 9.4|  1:13.0   0:20.0|  1:25.0   0:32.0|
 2.71  2.60 | 99.51|  1: 7.1   0:12.0|  1:21.0   0:25.9|  1:37.0   0:41.9|
 2.60  2.50 | 99.11|  1:13.0   0:15.2|  1:31.1   0:33.2|  1:52.5   0:54.6|
 2.50  2.42 | 99.52|  1:18.1   0:18.4|  1:40.6   0:40.9|  2: 8.2   1: 8.5|
 2.42  2.34 | 99.62|  1:24.5   0:21.6|  1:51.7   0:48.8|  2:25.8   1:22.5|
 2.34  2.27 |100.00|  1:31.7   0:25.9|  2: 5.4   0:59.6|  2:47.6   1:39.8|
 2.27  2.20 |100.00|  1:40.0   0:30.6|  2:20.9   1:11.5|  3:13.7   2: 0.3|
 2.20  2.14 | 99.62|  1:53.5   0:37.5|  2:45.2   1:28.6|  3:50.3   2:29.4|
 2.14  2.08 |100.00|  2: 5.0   0:44.6|  3: 6.8   1:46.4|  4:23.3   2:58.2|
 2.08  2.03 |100.00|  2:21.9   0:57.5|  3:44.3   2:19.7|  5:29.5   3:55.0|
 2.03  1.99 |100.00|  2:40.9   1:13.7|  4:29.3   2:58.4|  6:48.6   5: 4.1|
 1.99  1.94 |100.00|  3: 7.1   1:38.1|  5:39.1   3:59.1|  8:45.5   6:49.5|
 1.94  1.90 |100.00|  3:48.6   2:12.7|  7:17.2   5:27.2| 11:41.9   9:24.1|
 1.90  1.86 |100.00|  4:31.9   2:44.3|  8:50.3   6:46.6| 14:28.7  11:48.7|
 1.86  1.82 |100.00|  5:38.7   3:39.0| 11:31.1   9: 3.6| 18:57.0  15:39.5|
--------------------------------------------------------------------------
```

We do not have more than 12 hours for data collection, so the best statistic, which we can achieve, will be I/Sigma = 2 in the shell of resolution 1.82 Å

Ask BEST to print the plan of data collection and the data statistics that will be collected according to the plan (resolution =1.82Å, I/Sigma=2)

```
    ->>>Please give instruction (h - help) <<<-
plan 1.82 2

               Optimal  plan of data collection
               ================================
Resol. = 1.82   I/Sigma = 2 Overal Complet. =  99.1%  Redund. =  2.81
Total Data Collection time=  691.1 min ( 11.52 hour)
---------------------------------------------------------------------------
 N|phi_strt|n.of.img|width|   dose  |distans|det.diam|overlap|tot.time (s)|
---------------------------------------------------------------------------
 1   74.00     15    0.65    7094.94  104.6   240.0     No        2696.4
 2   83.75     49    0.52    9763.18   78.1   180.0     No        8773.6
 3  109.23     48    0.63    8884.08  104.6   240.0     No        9979.8
 4  139.47      5    0.94    7717.79  151.0   345.0     No        1436.4
 5  144.17     26    1.37    8115.32  151.0   345.0     No       10339.1
 6  179.79     10    1.49    7376.73  151.0   345.0     No        3940.4
 7  194.69     11    1.60    6807.15  151.0   345.0     No        4303.0
---------------------------------------------------------------------------
```

The plan has 7 entries. We can simplify the plan by reducing of number of plan segments.

Change the number of plan segments (not more then 3)

```
    ->>>Please give instruction (h - help) <<<-
split 3

          Table (Option: total time is minimal)
          =====================================
(D.C.Time - total data collection time  E.Time - total exposure time)
Phi spliting to take account of anisotropy =  60 degree
Allowable minimum of rotation width = 0.05 degree
Relative Error of estimation for last shell =  1.17%
--------------------------------------------------------------
Phi_start =  74.0  Phi_finish = 211.0
Overall Completeness =  99.1% and  Redundancy =  2.81

                                Ratio (I/Sigma)
```

```
                   |<===================================================>|
                   |         1       |         2       |         3       |
 Resolution |      |-----------------|-----------------|-----------------|
    shell   |Compl.|D.C.Time  E.Time |D.C.Time  E.Time |D.C.Time  E.Time |
  [Angst.]  |  %   | h: min   h: min | h: min   h: min| h: min   h: min |
------------|------|-----------------|-----------------|-----------------|
12.00  7.31 | 92.77|  0:30.1   0: 0.6|  0:30.8   0: 1.3|  0:31.4   0: 2.0|
 7.31  5.73 | 93.55|  0:30.9   0: 1.4|  0:32.3   0: 2.9|  0:33.8   0: 4.4|
 5.73  4.87 | 96.15|  0:33.4   0: 1.1|  0:34.5   0: 2.2|  0:35.7   0: 3.4|
 4.87  4.31 | 95.38|  0:35.5   0: 1.0|  0:36.5   0: 1.9|  0:37.5   0: 3.0|
 4.31  3.90 | 97.12|  0:38.6   0: 1.2|  0:39.9   0: 2.5|  0:41.2   0: 3.8|
 3.90  3.59 | 98.17|  0:41.3   0: 1.6|  0:43.0   0: 3.4|  0:44.8   0: 5.2|
 3.59  3.35 | 97.33|  0:50.2   0: 2.4|  0:52.7   0: 4.9|  0:55.4   0: 7.5|
 3.35  3.15 | 98.13|  0:53.6   0: 3.5|  0:57.3   0: 7.2|  1: 1.3   0:11.2|
 3.15  2.98 | 98.40|  0:57.4   0: 5.0|  1: 2.8   0:10.4|  1: 8.6   0:16.2|
 2.98  2.84 | 98.48|  1: 1.9   0: 7.2|  1: 9.7   0:15.0|  1:18.2   0:23.6|
 2.84  2.71 | 98.97|  1:13.3   0: 9.5|  1:23.6   0:19.8|  1:34.8   0:31.0|
 2.71  2.60 | 99.51|  1:18.1   0:12.0|  1:31.3   0:25.2|  1:46.1   0:40.0|
 2.60  2.50 | 99.11|  1:23.6   0:15.2|  1:40.7   0:32.3|  2: 0.1   0:51.7|
 2.50  2.42 | 99.52|  1:28.9   0:18.3|  1:49.9   0:39.3|  2:14.1   1: 3.5|
 2.42  2.34 | 99.62|  1:39.4   0:21.7|  2: 4.5   0:46.8|  2:33.7   1:16.0|
 2.34  2.27 |100.00|  1:45.0   0:25.2|  2:15.3   0:55.5|  2:50.8   1:31.0|
 2.27  2.20 |100.00|  1:52.9   0:29.7|  2:29.1   1: 6.0|  3:12.6   1:49.5|
 2.20  2.14 | 99.62|  2:25.9   0:38.3|  3:14.0   1:26.4|  4:13.3   2:25.7|
 2.14  2.08 |100.00|  2:36.3   0:45.9|  3:36.0   1:45.6|  4:50.0   2:58.8|
 2.08  2.03 |100.00|  2:55.6   1: 0.0|  4:16.2   2:20.7|  5:59.2   4: 1.3|
 2.03  1.99 |100.00|  3:27.8   1:14.4|  5: 6.1   2:51.8|  7: 7.7   4:51.0|
 1.99  1.94 |100.00|  3:55.6   1:38.3|  6:10.5   3:50.8|  9: 2.2   6:39.3|
 1.94  1.90 |100.00|  4:35.2   2:14.3|  7:47.8   5:23.0| 12: 4.8   9:33.7|
 1.90  1.86 |100.00|  5:17.7   2:50.9|  9:34.1   7: 4.0| 15:33.0  12:46.4|
 1.86  1.82 |100.00|  6:31.5   3:52.6| 12:49.6  10: 6.7| 21:37.5  18:10.8|
-------------------------------------------------------------------------

    ->>>Please give instruction (h - help) <<<-
```

pla 1.82 2

Again ask BEST to print the plan of data collection and the data statistics at the resolution =1.94Å and I/Sigma=2

```
               Optimal  plan of data collection
               ================================
Resol. = 1.82   I/Sigma = 2 Overal Complet. =  99.1%  Redund. =  2.81
Total Data Collection time=  769.6 min ( 12.83 hour)
---------------------------------------------------------------------------
 N|phi_strt|n.of.img|width|   dose  |distans|det.diam|overlap|tot.time (s)|
---------------------------------------------------------------------------
 1   74.00     120    0.50   10084.75   78.1   180.0     No       21368.1
 2  134.00     102    0.59    9311.68  104.6   240.0     No       20906.8
 3  194.18      10    1.70    6384.56  151.0   345.0     No        3901.1
-------------------------------------------------------------------------
```

The plan of optimal data collection consists of three segments according to behaviour of diffraction anisotropy and geometrical restrictions. Pay attention! BEST proposes the use a different detector diameter and crystal to detector distances for data collection runs. No overlaps will occur.

```
    ->>>Please give instruction (h - help) <<<-
```

stat

Print the prediction of data collection statistics

```
                   Statistical prediction
                   ======================
------------------------------------------------------------------------------------------
 Resolution      Average                             %  with I / Sigma less than     Overload
Lower Upper  Intensity  Error  I/Sigma  R-fact     1     2     3      5    10     20      %
------------------------------------------------------------------------------------------
12.00  7.31      9322.1   236.4   39.4     2.9     0.8   1.3   1.8   2.7   4.8   9.6   0.00
 7.31  5.73      4912.6   136.1   36.1     3.2     1.5   2.5   3.5   5.3   9.9  20.0   0.00
 5.73  4.87      6264.2   172.9   36.2     3.1     1.2   2.2   3.1   4.8   9.0  18.7   0.00
 4.87  4.31      8757.6   234.8   37.3     3.1     1.0   1.8   2.5   4.0   7.5  15.8   0.00
 4.31  3.90      8126.3   224.5   36.2     3.2     1.1   2.0   2.9   4.6   8.9  18.8   0.00
```

3.90	3.59	6684.4	196.4	34.0	3.3	1.5	2.7	3.9	6.2	11.9	24.6	0.00
3.59	3.35	5286.8	167.9	31.5	3.6	1.8	3.4	4.9	7.9	15.2	31.2	0.00
3.35	3.15	3884.9	140.2	27.7	4.1	2.6	4.8	6.9	10.9	20.7	40.8	0.00
3.15	2.98	2882.0	119.9	24.0	4.7	3.2	6.0	8.7	14.0	26.4	50.2	0.00
2.98	2.84	2183.1	105.8	20.6	5.4	4.2	7.8	11.2	17.8	32.8	59.5	0.00
2.84	2.71	1707.7	95.2	17.9	6.3	4.9	9.3	13.5	21.3	38.6	67.0	0.00
2.71	2.60	1419.9	91.6	15.5	7.1	6.0	11.2	16.2	25.3	44.7	74.0	0.00
2.60	2.50	1203.5	88.1	13.7	8.1	6.8	12.9	18.5	28.8	50.1	79.3	0.00
2.50	2.42	1049.5	86.9	12.1	9.1	7.9	14.8	21.2	32.7	55.4	83.8	0.00
2.42	2.34	934.9	86.7	10.8	10.2	8.9	16.7	23.8	36.3	60.2	87.3	0.00
2.34	2.27	837.6	86.8	9.7	11.4	10.1	18.8	26.6	40.1	64.7	90.1	0.00
2.27	2.20	754.2	87.4	8.6	12.7	11.2	20.9	29.4	44.0	69.2	92.5	0.00
2.20	2.14	655.1	87.9	7.5	14.8	13.0	23.9	33.5	49.3	74.8	94.9	0.00
2.14	2.08	571.9	88.0	6.5	16.9	14.9	27.2	37.7	54.4	79.5	96.5	0.00
2.08	2.03	481.1	87.4	5.5	19.7	17.5	31.5	43.1	60.7	84.6	97.9	0.00
2.03	1.99	399.5	85.9	4.6	23.3	20.3	36.2	48.8	67.0	89.0	98.8	0.00
1.99	1.94	324.1	83.4	3.9	27.9	24.0	41.8	55.3	73.5	92.6	99.4	0.00
1.94	1.90	258.7	83.2	3.1	34.6	29.1	49.2	63.4	80.8	95.8	99.7	0.00
1.90	1.86	209.7	81.4	2.6	42.5	34.0	55.8	70.2	86.1	97.6	99.9	0.00
1.86	1.82	169.9	83.6	2.0	52.5	40.9	64.4	78.2	91.4	98.9	100.0	0.00
All data		1903.5	107.0	17.8	6.2	13.7	23.8	31.7	43.2	60.0	76.4	0.00

```
------------------------------------------------------------------------------------------

   ->>>Please give instruction (h - help) <<<-
```

stop