Running d*TREK from the command line...

```
[prepare header]
dtextractheader image start.head
[update beam ctr] this is in pixels in start.head

dtfind start.head -seq 1 1 -sigma 3 -min 50 -filter 6 -out find.head
dtindex find.head dtfind.ref -maxresid 3.0 -sigma 5.0 -dps -nodiffs

... gives ...

FIND

dtfind:  Copyright (c) 1996 Molecular Structure Corporation
d*TREK version 9.5L -- Oct  4 2005
Command line:
 dtfind start.head -seq 1 1 -sigma 3 -min 50 -filter 6 -out find.head

     Header of file start.head successfully read.
A4_NONUNF_TYPE: >>Simple_mask<<
INFO in Cnonunf: using
     ../12287/12287_1_E1_001.img
     as the simple mask/nonunf file, was FirstScanImage.

     File ../12287/12287_1_E1_001.img successfully opened.
Min raw image pixel OK value in mask/nonunf/image file: 1


Command line string: >>-seq<<
Command line string: >>-sigma<<
Command line string: >>-min<<
Command line string: >>-filter<<
Command line string: >>-out<<

Resolution limits of an image are 979.65 to 1.37426
Resolution limits of peak search are 979.65 to 1.37426


dtfind: 2D method  used
...reading image ../12287/12287_1_E1_001.img...

     File ../12287/12287_1_E1_001.img successfully opened.
Find object listing:
     Sigma: 3
Resolution: 979.65 to 1.37426
   Minimum: 50
Circle lim: 1024, 1024, 0, 1448
  Rect lim: 20, 20, 2028, 2028
Spot wind.: 0, 0
Peak filt.: 6
```

```
Back. tile: 128, 128
 Seq. num.: 1, 1
Image dim.: 2048, 2048
   3D dump: 0
1339 preliminary spots found in 2D search with rotation angle 290.5 degs.

dtfind: There were 1074 spots found.
There were 1074 preliminary spots of which 4 were marked as saturated,
 or  0.37% of them.
Number of reflections written in 'dtfind.ref': 1074
dtfind: Spots written to dtfind.ref
dtfind - Wrote header file find.head

INDEX


dtindex:  Copyright (c) 1998, 1996 Molecular Structure Corporation
d*TREK version 9.5L -- Oct  4 2005
Command line:
 dtindex find.head dtfind.ref -maxresid 3.0 -sigma 5 -dps -nodiffs

     Header of file find.head successfully read.
Reflection list: dtfind.ref
Creflnlist::nRead with filename: dtfind.ref
INFO in Creflnlist::nRead, EOF after 1074 reflections read in
                                    (1074 total now in list).
Command line string: >>-maxresid<<
Command line string: >>-sigma<<
Command line string: >>-dps<<
Command line string: >>-nodiffs<<
INFO: deleted 0 reflns outside of resolution bounds.
      This leaves 1074 reflns for indexing.

INFO: 418 reflns deleted out of 1074 that might be in ice rings.
Max cell length allowed for reciprocal lattice vectors: 256.219


Method:     1D FFT with DPS algorithm
Out header: dtindex.head
Max cell:   256.219
Num vecs:   1000
Spacegroup: 0
Verbose:    1

Performing 1D FFT indexing (not cell reduction) with the DPS algorithm...see
  Steller, Bolotovsky, & Rossmann (1997) J. Appl. Cryst. 30, 1036-1040.

Max cell is:         256.219
Number of reflections/vectors used: 588
```

```
.....................................
...refining best 30 directions and lengths...
.............................  done.
Number of vectors used for integer residual calculation: 588
```

a	b	c	alpha	beta	gamma	Volume	Remarks	#Indexed	%Residual
196.09	52.05	51.42	90.02	122.45	104.58	422661	Okay	435	0.265
51.42	196.09	52.05	104.58	90.02	122.45	422661	Okay	435	0.265
52.05	51.42	196.09	122.45	104.58	90.02	422661	Okay	435	0.265
51.49	187.73	52.08	122.68	90.13	90.69	423682	Okay	432	0.268
187.73	52.08	51.49	90.13	90.69	122.68	423682	Okay	432	0.268
52.08	51.49	187.73	90.69	122.68	90.13	423682	Okay	432	0.268
51.42	196.09	73.15	123.80	45.36	122.45	422658	Okay	435	0.265
196.09	73.15	51.42	45.36	122.45	123.80	422661	Okay	435	0.265
73.15	51.42	196.09	122.45	123.80	45.36	422661	Okay	435	0.265
196.09	52.05	73.15	44.66	123.80	104.58	422661	Okay	435	0.265
52.05	73.15	196.09	123.80	104.58	44.66	422661	Okay	435	0.265
73.15	196.09	52.05	104.58	44.66	123.80	422661	Okay	435	0.265
73.15	51.50	187.74	90.69	113.13	45.40	423887	Okay	428	0.264
187.74	73.15	51.50	45.40	90.69	113.13	423887	Okay	428	0.264
51.50	187.74	73.15	113.13	45.40	90.69	423887	Okay	428	0.264
187.73	196.09	51.43	122.45	90.70	34.89	422913	Okay	437	0.274
73.15	187.71	52.06	122.67	44.67	113.16	422954	Okay	433	0.265
187.71	52.06	73.15	44.67	113.16	122.67	422954	Okay	433	0.265
52.06	73.15	187.71	113.16	122.67	44.67	422954	Okay	433	0.265

```
Executing beam refinement with
beam search radius, acceptable shift radius: 10 9 ...
A4_NONUNF_TYPE: >>Simple_mask<<
INFO in Cnonunf: using
     ../12287/12287_1_E1_001.img
     as the simple mask/nonunf file, was FirstScanImage.

     File ../12287/12287_1_E1_001.img successfully opened.
Min raw image pixel OK value in mask/nonunf/image file: 1
Original (input header) beam center: [1030.0 1066.0]

First Pass.  Search dim0 in [1020 1040] dim1 in [1056 1076]
.........................................
Second Pass.  Search dim0 in [1036 1038] dim1 in [1061 1063]
Calculated pre-reduced cell solution is in agreement with detector beam center!
Original (input header) beam center: [1030.0 1066.0]
New      (calculated)   beam center: [1036.5 1061.4]
Header updated to reflect beam center change.

WARNING!: Beam position moved more than 5 pixels!
=======
```

```
INFO: Restart with adjusted beam center.
Max cell length allowed for reciprocal lattice vectors: 256.219


Method:     1D FFT with DPS algorithm
Out header: dtindex.head
Max cell:   256.219
Num vecs:   1000
Spacegroup: 0
Verbose:    1

Performing 1D FFT indexing (not cell reduction) with the DPS algorithm...see
  Steller, Bolotovsky, & Rossmann (1997) J. Appl. Cryst. 30, 1036-1040.

Max cell is:         256.219
Number of reflections/vectors used: 588
.................................
...refining best 30 directions and lengths...
.............................  done.
Number of vectors used for integer residual calculation: 588
```

a	b	c	alpha	beta	gamma	Volume	Remarks	#Indexed	%Residual
174.05	166.20	157.98	18.20	24.83	17.27	423646	Okay	394	0.060
166.20	157.98	174.05	24.83	17.27	18.20	423646	Okay	394	0.060
157.99	166.21	174.09	39.69	24.82	18.19	423539	Okay	392	0.060
158.00	166.21	73.10	102.74	89.98	18.19	423234	Okay	388	0.059
157.98	195.63	73.09	55.96	89.99	36.17	423560	Okay	395	0.061
157.98	166.21	51.67	90.00	90.09	18.20	423833	Okay	389	0.059
166.21	51.67	157.98	90.09	18.20	90.00	423834	Okay	389	0.059
51.67	157.98	166.21	18.20	90.00	90.09	423834	Okay	389	0.059
51.64	195.60	157.98	36.17	90.09	58.27	423209	Okay	385	0.059
157.98	51.64	195.60	58.27	36.17	90.09	423209	Okay	385	0.059
195.60	157.98	51.64	90.09	58.27	36.17	423209	Okay	385	0.059
51.66	157.99	174.06	24.83	107.28	90.08	423467	Okay	396	0.061
174.06	51.66	157.99	90.08	24.83	107.28	423468	Okay	396	0.061
157.99	174.06	51.66	107.28	90.08	24.83	423472	Okay	396	0.061
158.00	51.64	174.09	72.86	24.83	90.07	423231	Okay	383	0.059
174.09	158.00	51.64	90.07	72.86	24.83	423232	Okay	383	0.059
51.64	174.09	158.00	24.83	90.07	72.86	423231	Okay	383	0.059
73.09	157.99	51.66	90.08	45.23	89.99	423468	Okay	396	0.061
157.99	51.66	73.09	45.23	89.99	90.08	423468	Okay	396	0.061
51.66	73.09	157.99	89.99	90.08	45.23	423468	Okay	396	0.061
174.06	166.20	73.09	102.75	114.82	17.26	423434	Okay	396	0.061
174.10	166.21	73.09	102.75	65.16	39.69	423362	Okay	393	0.060
73.10	166.20	51.64	90.03	45.22	102.75	423344	Okay	393	0.060
166.20	51.64	73.10	45.22	102.75	90.03	423344	Okay	393	0.060
51.64	73.10	166.20	102.75	90.03	45.22	423345	Okay	393	0.060
51.66	73.09	195.63	55.96	58.26	45.23	423468	Okay	396	0.061

```
 73.09 195.63  51.66  58.26  45.23  55.96   423468     Okay      396     0.061
195.63  51.66  73.09  45.23  55.96  58.26   423468     Okay      396     0.061
174.06  51.66  73.09  45.23 114.82 107.28   423468     Okay      396     0.061
 73.09 174.06  51.66 107.28  45.23 114.82   423468     Okay      396     0.061
 51.66  73.09 174.06 114.82 107.28  45.23   423468     Okay      396     0.061
 73.09 174.09  51.65  72.88  45.23  65.16   423432     Okay      396     0.061
 51.65  73.09 174.09  65.16  72.88  45.23   423432     Okay      396     0.061
174.09  51.65  73.09  45.23  65.16  72.88   423432     Okay      396     0.061


Least square fit to lattice characters...see
  Andrews & Bernstein (1988) Acta Cryst. A44, 1009-1018 and
  Paciorek & Bonin (1992) J. Appl. Cryst. 25, 632-637.
.....................................................
.....................................................
done.

Least-squares fit of reduced primitive cell to 44 lattice characters
sorted on decreasing (highest to lowest) symmetry.
Only solutions with residuals <=   3.0 are listed.
=======================================================================
 Soln  LeastSq Spgrp Cent    Bravais type         a         b         c
  num residual  num* type     Cell volume     alpha      beta     gamma
=======================================================================
   7     0.190    75    P      tetragonal    51.796    51.796   157.982
                                   423844    90.000    90.000    90.000

   9     0.166    21    C    orthorhombic    73.093    73.409   157.982
                                   847680    90.000    90.000    90.000

  11     0.175    16    P    orthorhombic    51.669    51.923   157.982
                                   423839    90.000    90.000    90.000

  12     0.064     5    C      monoclinic    73.691    73.168   157.982
                                   851816    90.000    90.141    90.000

  12b    0.075     5    C      monoclinic    73.409    73.093   157.982
                                   847678    90.000    90.131    90.000

  13     0.092     3    P      monoclinic    51.923    51.669   157.982
                                   423838    90.000    90.100    90.000

  14     0.000     1    P       triclinic    51.669    51.923   157.982
                                   423834    89.900    89.915    89.753

=======================================================================
*Suggested spacegroup number until systematic absences are examined.
...determining orientation angles...
.
```

Unit cell parameters and orientation angles

Num	Integer residual	a alpha	b beta	c gamma	Rot1	Rot2	Rot3
1	0.001	51.796 90.000	51.796 90.000	157.982 90.000	-75.915	20.479	-78.321
2	0.001	51.796 90.000	51.796 90.000	157.982 90.000	75.915	-20.479	101.679
3	0.001	51.796 90.000	51.796 90.000	157.982 90.000	104.085	20.479	-78.321
4	0.001	51.796 90.000	51.796 90.000	157.982 90.000	-104.085	-20.479	101.679
5	0.001	51.796 90.000	51.796 90.000	157.982 90.000	56.911	65.317	66.033
6	0.001	51.796 90.000	51.796 90.000	157.982 90.000	-56.911	-65.317	-113.967
7	0.001	51.796 90.000	51.796 90.000	157.982 90.000	-123.089	65.317	66.033
8	0.001	51.796 90.000	51.796 90.000	157.982 90.000	123.089	-65.317	-113.967

The above table shows symmetry EQUIVALENT crystal orientation angles for the indexing orientation. All the solutions are equivalent for the selected Bravais lattice. The default selection usually has the values closest to crystal orientation found in the input .head file or the one where (|Rot1| + |Rot2| + |Rot3|) is a minimum.
Orientation angles choice 1 selected.

Crystal listing:

```
 Unit cell lengths:   51.7964   51.7964  157.9819
 Unit cell  angles:   90.0000   90.0000   90.0000
 Unit cell  volume: 423843.915
Orientation angles:  -75.9149   20.4794  -78.3208
         Mosaicity:     0.300
       Description: unknown

Spacegroup number: 75
             name: P4
```

```
Num. equiv. posns: 4
dtindex - Wrote header file dtindex.head
```