```
dtindex:  Copyright (c) 1998, 1996 Molecular Structure Corporation
d*TREK version 8.0SSI -- Oct 31 2003
Command line:
 dtindex input.head dtfind.ref -dps -sigma 5.000000 -reso 100.00 3.00 ¥
    -diffs -nodeice -maxresid 3.00 -prompt -nobeamcheck -out ¥
    output.head
     Header of file input.head successfully read.
Reflection list: dtfind.ref
CrefInlist::nRead with filename: dtfind.ref
INFO in CrefInlist::nRead, EOF after 129 reflections read in
                                    (129 total now in list).
Command line string: >>-dps<<
Command line string: >>-sigma<<
Command line string: >>-reso<<
Command line string: >>-diffs<<
Command line string: >>-nodeice<<
Command line string: >>-maxresid<<
Command line string: >>-prompt<<
Command line string: >>-nobeamcheck<<
Command line string: >>-out<<
Max cell length allowed for reciprocal lattice vectors: 355.8
...calculating difference vectors...


Method:     1D FFT with DPS algorithm
Out header: output.head
Max cell:   355.8
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: 355.8

Number of reflections/vectors used: 414

.....

...refining best 30 directions and lengths...

..... done.

Number of vectors used for integer residual calculation: 414

a	b	c	alpha	beta	gamma	Volume	Remarks	#Indexed	%Residual
73.82	103.35	31.79	90.88	90.09	44.73	170636	Okay	104	1.626
31.79	73.82	103.35	44.73	90.88	90.09	170636	Okay	104	1.626
31.79	164.22	103.35	18.44	90.88	90.59	170636	Okay	104	1.626
164.22	103.35	31.79	90.88	90.59	18.44	170636	Okay	104	1.626
166.92	103.33	31.78	90.86	79.59	21.54	170572	Okay	114	2.815
31.78	166.92	103.33	21.54	90.86	79.59	170572	Okay	114	2.815
73.82	107.66	31.79	73.71	90.09	47.04	170636	Okay	104	1.626
31.79	73.82	107.66	47.04	73.71	90.09	170636	Okay	104	1.626
107.66	31.79	73.82	90.09	47.04	73.71	170636	Okay	104	1.626
164.20	107.66	31.78	73.70	90.56	24.81	170567	Okay	104	1.626
31.78	164.20	107.66	24.81	73.70	90.56	170567	Okay	104	1.626
31.79	73.82	108.59	47.42	107.90	90.09	170636	Okay	104	1.626
73.82	108.59	31.79	107.90	90.09	47.42	170636	Okay	104	1.626
108.59	31.79	73.82	90.09	47.42	107.90	170636	Okay	104	1.626
107.66	31.77	166.91	79.55	18.87	73.67	170499	Okay	114	2.795
31.77	166.91	107.66	18.87	73.67	79.55	170499	Okay	114	2.795
166.91	107.66	31.77	73.67	79.55	18.87	170499	Okay	114	2.795
31.79	164.22	108.59	25.06	107.90	90.59	170636	Okay	104	1.626
108.59	31.79	164.22	90.59	25.06	107.90	170636	Okay	104	1.626
164.22	108.59	31.79	107.90	90.59	25.06	170636	Okay	104	1.626
167.01	108.55	31.79	107.84	79.56	33.63	170585	Okay	104	1.664
108.55	31.79	167.01	79.56	33.63	107.84	170585	Okay	104	1.664

31.79	167.01	108.55	33.63	107.84	79.56	170585	Okay	104	1.664
73.82	103.35	107.66	17.17	47.04	44.73	170636	Okay	104	1.626
164.22	103.35	107.66	17.17	24.82	18.44	170636	Okay	104	1.626
108.59	103.35	73.82	44.73	47.42	17.02	170636	Okay	104	1.626
73.82	108.59	103.35	17.02	44.73	47.42	170636	Okay	104	1.626
108.59	103.35	164.22	18.44	25.06	17.02	170636	Okay	104	1.626
108.56	103.33	166.92	21.54	33.65	17.02	170573	Okay	114	2.815
73.82	120.50	31.79	59.04	90.09	52.52	170636	Okay	104	1.626
31.79	73.82	120.50	52.52	59.04	90.09	170636	Okay	104	1.626
120.50	31.79	73.82	90.09	52.52	59.04	170636	Okay	104	1.626
120.50	31.79	164.22	90.59	36.09	59.04	170636	Okay	104	1.626
31.79	164.22	120.50	36.09	59.04	90.59	170636	Okay	104	1.626
164.22	120.50	31.79	59.04	90.59	36.09	170636	Okay	104	1.626
31.77	166.92	120.50	26.72	59.02	79.55	170441	Okay	114	2.785
166.92	120.50	31.77	59.02	79.55	26.72	170441	Okay	114	2.785
120.50	31.77	166.92	79.55	26.72	59.02	170441	Okay	114	2.785
31.79	73.82	164.22	26.29	90.59	90.09	170636	Okay	104	1.626
73.82	164.22	31.79	90.59	90.09	26.29	170636	Okay	104	1.626
164.22	31.79	73.82	90.09	26.29	90.59	170636	Okay	104	1.626
166.91	31.77	73.78	90.00	28.16	79.55	170499	Okay	104	1.625
31.77	73.78	166.91	28.16	79.55	90.00	170499	Okay	104	1.625
73.78	166.91	31.77	79.55	90.00	28.16	170499	Okay	104	1.625
166.92	73.79	103.33	44.75	21.54	28.17	170572	Okay	104	1.626
164.22	107.66	73.82	47.04	26.29	24.82	170636	Okay	104	1.626
73.82	164.22	107.66	24.82	47.04	26.29	170636	Okay	104	1.626
108.59	164.22	73.82	26.29	47.42	25.06	170636	Okay	104	1.626
164.22	73.82	108.59	47.42	25.06	26.29	170636	Okay	104	1.626
166.91	120.51	73.78	52.49	28.16	26.73	170499	Okay	104	1.625

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 num	LeastSq residual	Spgrp num*	Cent type	Bravais type Cell volume	a alpha	b beta	c gamma
7	2.048	75	P	tetragonal 170623	73.277 90.000	73.277 90.000	31.777 90.000
9	1.898	21	C	orthorhombic 341242	103.344 90.000	103.913 90.000	31.777 90.000
11	1.464	16	P	orthorhombic 170605	31.777 90.000	72.745 90.000	73.805 90.000
12	1.391	5	C	monoclinic 351294	103.392 90.000	103.102 90.321	32.955 90.000
12b	1.699	5	C	monoclinic 341242	103.344 90.000	103.913 90.000	31.777 90.000
13	0.725	3	P	monoclinic 170569	31.777 90.000	73.805 91.182	72.745 90.000
13b	0.770	3	P	monoclinic 170569	31.777 90.000	73.805 91.182	72.745 90.000
14	0.000	1	P	triclinic	31.777	72.745	73.805

170567 90.314 90.043 91.182

==========

*Suggested spacegroup number until systematic absences are examined.

To view least-squares fits to other lattices,
enter a new residual between 17 and 100 at the following prompt.
Enter solution number of your choice (1-14)
or new max residual (>=17) or get lattice listing (L)
<Enter> or <cr> will select the 'P tetragonal' lattice.
...determining orientation angles...
.

Unit cell parameters and orientation angles

Num	Integer residual	a alpha	b beta	c gamma	Rot1	Rot2	Rot3
1	0.001	73.277 90.000	73.277 90.000	31.777 90.000	-178.539	-3.934	48.568
2	0.001	73.277 90.000	73.277 90.000	31.777 90.000	178.539	3.934	-131.432
3	0.001	73.277 90.000	73.277 90.000	31.777 90.000	1.461	-3.934	48.568
4	0.001	73.277 90.000	73.277 90.000	31.777 90.000	-1.461	3.934	-131.432
5	0.001	73.277 90.000	73.277 90.000	31.777 90.000	-176.065	1.457	-41.332

```
  6      0.001     73.277     73.277     31.777   176.065    -1.457   138.668
                   90.000     90.000     90.000

  7      0.001     73.277     73.277     31.777     3.935     1.457   -41.332
                   90.000     90.000     90.000

  8      0.001     73.277     73.277     31.777    -3.935    -1.457   138.668
                   90.000     90.000     90.000

================================================================================
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.
Enter your choice 0=Abort [7]: Orientation angles choice 1 selected.

Crystal listing:

 Unit cell lengths:   73.2767   73.2767   31.7765
 Unit cell  angles:   90.0000   90.0000   90.0000
 Unit cell  volume: 170623.326
Orientation angles: -178.5394   -3.9337   48.5679
         Mosaicity:     0.300
       Description: unknown

Spacegroup number: 75
             name: P4
Num. equiv. posns: 4
dtindex - Wrote header file output.head
```