Supplementary material

(to '*Ind_X*: program for indexing single crystal diffraction patterns' by A. Morawiec)

Tables below show high quality solutions (parts of output files) obtained by running *Ind_X* for data of Duisenberg (1992). In response to a recommendation by an anonymous reviewer, also results for unpublished "examples 6 and 7" are listed. In all cases, the limit on the allowed deviation of Miller indices from integers was the *Ind_X* default of 0.12; reflections within this limit are denoted by `-h` and reflections within half of the limit are denoted by `H-`. The unit of length is Ångström, and angles are in degrees.

Example 1:

```
 Solution nr   2 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            -0.41624538    0.04542523    5.05672819
            -2.24425594   -7.88469324   -0.11196100
           -11.93485938    1.08178703   -0.99071084

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   2   0  -8 |   2.01   0.00  -8.03  |  0.032
  2  H- |   2  -5  -7 |   2.00  -5.00  -6.96  |  0.037
  3     |             |   1.97  -0.01  -9.20  |  0.205
  4
  5  H- |   1  -1  -7 |   0.99  -1.00  -6.94  |  0.058
  6
  7  H- |   1   0  -7 |   1.00   0.00  -7.03  |  0.032
  8  H- |   1  -2  -7 |   1.00  -2.00  -7.00  |  0.004
  9  -h |   2  -3   3 |   1.93  -3.00   2.93  |  0.093
 10  H- |   3  -4   0 |   3.01  -4.00   0.04  |  0.039
 11  H- |   1  -4   1 |   1.01  -4.00   0.95  |  0.055
 12  H- |   1  -4   0 |   0.99  -4.00   0.04  |  0.044
 13  -h |   1  -4   0 |   1.01  -4.00  -0.07  |  0.074
 14  H- |   2  -1   4 |   2.01  -1.00   4.02  |  0.026
 15     |             |   1.93   0.00   4.22  |  0.232
 16  H- |   2  -3  -2 |   2.01  -3.00  -1.98  |  0.025
 17  H- |   3   1   6 |   3.02   1.00   5.99  |  0.021
 18  -h |   2   0   8 |   2.01   0.01   8.07  |  0.073
 19
 20  H- |   1   1   6 |   1.00   1.00   6.00  |  0.004
 21  H- |   1   4  -1 |   0.98   4.01  -0.99  |  0.026
 22     |             |   1.97   1.99   2.22  |  0.226
 23  H- |   2   1   1 |   1.99   0.99   0.94  |  0.061
 24  H- |   3   2   1 |   3.00   2.00   0.99  |  0.011
 25     |             |   3.04   1.99  -2.16  |  0.166
-------------------------------------------------------
  18h and  15H vectors out of  25.    Quality : 0.684

 Primitive cell :
                         5.074    8.199   12.025
                        79.26    89.99    89.99

 Volume of the cell  :      491.47
```

Example 2:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            22.39827411   23.67373447   19.86433441
           -55.72013365   53.74568735    2.85453230
            27.36701652   32.99645419  -66.67913680

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
 1  -h |   0   4   7 |  -0.02   3.92   6.89  |  0.134
 2  H- |   3  15  11 |   3.01  15.01  10.99  |  0.017
 3  H- |   4  24  14 |   4.01  24.03  14.01  |  0.031
 4  -h |   1   6   7 |   0.99   5.94   6.91  |  0.105
 5  H- |   6  15   0 |   6.00  14.95  -0.04  |  0.059
 6  -h |   5  22  10 |   4.99  22.05  10.09  |  0.100
 7  H- |   4  27  15 |   4.01  27.00  14.97  |  0.037
 8  -h |   7  26   5 |   7.00  26.05   5.07  |  0.090
 9  -h |   9  27  -6 |   9.00  26.91  -6.10  |  0.131
10  -h |   6  29  10 |   6.01  29.11  10.03  |  0.116
11  -h |   5  24  11 |   4.99  24.03  11.08  |  0.090
12  -h |   1  26  21 |   0.98  25.90  20.92  |  0.126
13  -h |   6  13  -3 |   6.01  12.98  -3.08  |  0.079
14  H- |   4  15   8 |   4.00  15.02   8.03  |  0.030
15  -h |   3   5  -2 |   3.00   4.98  -2.06  |  0.066
16  H- |   4   7  -3 |   4.00   6.99  -3.05  |  0.054
17  H- |   4   8  -1 |   4.00   8.00  -1.02  |  0.020
18  H- |   7  23   3 |   7.00  22.98   3.03  |  0.040
19  H- |   6  10 -11 |   5.98   9.96 -11.02  |  0.051
20  H- |   5  13   2 |   5.00  12.98   1.99  |  0.021
21  H- |   6  20   5 |   6.00  20.00   5.05  |  0.049
22  -h |   2  26  19 |   2.00  25.93  18.93  |  0.101
23  H- |   8  28   1 |   8.01  28.01   1.02  |  0.023
24  -h |   8  30   2 |   8.00  30.09   2.08  |  0.118
25  H- |   3  13   9 |   3.00  13.00   9.01  |  0.008
26  H- |   7  16  -5 |   7.00  15.95  -5.05  |  0.074
-------------------------------------------------------
  26h and  14H vectors out of  26.    Quality : 0.862

 Primitive cell :
                         38.167   77.469   79.271
                         89.46    88.68    88.43

 Volume of the cell  :   234225.58
```

Example 3, solution *a*:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            -0.08757438    2.89242892   -3.33163710
            18.02074562   -1.42129210    1.17612284
            -3.89689517  -16.76216719  -11.52746836

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   1   3  -7 |   1.00   3.02  -6.99  |  0.023
  2  H- |   1  -3  -4 |   1.00  -2.99  -4.00  |  0.008
  3  H- |   0   5  -5 |   0.00   5.00  -5.00  |  0.004
  4  H- |   1  -3  -8 |   1.00  -3.00  -8.00  |  0.007
  5  H- |   0   0  -8 |   0.00   0.00  -8.00  |  0.003
  6  H- |   0  -5  -7 |   0.00  -5.00  -7.00  |  0.003
  7  H- |   0  -5  -3 |   0.00  -5.00  -3.00  |  0.005
  8  H- |   0   0 -12 |   0.00   0.00 -11.99  |  0.006
  9  H- |  -1   4  -6 |  -1.00   4.02  -6.00  |  0.016
 10  H- |  -1  -6  -8 |  -1.00  -5.99  -8.00  |  0.012
 11  H- |  -1  -7  -6 |  -1.00  -7.01  -6.00  |  0.012
 12  H- |   0   0 -12 |   0.00  -0.01 -12.01  |  0.016
 13  H- |   0   5 -13 |   0.00   5.00 -13.00  |  0.007
 14  H- |   1   2 -13 |   1.00   2.00 -13.00  |  0.003
 15  H- |   1   0 -13 |   1.00  -0.04 -13.01  |  0.036
 16  H- |   1  -3 -12 |   1.00  -3.00 -11.99  |  0.005
 17  H- |   1   1 -11 |   1.00   0.98 -11.01  |  0.019
 18  H- |  -1   3  -8 |  -1.00   3.00  -8.00  |  0.007
 19  H- |  -1   4 -10 |  -1.00   4.01  -9.99  |  0.014
 20  H- |   0  10 -10 |   0.00  10.00 -10.00  |  0.003
 21  H- |   1  -7  -9 |   1.00  -6.98  -9.00  |  0.023
 22  H- |   1   3 -11 |   1.00   3.02 -11.00  |  0.025
 23  H- |   1  -3  -8 |   1.00  -3.00  -8.00  |  0.003
 24  H- |   1   2  -9 |   1.00   2.01  -9.00  |  0.006
 25  H- |   1   1  -7 |   1.00   0.98  -7.00  |  0.016
-------------------------------------------------------
  25h and  25H vectors out of  25.    Quality : 1.000

 Primitive cell :
                          4.413   18.115   20.713
                         99.20    96.11    96.90

 Volume of the cell  :     1609.27
```

Example 4:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            1.20056709    1.71918935  -10.94962184
           -0.92071771  -22.25549176   -3.59537022
           97.65751543   -5.77590232    9.77179118

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   0  -3 -21 |   0.00  -3.02 -21.06  |  0.059
  2  H- |   0  -3 -24 |   0.00  -3.01 -23.99  |  0.011
  3     |             |   0.00  -3.04 -22.14  |  0.143
  4  H- |   0  -3 -23 |   0.00  -3.00 -22.98  |  0.023
  5  H- |   0  -5 -16 |   0.00  -5.00 -15.99  |  0.009
  6  H- |   0  -4 -26 |   0.00  -4.00 -25.95  |  0.050
  7  H- |   0  -1 -29 |   0.00  -1.01 -28.97  |  0.031
  8  -h |   0  -1 -31 |  -0.01  -0.89 -31.03  |  0.112
  9  H- |   0   0 -22 |   0.00  -0.01 -21.97  |  0.035
 10  H- |  -1  -4  18 |  -1.00  -3.99  17.98  |  0.022
 11  H- |  -1  -4  17 |  -1.00  -3.99  16.99  |  0.014
 12  H- |  -1  -5  11 |  -1.00  -4.99  11.00  |  0.007
 13  H- |  -1  -5  10 |  -1.00  -5.01  10.02  |  0.025
 14  H- |  -2   1 -19 |  -2.00   1.00 -18.97  |  0.025
 15  H- |  -2   0 -21 |  -2.00   0.00 -20.99  |  0.010
 16  H- |  -2   1 -23 |  -2.00   1.00 -22.96  |  0.037
 17  H- |  -2   0 -23 |  -2.00   0.00 -22.98  |  0.020
 18  H- |  -1  -3  27 |  -1.00  -2.99  27.00  |  0.015
 19  H- |   2  -2  19 |   2.00  -2.00  19.00  |  0.004
 20  H- |   2  -3  16 |   2.00  -3.00  16.01  |  0.011
 21  H- |   2  -4  11 |   2.00  -4.00  11.05  |  0.047
 22  H- |   2  -3  17 |   2.00  -3.00  17.01  |  0.013
 23  H- |   2  -4   9 |   2.00  -4.00   9.01  |  0.010
 24  H- |   2  -5   0 |   2.00  -5.01   0.01  |  0.014
 25  H- |   2  -4  15 |   2.00  -3.99  15.00  |  0.007
-------------------------------------------------------
  24h and  23H vectors out of  25.    Quality : 0.948

 Primitive cell :
                        11.149   22.563   98.315
                        89.91    89.98    90.00

 Volume of the cell  :    24730.50
```

The diffraction data of Example 3 were known to originate from an incommensurate structure. According to (Duisenberg 1992), a "supercell" fitting all reflections has the "volume $3942.00 = 49 \times 80.44$". The quite accurate *Ind_X* solution (a) shown above gives a smaller volume ($1609.27 \approx 20 \times 80.46$). If 100 is the upper limit on the cell volume, *Ind_X* gives the solution (b) with the volume of 80.43; see below. The relationship between the two solutions is $\mathbf{M}_a \approx \mathbf{T} \times \mathbf{M}_b$, where $\mathbf{M}_a$ and $\mathbf{M}_b$ are the matrices of direct lattice vectors (in rows) for each of the solutions, and

$$\mathbf{T} = \begin{bmatrix} 1 & -1 & 0 \\ -3 & -2 & 0 \\ 0 & 1 & 4 \end{bmatrix};$$

Miller indices of the solution (a) can be obtained by multiplying $\mathbf{T}$ and the column of indices of the solution (b). The smallest-volume solution accepting all reflections with the default *Ind_X* parameters is listed below as (c).

Example 3, solution *b*:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            -3.63857749    1.44382309   -1.57287407
            -3.55149346   -1.44846389    1.75859322
            -0.08637420   -3.83006631   -3.31877056

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1
  2  H- |   1   0  -1 |   1.00   0.00  -1.00  |  0.001
  3  H- |  -1  -1  -1 |  -1.00  -1.00  -1.00  |  0.001
  4  H- |   1   0  -2 |   1.00   0.00  -2.00  |  0.001
  5  H- |   0   0  -2 |   0.00   0.00  -2.00  |  0.001
  6  H- |   1   1  -2 |   1.00   1.00  -2.00  |  0.001
  7  H- |   1   1  -1 |   1.00   1.00  -1.00  |  0.002
  8  H- |   0   0  -3 |   0.00   0.00  -3.00  |  0.002
  9
 10
 11  H- |   1   2  -2 |   1.00   2.00  -2.00  |  0.001
 12  H- |   0   0  -3 |   0.00   0.00  -3.00  |  0.003
 13  H- |  -1  -1  -3 |  -1.00  -1.00  -3.00  |  0.001
 14  H- |   0  -1  -3 |   0.00  -1.00  -3.00  |  0.000
 15
 16  H- |   1   0  -3 |   1.00   0.00  -3.00  |  0.001
 17
 18  H- |  -1   0  -2 |  -1.00   0.00  -2.00  |  0.001
 19
 20  H- |  -2  -2  -2 |  -2.00  -2.00  -2.00  |  0.001
 21
 22
 23  H- |   1   0  -2 |   1.00   0.00  -2.00  |  0.001
 24  H- |   0  -1  -2 |   0.00  -1.00  -2.00  |  0.000
 25
-------------------------------------------------------
  16h and  16H vectors out of  25.    Quality : 0.640

 Primitive cell :
                         4.219    4.219    5.069
                        89.95    89.99    63.06

 Volume of the cell  :       80.43
```

Example 3, solution *c*:

```
 Solution nr   9 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
             0.08764924   -2.89243836    3.33158017
            -7.09574696    3.84139431    3.45898860
            10.99137244   12.92062820    8.06968392

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |  -1   0   7 |  -1.00   0.05   6.94  |  0.076
  2  H- |  -1   2   2 |  -1.00   2.00   2.00  |  0.007
  3  H- |   0  -1   6 |   0.00  -1.00   6.00  |  0.003
  4  H- |  -1   3   5 |  -1.00   3.00   4.99  |  0.005
  5  H- |   0   2   6 |   0.00   1.99   6.01  |  0.010
  6  H- |   0   4   3 |   0.00   3.99   3.01  |  0.016
  7  H- |   0   3   0 |   0.00   2.99   0.01  |  0.010
  8  H- |   0   3   9 |   0.00   2.99   9.01  |  0.015
  9  H- |   1   0   6 |   1.00   0.02   5.97  |  0.037
 10  H- |   1   5   3 |   1.00   5.02   2.98  |  0.025
 11  H- |   1   5   1 |   1.00   4.98   1.02  |  0.032
 12  H- |   0   3   9 |   0.00   2.99   9.02  |  0.019
 13  H- |   0   1  12 |   0.00   0.99  12.01  |  0.013
 14  H- |  -1   2  11 |  -1.00   2.00  11.00  |  0.003
 15  -h |  -1   3  10 |  -1.00   2.92  10.09  |  0.121
 16  H- |  -1   4   8 |  -1.00   4.00   8.00  |  0.003
 17  H- |  -1   2   9 |  -1.00   1.96   9.04  |  0.057
 18  H- |   1   1   7 |   1.00   0.98   7.02  |  0.028
 19  H- |   1   1   9 |   1.00   1.02   8.97  |  0.036
 20  H- |   0  -2  12 |   0.00  -2.00  12.00  |  0.003
 21  H- |  -1   5   4 |  -1.00   5.04   3.96  |  0.058
 22  H- |  -1   1  10 |  -1.00   1.04   9.96  |  0.062
 23  H- |  -1   3   5 |  -1.00   3.00   5.00  |  0.004
 24  H- |  -1   1   8 |  -1.00   1.00   7.99  |  0.008
 25  H- |  -1   1   6 |  -1.00   0.97   6.04  |  0.049
-------------------------------------------------------
  25h and  24H vectors out of  25.    Quality : 0.988

 Primitive cell :
                         4.413    8.779   18.785
                        90.15    96.60    90.31

 Volume of the cell  :      722.90
```

Examples 6 and 7 are described at http://www.crystal.chem.uu.nl/distr/dirax/examples.html as "inaccurate data" and "not very accurate data", respectively. *DirAx* solutions to these examples are available at the same web page. The first solution given by *Ind_X* to example 6 is similar to that given by *DirAx*; in both cases, one reflection is not indexed. Example 7 is fully indexable (solution no 1). However, solutions 2 and 3 of *Ind_X* indicate that the data originate from a twinned crystal. Only solutions similar to 1 and 2 are listed at http://www.crystal.chem.uu.nl/distr/dirax/examples.html and, in consequence, the possibility of twinning is overlooked.

Example 6:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            -0.22772791    0.41128973    3.87525272
            -0.28186242   -5.94601285    1.00932446
            16.69620088   -2.75388915    1.71750269

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   2   0  10 |   2.00   0.00  10.00  |  0.007
  2  H- |   2   2   9 |   2.00   2.00   9.01  |  0.011
  3  H- |   1  -1  13 |   1.00  -1.01  13.00  |  0.007
  4  H- |   0   2   6 |  -0.03   2.00   5.98  |  0.033
  5  H- |   0   3   4 |  -0.03   3.00   3.96  |  0.049
  6  H- |   0   1   9 |  -0.02   1.00   9.01  |  0.022
  7  H- |   1   1   5 |   0.99   1.00   4.98  |  0.021
  8  H- |   1   0   5 |   0.99   0.01   5.00  |  0.016
  9  H- |   2  -2  -2 |   2.02  -2.00  -2.02  |  0.028
 10
 11  H- |   1  -2   2 |   0.99  -2.00   2.01  |  0.012
 12  H- |   0  -2  -6 |  -0.02  -2.00  -6.00  |  0.022
 13  H- |   0  -1  -3 |  -0.02  -1.01  -2.99  |  0.026
 14  H- |   1  -1  -1 |   1.01  -1.00  -1.01  |  0.013
 15  H- |   0  -3   5 |  -0.01  -3.00   5.02  |  0.022
 16  H- |   0  -3  -4 |  -0.02  -3.00  -3.99  |  0.020
 17  H- |   2   1  -7 |   2.00   1.00  -7.00  |  0.005
 18  H- |   1   4  -1 |   0.98   4.00  -0.99  |  0.019
 19  H- |   2   3  -2 |   2.00   3.00  -1.99  |  0.013
 20  H- |   1   5   4 |   0.98   5.00   4.05  |  0.052
 21  -h |   1   4  -4 |   0.99   4.01  -4.12  |  0.120
 22  H- |   1   0  -8 |   0.99   0.00  -8.00  |  0.012
 23  -h |   1   2  -5 |   0.98   2.01  -5.12  |  0.117
 24  H- |   1   4  -7 |   0.98   4.02  -6.97  |  0.041
 25  H- |   0  -1  -6 |  -0.03  -1.01  -6.02  |  0.035
-------------------------------------------------------
  24h and  22H vectors out of  25.    Quality : 0.936

 Primitive cell :
                         3.904    6.038   17.009
                        82.50    88.51    86.28

 Volume of the cell  :      396.55
```

Example 7:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            1.84344954    3.25703922    8.82866263
           22.22374211    1.60108683   -5.22574341
           16.66747588  -35.84753215    9.80100707

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   4  10  24 |   4.01   9.99  23.98  |  0.024
  2  H- |   6  12  16 |   6.00  12.00  16.02  |  0.018
  3  H- |   4  12  22 |   4.01  11.99  21.97  |  0.034
  4  H- |   4   8  20 |   4.00   8.00  19.99  |  0.015
  5  H- |   6   7   1 |   6.00   7.02   1.04  |  0.049
  6  H- |   7  10   6 |   6.99  10.02   6.00  |  0.021
  7  H- |   5  15  15 |   5.00  14.99  14.98  |  0.017
  8  H- |   5  15  16 |   4.99  14.99  15.96  |  0.041
  9  H- |   4 -14 -16 |   4.00 -14.00 -16.03  |  0.033
 10  H- |   5 -11 -17 |   5.00 -11.00 -17.01  |  0.014
 11  H- |   5 -13 -21 |   5.00 -13.00 -21.02  |  0.023
 12  H- |   7   4 -14 |   7.00   4.00 -14.00  |  0.005
 13  H- |   6   2 -12 |   6.01   2.00 -11.97  |  0.029
 14  H- |   4 -13  -9 |   4.00 -13.00  -9.06  |  0.055
 15  H- |   5  -9 -14 |   5.00  -9.00 -13.96  |  0.041
 16  H- |   7  -4 -18 |   7.00  -4.01 -17.96  |  0.044
 17  H- |   2  -4  30 |   2.00  -4.00  30.02  |  0.020
 18  H- |   2  -5  29 |   2.00  -5.00  29.03  |  0.027
 19  H- |   2 -16   8 |   1.99 -16.01   8.00  |  0.010
 20  H- |   2 -16  10 |   1.99 -16.00   9.96  |  0.038
 21  H- |   1 -10  20 |   1.00  -9.99  19.99  |  0.013
 22  H- |   1 -12  16 |   1.00 -11.99  16.03  |  0.034
 23  H- |   2 -17  -5 |   2.01 -17.01  -5.04  |  0.039
 24  H- |   1 -13   8 |   1.00 -13.00   8.06  |  0.058
 25  H- |   1 -12  10 |   1.00 -11.99  10.01  |  0.012
-------------------------------------------------------
  25h and  25H vectors out of  25.    Quality : 1.000

 Primitive cell :
                         9.589   22.886   40.730
                        73.69    89.93    89.99

 Volume of the cell  :     8578.63
```

Example 7:

```
 Solution nr   2 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            -1.84244579   -3.25710729   -8.82838295
            -2.78455888  -18.72373301    7.51579641
            22.22271405    1.60042838   -5.22626771

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |  -4   7  10 |  -4.01   6.99   9.99  |  0.015
  2  H- |  -6   2  12 |  -5.99   2.01  12.00  |  0.010
  3  H- |  -4   5  12 |  -4.01   4.98  11.99  |  0.019
  4  H- |  -4   6   8 |  -4.00   5.99   8.00  |  0.012
  5  H- |  -6  -3   7 |  -6.00  -2.99   7.02  |  0.022
  6  H- |  -7  -2  10 |  -6.99  -2.01  10.02  |  0.024
  7  H- |  -5   0  15 |  -5.00  -0.01  14.99  |  0.011
  8
  9  H- |  -4  -1 -14 |  -4.00  -1.01 -13.99  |  0.015
 10  H- |  -5  -3 -11 |  -5.00  -3.00 -11.00  |  0.003
 11  H- |  -5  -4 -13 |  -5.00  -4.00 -13.00  |  0.006
 12  H- |  -7  -9   4 |  -7.00  -9.00   4.00  |  0.003
 13  H- |  -6  -7   2 |  -6.01  -6.99   2.00  |  0.014
 14  H- |  -4   2 -13 |  -4.00   1.98 -13.00  |  0.023
 15
 16  H- |  -7  -7  -4 |  -7.00  -6.97  -4.01  |  0.030
 17  H- |  -2  17  -4 |  -2.00  17.01  -4.00  |  0.013
 18  H- |  -2  17  -5 |  -2.00  17.02  -5.00  |  0.018
 19  H- |  -2  12 -16 |  -2.00  12.01 -16.01  |  0.012
 20  H- |  -2  13 -16 |  -1.99  12.99 -16.00  |  0.015
 21  H- |  -1  15 -10 |  -1.00  14.99  -9.99  |  0.012
 22  H- |  -1  14 -12 |  -1.00  14.01 -11.99  |  0.019
 23  H- |  -2   6 -17 |  -2.01   5.99 -17.01  |  0.015
 24
 25  H- |  -1  11 -12 |  -1.00  11.00 -11.99  |  0.009
-------------------------------------------------------
  22h and  22H vectors out of  25.    Quality : 0.880

 Primitive cell :
                          9.589   20.367   22.885
                        106.34    90.00    90.07

 Volume of the cell  :     4288.81
```

Example 7:

```
 Solution nr   3 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            1.84235217    3.25747591    8.82920015
            8.34452110  -17.93160379    4.89513606
           22.22639387    1.60217130   -5.22661136

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   4  12  10 |   4.01  12.00   9.99  |  0.012
  2  H- |   6   8  12 |   6.00   8.01  12.00  |  0.014
  3  H- |   4  11  12 |   4.01  10.99  11.99  |  0.014
  4  H- |   4  10   8 |   4.00  10.00   8.00  |  0.006
  5
  6  H- |   7   3  10 |   6.99   3.00  10.02  |  0.022
  7
  8  H- |   5   8  15 |   4.99   7.99  15.00  |  0.016
  9  H- |   4  -8 -14 |   4.00  -8.03 -14.00  |  0.028
 10
 11
 12  H- |   7  -7   4 |   7.00  -7.00   4.00  |  0.003
 13  H- |   6  -6   2 |   6.01  -5.99   2.00  |  0.012
 14
 15  H- |   5  -7  -9 |   5.00  -6.99  -9.00  |  0.012
 16  H- |   7  -9  -4 |   7.00  -8.99  -4.01  |  0.016
 17  H- |   2  15  -4 |   2.00  15.01  -4.01  |  0.014
 18
 19  H- |   2   4 -16 |   2.00   3.99 -16.01  |  0.013
 20  H- |   2   5 -16 |   1.99   4.98 -16.00  |  0.026
 21  H- |   1  10 -10 |   1.00   9.99  -9.99  |  0.010
 22  H- |   1   8 -12 |   1.00   8.01 -11.99  |  0.018
 23
 24  H- |   1   4 -13 |   1.00   4.02 -13.00  |  0.025
 25  H- |   1   5 -12 |   1.00   5.00 -12.00  |  0.005
-------------------------------------------------------
  18h and  18H vectors out of  25.    Quality : 0.720

 Primitive cell :
                         9.590   20.375   22.889
                        73.67    89.99    89.95

 Volume of the cell  :     4291.67
```

Output of LePage.exe for solution no. 3 of example 7 (cf. solution no 2):

	LATO	LATT	A	B	C	ALFA	BET	GAM	VOL
INPUT CELL		P	9.590	20.375	22.889	73.67	89.99	89.95	4292.00
REDUC CELL		P	9.590	20.375	22.889	73.67	89.99	89.95	4292.00
CONV. CELL	M	P	20.375	9.590	22.889	90.01	106.33	89.95	4292.00