QUESTIONNAIRE FOR the
STRUCTURE DETERMINATION BY POWDER DIFFRACTOMETRY ROUND ROBIN - 3

Calcium tartrate

0.0 Precise date of
- data download : Fri, 4 Feb 2008
- results submission : 30 April 2008

0.1 Is the first sample structure solvable with this quality of data ? Yes

1. Preliminary work

1.1 Did you obtained additional informations ? no
(for instance from CSD or ICSD or ICDD databases)

1.2 Did you obtained additional informations from the powder pattern ? no
(for instance using the JCPDS-ICDD database)

1.3 Did you extract the structure factors ? Yes

1.3.1 If yes, which program(s) did you use Fullprof
1.3.2 Give the angular range: 7-90°
1.3.3 Give the number of extracted structure factors: 1559
1.3.4 Give the Rp and Rwp (conventional Rietveld, background subtracted):8.15% 8.50%
1.3.5 Give the Rp and Rwp (background not subtracted): 2.95%, 3.97%

2- Structure solution

2.1 Did you use direct methods ? No

2.2 Did you use Patterson methods ? No

2.3 Did you use another method ? Yes

2.3.1 reverse Monte Carlo and pseudo simulated annealing code

2.3.2 Which program(s) did you use (name and reference) ESPOIR A. Le Bail

2.3.3 I used one CaO8 polyedra with free torsion angles, a C4 molecule (tartrate without oxygen) fragment with free torsion angles and two oxygen atoms.

2.4 Did you first locate the whole structure ? Yes

Ca1	1	0.82613	0.23028	0.14772	11.00000	10.05000
O1	3	0.63230	0.12989	0.30893	11.00000	10.05000
O2	3	1.02361	0.41504	0.16112	11.00000	10.05000
O3	3	1.04694	0.10496	0.31236	11.00000	10.05000
O4	3	0.94445	0.17538	-0.12679	11.00000	10.05000
O5	3	0.68628	-0.00614	-0.11182	11.00000	10.05000
O6	3	0.57420	0.26917	-0.14694	11.00000	10.05000
O7	3	0.65897	0.41042	0.29716	11.00000	10.05000
O8	3	0.95530	0.33198	0.60292	11.00000	10.05000
C1	2	0.81324	0.63712	0.94250	11.00000	10.05000
C2	2	0.92879	0.75730	1.15273	11.00000	10.05000
C3	2	0.84103	0.81702	1.33016	11.00000	10.05000
C4	2	0.82056	0.71744	1.46449	11.00000	10.05000
O1	3	0.74903	0.89792	0.41213	11.00000	10.05000

```
          O2    3    0.27325    0.49017    0.19958   11.00000  10.05000
```

3- Structure completion

3.1 Did you performed Fourier difference syntheses before refining the structure by the Rietveld method ? No

3.5 Did you made first Rietveld refinements without preliminary Fourier difference syntheses ? Yes

3.5.1 If yes, with what program ? Fullprof

3.5.2 What were the Rp and Rwp (background subtracted AND not subtracted) and RB and RF that you obtained at the first Rietveld application ?

```
==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS FOR PATTERN:  1

 => Cycle:  2 => MaxCycle: 10
 => N-P+C:  4754
 =>  R-factors (not corrected for background) for Pattern:  1
 => Rp: 4.23     Rwp: 5.86     Rexp:    1.98 Chi2:  8.76      M.L. refinement
 => Conventional Rietveld R-factors for Pattern:  1
 => Rp: 11.4     Rwp: 12.3     Rexp:    4.16 Chi2:  8.76
 => Deviance: 0.408E+05     Dev*  :  8.579
 => DW-Stat.:    0.2803     DW-exp:     1.9401
 => N-sigma of the GoF:  378.194

 ==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN:  1

 => N-P+C:  4708
 =>  R-factors (not corrected for background) for Pattern:  1
 => Rp: 4.28     Rwp: 5.91     Rexp:    1.99 Chi2:  8.83      M.L. refinement
 => Conventional Rietveld R-factors for Pattern:  1
 => Rp: 11.3     Rwp: 12.3     Rexp:    4.14 Chi2:  8.83
 => Deviance: 0.407E+05     Dev*  :  8.651
 => DW-Stat.:    0.2807     DW-exp:     1.9399
 => N-sigma of the GoF:      379.924

 => Global user-weigthed Chi2 (Bragg contrib.):  8.84

     ------------------------------------------------------
     BRAGG R-Factors and weight fractions for Pattern #  1
     ------------------------------------------------------

 => Phase:  1
 => Bragg R-factor:  5.62       Vol:  483.286( 0.000)  Fract(%):  100.00( 0.80)
 => Rf-factor= 5.61             ATZ:        2795.410   Brindley:  1.0000
```

3.5.3 Did you get the structure factors from this result and performed a Fourier difference synthesis No

3.5.4 Did you locate additional atoms at this stage No

4- Final refinement

- Give the final atomic coordinates, thermal parameters, standard deviations, Reliability factors.....

```
      70    !Number of refined parameters
!
!  Zero    Code    SyCos    Code   SySin    Code  Lambda     Code MORE ->Patt# 1
 -0.00031  0.0  0.00000    0.0  0.00000    0.0 0.000000    0.00   0
```

```
!-------------------------------------------------------------------------------
!  Data for PHASE number:   1  ==> Current R_Bragg for Pattern#  1:     5.62
!-------------------------------------------------------------------------------
Calcium tartrate
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ    Nvk Npr More
  15   0   0 0.0 0.0 1.0   0   0   0   0   0       2795.410   0   5   0
!
P -1                     <--Space group symbol
!Atom Typ       X         Y         Z      Biso       Occ     In Fin N_t Spc /Codes
Ca1  CA      0.81637   0.23059   0.16270  4.23076   1.00000   0   0   0    0
               21.00     31.00     41.00   471.00      0.00
O1   O       0.66479   0.11899   0.37022  1.42714   1.00000   0   0   0    0
               51.00     61.00     71.00   481.00      0.00
O2   O       0.02247   0.42074   0.20859  1.42714   1.00000   0   0   0    0
               81.00     91.00    101.00   481.00      0.00
O3   O       0.03189   0.09821   0.32157  1.42714   1.00000   0   0   0    0
              111.00    121.00    131.00   481.00      0.00
O4   O       0.98127   0.15332  -0.12504  1.42714   1.00000   0   0   0    0
              141.00    151.00    161.00   481.00      0.00
O5   O       0.68205  -0.01073  -0.11545  1.42714   1.00000   0   0   0    0
              171.00    181.00    191.00   481.00      0.00
O6   O       0.62759   0.28052  -0.19129  1.42714   1.00000   0   0   0    0
              201.00    211.00    221.00   481.00      0.00
O7   O       0.64782   0.40327   0.31811  1.42714   1.00000   0   0   0    0
              231.00    241.00    251.00   481.00      0.00
O8   O       0.97928   0.32341   0.59543  1.42714   1.00000   0   0   0    0
              261.00    271.00    281.00   481.00      0.00
C1   C       0.89545   0.62569   0.91874  1.33657   1.00000   0   0   0    0
              291.00    301.00    311.00   491.00      0.00
C2   C       0.86565   0.75771   0.08168  1.33657   1.00000   0   0   0    0
              321.00    331.00    341.00   491.00      0.00
C3   C       0.85904   0.82440   0.49106  1.33657   1.00000   0   0   0    0
              351.00    361.00    371.00   491.00      0.00
C4   C       0.89041   0.70940   0.29607  1.33657   1.00000   0   0   0    0
              381.00    391.00    401.00   491.00      0.00
O9   O       0.70536   0.87492   0.41978  1.42714   1.00000   0   0   0    0
              411.00    421.00    431.00   481.00      0.00
O10  O       0.29803   0.46451   0.20520  1.42714   1.00000   0   0   0    0
              441.00    451.00    461.00   481.00      0.00
```

The final refinement was performed without any constraints

5- You will find below the ESPOIR starting file

```
! title
tartrate clacium
!    a,     b,     c,    alpha,    beta,    gamma
8.220435  10.435094   6.248580 105.966553 107.523972  94.935944
! space group
P -1
! lambda, radiation, N of atoms, types of atoms, N of objects, "|Fobs|" or
patterns, iprint
1.54056   4  15   3  3   1   1
! U,     V,     W,    STEP
 -0.073016   0.093399   0.000298     5.
! atom names, in 8A4
Ca  C   O
! code for minimal distance contraints
 0
! maximum moves for each type of atom
   10 10 10
! annealing law, sigma, reject
```

```
1.50000  1.0000  0.0010
! number of events for : print, maximum, save
     20000    2000000    100000
! events for restart, rmax, ichi, number of runs
 1000000  0.300   2  300
3 4
1 0 8
3.0 0 0
1 1 1 90 90 90
3.12 7.11 11.022 1
3.672 6.245 13.226 1
2.061 6.903 8.904 1
1.398 8.54 12.06 1
3.265 8.938 9.833 1
4.572 8.721 12.256 1
5.367 6.483 10.209 1
3.645 4.618 10.778 1
1.112 5.694 11.818 1
3 4
0 4 0
3.0 0 0
1 1 1 90 90 90
4.20995        2.26348        4.11425 1
2.73238        2.10996        3.75226 1
2.49626        1.53078        2.36454 1
0.98788        1.42993        2.11528 1
1 0
0 0 2
3.0 0 0
```

The better solution was found after 91 tests

The output file :

```
Test number :  91
Ca1     0.93927    1.03800    1.95022      1.000
O1      1.09433    1.02561    2.34019      1.000
O2      0.71507    0.95004    1.57546      1.000
O3      0.79050    1.20890    2.13388      1.000
O4      0.92379    1.17563    1.73984      1.000
O5      1.18714    1.23260    2.16856      1.000
O6      1.17025    0.95157    1.80637      1.000
O7      0.96622    0.79046    1.90705      1.000
O8      0.71516    0.92737    2.09106      1.000
C1      0.71696    0.34990    0.72797      1.000
C2      0.51968    0.32350    0.66392      1.000
C3      0.42380    0.22321    0.41838      1.000
C4      0.22828    0.20550    0.37428      1.000

 Starting coordinates x,y,z and occupation numbers

O1      0.38992    0.32684    0.74884      1.000
O2      0.51443    0.33055    0.83251      1.000

  Object number  1 at test 91.  Previous minimum R=0.245 at test 24
      0 rot. acc.       0 gen. and       0 tested; Chi**2=0.777    , R=0.777
      0 trans. acc.       0 tested
      0 events did not improve the fit, DAMP = 1.000000
  Object number  2 at test 91.  Previous minimum R=0.245 at test 24
      0 rot. acc.       0 gen. and       0 tested; Chi**2=0.777    , R=0.777
      0 trans. acc.       0 tested
      0 events did not improve the fit, DAMP = 1.000000
  Object number  3 at test 91.  Previous minimum R=0.245 at test 24
      0 moves acc.       0 tested; Chi**2=0.777    , R=0.777
      0 perm. acc.       0 tested
      0 events did not improve the fit, DAMP = 1.000000

  Object number  1 at test 91.  Previous minimum R=0.245 at test 24
      6 rot. acc.   34189 gen. and   34189 tested; Chi**2=0.435    , R=0.435
      2 trans. acc.   11396 tested
      1 events did not improve the fit, DAMP = 0.899210
  Object number  2 at test 91.  Previous minimum R=0.245 at test 24
      6 rot. acc.   34106 gen. and   34106 tested; Chi**2=0.435    , R=0.435
      1 trans. acc.   11368 tested
      0 events did not improve the fit, DAMP = 0.899449
  Object number  3 at test 91.  Previous minimum R=0.245 at test 24
      5 moves acc.   45720 tested; Chi**2=0.435    , R=0.435
      0 perm. acc.       0 tested
      0 events did not improve the fit, DAMP = 0.898914

  Object number  1 at test 91.  Previous minimum R=0.245 at test 24
      6 rot. acc.   34189 gen. and   34189 tested; Chi**2=0.434    , R=0.434
      2 trans. acc.   11396 tested
      1 events did not improve the fit, DAMP = 0.899210
  Object number  2 at test 91.  Previous minimum R=0.245 at test 24
      7 rot. acc.   34108 gen. and   34108 tested; Chi**2=0.434    , R=0.434
      1 trans. acc.   11368 tested
      0 events did not improve the fit, DAMP = 0.899444
  Object number  3 at test 91.  Previous minimum R=0.245 at test 24
      6 moves acc.   45723 tested; Chi**2=0.434    , R=0.434
      0 perm. acc.       0 tested
      0 events did not improve the fit, DAMP = 0.898908
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```
Object number  1 at test 91.  Previous minimum R=0.245 at test 24
    6 rot. acc.   38563 gen. and   38563 tested; Chi**2=0.430    , R=0.430
    3 trans. acc.   12854 tested
    1 events did not improve the fit, DAMP = 0.886574
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
    7 rot. acc.   38531 gen. and   38531 tested; Chi**2=0.430    , R=0.430
    1 trans. acc.   12843 tested
    0 events did not improve the fit, DAMP = 0.886665
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    6 moves acc.   51646 tested; Chi**2=0.430    , R=0.430
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.886077

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
    9 rot. acc.   58763 gen. and   58763 tested; Chi**2=0.390    , R=0.390
    3 trans. acc.   19587 tested
    1 events did not improve the fit, DAMP = 0.828998
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
    8 rot. acc.   58998 gen. and   58998 tested; Chi**2=0.390    , R=0.390
    1 trans. acc.   19665 tested
    0 events did not improve the fit, DAMP = 0.828337
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    6 moves acc.   78448 tested; Chi**2=0.390    , R=0.390
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.828791

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   10 rot. acc.   62549 gen. and   62549 tested; Chi**2=0.387    , R=0.387
    3 trans. acc.   20849 tested
    1 events did not improve the fit, DAMP = 0.818351
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
    8 rot. acc.   62802 gen. and   62802 tested; Chi**2=0.387    , R=0.387
    1 trans. acc.   20933 tested
    0 events did not improve the fit, DAMP = 0.817642
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    6 moves acc.   83443 tested; Chi**2=0.387    , R=0.387
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.818257

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   10 rot. acc.   85961 gen. and   85961 tested; Chi**2=0.380    , R=0.380
    3 trans. acc.   28653 tested
    1 events did not improve the fit, DAMP = 0.753542
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
    8 rot. acc.   86295 gen. and   86295 tested; Chi**2=0.380    , R=0.380
    1 trans. acc.   28764 tested
    0 events did not improve the fit, DAMP = 0.752631
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    7 moves acc.  114821 tested; Chi**2=0.380    , R=0.380
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.753119

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   11 rot. acc.   90343 gen. and   90343 tested; Chi**2=0.355    , R=0.355
    3 trans. acc.   30113 tested
    1 events did not improve the fit, DAMP = 0.741613
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
    8 rot. acc.   90703 gen. and   90703 tested; Chi**2=0.355    , R=0.355
    1 trans. acc.   30233 tested
    0 events did not improve the fit, DAMP = 0.740635
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  120600 tested; Chi**2=0.355    , R=0.355
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.741319
```

```
Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   12 rot. acc.   99307 gen. and   99307 tested; Chi**2=0.340    , R=0.340
    3 trans. acc.   33101 tested
    1 events did not improve the fit, DAMP = 0.717405
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
    9 rot. acc.   99787 gen. and   99787 tested; Chi**2=0.340    , R=0.340
    1 trans. acc.   33261 tested
    1 events did not improve the fit, DAMP = 0.716116
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  132768 tested; Chi**2=0.340    , R=0.340
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.716680

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   15 rot. acc.  154978 gen. and  154978 tested; Chi**2=0.324    , R=0.324
    3 trans. acc.   51658 tested
    1 events did not improve the fit, DAMP = 0.573214
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
    9 rot. acc.  155251 gen. and  155251 tested; Chi**2=0.324    , R=0.324
    1 trans. acc.   51749 tested
    1 events did not improve the fit, DAMP = 0.572534
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  206688 tested; Chi**2=0.324    , R=0.324
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.573117

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   16 rot. acc.  170250 gen. and  170250 tested; Chi**2=0.316    , R=0.316
    4 trans. acc.   56749 tested
    1 events did not improve the fit, DAMP = 0.535579
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
    9 rot. acc.  170728 gen. and  170728 tested; Chi**2=0.316    , R=0.316
    1 trans. acc.   56908 tested
    1 events did not improve the fit, DAMP = 0.534416
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  226930 tested; Chi**2=0.316    , R=0.316
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.535705

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   17 rot. acc.  182562 gen. and  182562 tested; Chi**2=0.315    , R=0.315
    4 trans. acc.   60853 tested
    1 events did not improve the fit, DAMP = 0.505865
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
    9 rot. acc.  183012 gen. and  183012 tested; Chi**2=0.315    , R=0.315
    1 trans. acc.   61003 tested
    1 events did not improve the fit, DAMP = 0.504790
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  243143 tested; Chi**2=0.315    , R=0.315
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.506353

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   17 rot. acc.  213202 gen. and  213202 tested; Chi**2=0.307    , R=0.307
    5 trans. acc.   71067 tested
    1 events did not improve the fit, DAMP = 0.434422
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
    9 rot. acc.  213687 gen. and  213687 tested; Chi**2=0.307    , R=0.307
    1 trans. acc.   71228 tested
    1 events did not improve the fit, DAMP = 0.433320
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  284127 tested; Chi**2=0.307    , R=0.307
    0 perm. acc.       0 tested
```

```
    0 events did not improve the fit, DAMP = 0.434662

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   19 rot. acc.  244531 gen. and  244531 tested; Chi**2=0.301    , R=0.301
    5 trans. acc.   81509 tested
    1 events did not improve the fit, DAMP = 0.365220
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
    9 rot. acc.  244823 gen. and  244823 tested; Chi**2=0.301    , R=0.301
    1 trans. acc.   81607 tested
    1 events did not improve the fit, DAMP = 0.364593
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  325242 tested; Chi**2=0.301    , R=0.301
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.366504

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   19 rot. acc.  282415 gen. and  282415 tested; Chi**2=0.298    , R=0.298
    5 trans. acc.   94138 tested
    1 events did not improve the fit, DAMP = 0.287072
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
   10 rot. acc.  282702 gen. and  282702 tested; Chi**2=0.298    , R=0.298
    1 trans. acc.   94233 tested
    1 events did not improve the fit, DAMP = 0.286504
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  375755 tested; Chi**2=0.298    , R=0.298
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.288256

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   19 rot. acc.  382363 gen. and  382363 tested; Chi**2=0.284    , R=0.284
    5 trans. acc.  127453 tested
    1 events did not improve the fit, DAMP = 0.114121
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
   10 rot. acc.  383575 gen. and  383575 tested; Chi**2=0.284    , R=0.284
    2 trans. acc.  127858 tested
    1 events did not improve the fit, DAMP = 0.112362
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  509560 tested; Chi**2=0.284    , R=0.284
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.114401

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   19 rot. acc.  385177 gen. and  385177 tested; Chi**2=0.281    , R=0.281
    6 trans. acc.  128392 tested
    1 events did not improve the fit, DAMP = 0.110051
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
   10 rot. acc.  386463 gen. and  386463 tested; Chi**2=0.281    , R=0.281
    2 trans. acc.  128820 tested
    1 events did not improve the fit, DAMP = 0.108207
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  513351 tested; Chi**2=0.281    , R=0.281
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.110285

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   19 rot. acc.  401866 gen. and  401866 tested; Chi**2=0.267    , R=0.267
    8 trans. acc.  133955 tested
    1 events did not improve the fit, DAMP = 0.086952
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
   11 rot. acc.  402959 gen. and  402959 tested; Chi**2=0.267    , R=0.267
    2 trans. acc.  134319 tested
    1 events did not improve the fit, DAMP = 0.085503
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  535573 tested; Chi**2=0.267    , R=0.267
```

```
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.087199

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   19 rot. acc.  410101 gen. and  410101 tested; Chi**2=0.264    , R=0.264
    9 trans. acc.  136700 tested
    1 events did not improve the fit, DAMP = 0.076240
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
   11 rot. acc.  411215 gen. and  411215 tested; Chi**2=0.264    , R=0.264
    2 trans. acc.  137071 tested
    1 events did not improve the fit, DAMP = 0.074827
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  546514 tested; Chi**2=0.264    , R=0.264
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.076513

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   19 rot. acc.  420520 gen. and  420520 tested; Chi**2=0.264    , R=0.264
    9 trans. acc.  140173 tested
    1 events did not improve the fit, DAMP = 0.063378
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
   12 rot. acc.  421728 gen. and  421728 tested; Chi**2=0.264    , R=0.264
    2 trans. acc.  140575 tested
    1 events did not improve the fit, DAMP = 0.061939
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  560376 tested; Chi**2=0.264    , R=0.264
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.063662

Object number  1 at test 91.  Previous minimum R=0.245 at test 24
   19 rot. acc.  430963 gen. and  430963 tested; Chi**2=0.243    , R=0.243
   10 trans. acc.  143654 tested
    1 events did not improve the fit, DAMP = 0.051307
Object number  2 at test 91.  Previous minimum R=0.245 at test 24
   15 rot. acc.  432061 gen. and  432061 tested; Chi**2=0.243    , R=0.243
    2 trans. acc.  144020 tested
    1 events did not improve the fit, DAMP = 0.050088
Object number  3 at test 91.  Previous minimum R=0.245 at test 24
    8 moves acc.  574168 tested; Chi**2=0.243    , R=0.243
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.051682

Object number  1 at test 91.  Previous minimum R=0.237 at test 91
   19 rot. acc.  443554 gen. and  443554 tested; Chi**2=0.230    , R=0.230
   11 trans. acc.  147850 tested
    1 events did not improve the fit, DAMP = 0.037932
Object number  2 at test 91.  Previous minimum R=0.237 at test 91
   15 rot. acc.  444694 gen. and  444694 tested; Chi**2=0.230    , R=0.230
    3 trans. acc.  148231 tested
    1 events did not improve the fit, DAMP = 0.036789
Object number  3 at test 91.  Previous minimum R=0.237 at test 91
    8 moves acc.  591058 tested; Chi**2=0.230    , R=0.230
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.038194

Object number  1 at test 91.  Previous minimum R=0.230 at test 91
   20 rot. acc.  450700 gen. and  450700 tested; Chi**2=0.227    , R=0.227
   11 trans. acc.  150232 tested
    1 events did not improve the fit, DAMP = 0.030962
Object number  2 at test 91.  Previous minimum R=0.230 at test 91
   15 rot. acc.  451991 gen. and  451991 tested; Chi**2=0.227    , R=0.227
    3 trans. acc.  150663 tested
    1 events did not improve the fit, DAMP = 0.029753
Object number  3 at test 91.  Previous minimum R=0.230 at test 91
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    8 moves acc.  600713 tested; Chi**2=0.227    , R=0.227
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.031117

Object number  1 at test 91.  Previous minimum R=0.227 at test 91
   20 rot. acc.  451288 gen. and  451288 tested; Chi**2=0.225    , R=0.225
   11 trans. acc.  150429 tested
    1 events did not improve the fit, DAMP = 0.030410
Object number  2 at test 91.  Previous minimum R=0.227 at test 91
   15 rot. acc.  452545 gen. and  452545 tested; Chi**2=0.225    , R=0.225
    3 trans. acc.  150847 tested
    1 events did not improve the fit, DAMP = 0.029240
Object number  3 at test 91.  Previous minimum R=0.227 at test 91
    9 moves acc.  601501 tested; Chi**2=0.225    , R=0.225
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.030561

Object number  1 at test 91.  Previous minimum R=0.223 at test 91
   20 rot. acc.  455602 gen. and  455602 tested; Chi**2=0.219    , R=0.219
   11 trans. acc.  151867 tested
    1 events did not improve the fit, DAMP = 0.026461
Object number  2 at test 91.  Previous minimum R=0.223 at test 91
   16 rot. acc.  456743 gen. and  456743 tested; Chi**2=0.219    , R=0.219
    3 trans. acc.  152247 tested
    1 events did not improve the fit, DAMP = 0.025447
Object number  3 at test 91.  Previous minimum R=0.223 at test 91
   10 moves acc.  607333 tested; Chi**2=0.219    , R=0.219
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.026551

Object number  1 at test 91.  Previous minimum R=0.216 at test 91
   20 rot. acc.  464379 gen. and  464379 tested; Chi**2=0.216    , R=0.216
   12 trans. acc.  154792 tested
    1 events did not improve the fit, DAMP = 0.019016
Object number  2 at test 91.  Previous minimum R=0.216 at test 91
   18 rot. acc.  465586 gen. and  465586 tested; Chi**2=0.216    , R=0.216
    3 trans. acc.  155194 tested
    1 events did not improve the fit, DAMP = 0.018058
Object number  3 at test 91.  Previous minimum R=0.216 at test 91
   12 moves acc.  619067 tested; Chi**2=0.216    , R=0.216
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.019078

Object number  1 at test 91.  Previous minimum R=0.216 at test 91
   20 rot. acc.  465277 gen. and  465277 tested; Chi**2=0.214    , R=0.214
   12 trans. acc.  155092 tested
    1 events did not improve the fit, DAMP = 0.018302
Object number  2 at test 91.  Previous minimum R=0.216 at test 91
   19 rot. acc.  466489 gen. and  466489 tested; Chi**2=0.214    , R=0.214
    3 trans. acc.  155496 tested
    1 events did not improve the fit, DAMP = 0.017352
Object number  3 at test 91.  Previous minimum R=0.216 at test 91
   13 moves acc.  620300 tested; Chi**2=0.214    , R=0.214
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.018342

Object number  1 at test 91.  Previous minimum R=0.214 at test 91
   20 rot. acc.  467671 gen. and  467671 tested; Chi**2=0.213    , R=0.213
   13 trans. acc.  155890 tested
    1 events did not improve the fit, DAMP = 0.016442
Object number  2 at test 91.  Previous minimum R=0.214 at test 91
   19 rot. acc.  468913 gen. and  468913 tested; Chi**2=0.213    , R=0.213
    3 trans. acc.  156304 tested
    1 events did not improve the fit, DAMP = 0.015504
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Object number  3 at test 91.  Previous minimum R=0.214 at test 91
   13 moves acc.  623437 tested; Chi**2=0.213    , R=0.213
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.016512

Object number  1 at test 91.  Previous minimum R=0.208 at test 91
   21 rot. acc.  478867 gen. and  478867 tested; Chi**2=0.208    , R=0.208
   15 trans. acc.  159622 tested
    1 events did not improve the fit, DAMP = 0.010000
Object number  2 at test 91.  Previous minimum R=0.208 at test 91
   22 rot. acc.  480121 gen. and  480121 tested; Chi**2=0.208    , R=0.208
    4 trans. acc.  160039 tested
    1 events did not improve the fit, DAMP = 0.010000
Object number  3 at test 91.  Previous minimum R=0.208 at test 91
   15 moves acc.  638392 tested; Chi**2=0.208    , R=0.208
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.010000

Object number  1 at test 91.  Previous minimum R=0.208 at test 91
   21 rot. acc.  480166 gen. and  480166 tested; Chi**2=0.207    , R=0.207
   16 trans. acc.  160055 tested
    1 events did not improve the fit, DAMP = 0.010000
Object number  2 at test 91.  Previous minimum R=0.208 at test 91
   25 rot. acc.  481369 gen. and  481369 tested; Chi**2=0.207    , R=0.207
    4 trans. acc.  160456 tested
    1 events did not improve the fit, DAMP = 0.010000
Object number  3 at test 91.  Previous minimum R=0.208 at test 91
   15 moves acc.  640126 tested; Chi**2=0.207    , R=0.207
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.010000

Object number  1 at test 91.  Previous minimum R=0.206 at test 91
   21 rot. acc.  484627 gen. and  484627 tested; Chi**2=0.205    , R=0.205
   16 trans. acc.  161542 tested
    1 events did not improve the fit, DAMP = 0.010000
Object number  2 at test 91.  Previous minimum R=0.206 at test 91
   26 rot. acc.  485584 gen. and  485584 tested; Chi**2=0.205    , R=0.205
    4 trans. acc.  161860 tested
    1 events did not improve the fit, DAMP = 0.010000
Object number  3 at test 91.  Previous minimum R=0.206 at test 91
   16 moves acc.  646062 tested; Chi**2=0.205    , R=0.205
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.010000

Object number  1 at test 91.  Previous minimum R=0.205 at test 91
   21 rot. acc.  494938 gen. and  494938 tested; Chi**2=0.205    , R=0.205
   17 trans. acc.  164979 tested
    1 events did not improve the fit, DAMP = 0.010000
Object number  2 at test 91.  Previous minimum R=0.205 at test 91
   28 rot. acc.  495724 gen. and  495724 tested; Chi**2=0.205    , R=0.205
    4 trans. acc.  165240 tested
    1 events did not improve the fit, DAMP = 0.010000
Object number  3 at test 91.  Previous minimum R=0.205 at test 91
   16 moves acc.  659766 tested; Chi**2=0.205    , R=0.205
    0 perm. acc.       0 tested
    0 events did not improve the fit, DAMP = 0.010000

Object number  1 at test 91.  Previous minimum R=0.205 at test 91
   21 rot. acc.  499798 gen. and  499798 tested; Chi**2=0.354    , R=0.205
   17 trans. acc.  166598 tested
    1 events did not improve the fit, DAMP = 0.010000
Object number  2 at test 91.  Previous minimum R=0.205 at test 91
   28 rot. acc.  500597 gen. and  500597 tested; Chi**2=0.354    , R=0.205
    4 trans. acc.  166865 tested
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     1 events did not improve the fit, DAMP = 0.010000
  Object number  3 at test 91.  Previous minimum R=0.205 at test 91
    16 moves acc.  666141 tested; Chi**2=0.354    , R=0.205
     0 perm. acc.       0 tested
     0 events did not improve the fit, DAMP = 0.010000

 Final coordinates x,y,z and occupation numbers

Ca1     0.82613    0.23028    0.14772      1.000
O1      0.63230    0.12989    0.30893      1.000
O2      1.02361    0.41504    0.16112      1.000
O3      1.04694    0.10496    0.31236      1.000
O4      0.94445    0.17538   -0.12679      1.000
O5      0.68628   -0.00614   -0.11182      1.000
O6      0.57420    0.26917   -0.14694      1.000
O7      0.65897    0.41042    0.29716      1.000
O8      0.95530    0.33198    0.60292      1.000
C1      0.81324    0.63712    0.94250      1.000
C2      0.92879    0.75730    1.15273      1.000
C3      0.84103    0.81702    1.33016      1.000
C4      0.82056    0.71744    1.46449      1.000
O1      0.74903    0.89792    0.41213      1.000
O2      0.27325    0.49017    0.19958      1.000
 28-Apr-2008     19 hour 13 min  2 Sec

 End of this test
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