```
$ fliprot 1mfm-sf.cif SG=19 name=mfm

 ==================================================
 !      Ab initio phasing by Charge flipping      !
 !         Biological macromolecule crystal       !
 !           version   january 15, 2012           !
 ==================================================

Enter the 6 unit cell parameters a, b,c,alpha,beta,gamma:
 enter a: 34.99
 enter b: 48.11
 enter c: 81.08
 enter alpha: 90
 enter beta: 90
 enter gamma: 90

Cell parameters are 34.99 48.11 81.08 90 90 90
Now converting 1mfm-sf.cif file to MTZ format
Generate a Fobs/SIGFobs columns from Iobs in the MTZ file

-------------------  Crystal data --------------------
cifin file  or           .......  1mfm-sf.cif
mtzin file               .......  mfm_fromcif.mtz
label for amplitude or I .......  I
generic name             .......  mfm
dmin resolution limit    .......  1.020 A
dmax resolution limit    .......  30.0 A
unit cell parameters     .......  34.9900 48.1100 81.0800 90.0000 90.0000 90.0000
SG symmetry number       .......  19

----------------  CF parameters used  -----------------
ked coefficient          .......  1.3
weak threshold           .......  0.05
convergence mode         .......  symmetry
convergence threshold    .......  75.0
polishing LDE cycles    ........  50
maximum cycles / trial   ......  10000
additional cycles        .......  100
number of repeated trials  .....  never
--------------------------------------------------

Press ENTER to continue

Preparing input hkl file for SUPERFLIP using observed intensity


             ***  SUPERFLIP running  ***
           version 09/05/11 14:22 required

The input file mfm.inflip was succesfully read.
Start of the calculation: 18.JAN 2012, 10:55:19
Processing the reflections...
Coverage statistics of the expanded reflections by shells:
Resolution (sin(th)/l):    0.050    0.100    0.150    0.200    0.250    0.300    0.350    0.400
Resolution (d_min):       10.000    5.000    3.333    2.500    2.000    1.667    1.429    1.250
Obs. refl. in shell:         267     2040     5578    10679    17802    26372    36628    48013
Total refl. in shell:        329     2162     5770    10935    18006    26658    37118    49161
Coverage in shell:         81.2%    94.4%    96.7%    97.7%    98.9%    98.9%    98.7%    97.7%
Cummulative coverage:      81.2%    92.6%    95.4%    96.7%    97.8%    98.2%    98.4%    98.2%

Resolution (sin(th)/l):    0.450    0.490
Resolution (d_min):        1.111    1.020
Obs. refl. in shell:       60175    54936
Total refl. in shell:      63164    61794
Coverage in shell:         95.3%    88.9%
Cummulative coverage:      97.3%    95.4%

...successfully finished.

Starting iteration:

Estimated delta:  0.0052
Random seed: 105521824

Current k_ed =    1.30000  (absolute delta =   0.00682)
   10  R: 54.396  Charge:     203.17   Peaks:  1.00  Sym:100.00   Score:    ---
   20  R: 54.349  Charge:     200.39   Peaks:  1.21  Sym: 99.78   Score:    ---
   30  R: 54.163  Charge:     197.41   Peaks:  1.40  Sym: 99.78   Score:    ---
   40  R: 54.131  Charge:     194.42   Peaks:  1.58  Sym: 99.75   Score:    ---
```

Commentaire: Input shell command using all default parameters except SG and unit cell parameters (space-group information not present in the CIF file)

Commentaire: Enter unit-cell parameters

Commentaire: Default parameters for ked and weak

Commentaire: sym score is used to detect convergence and is computed at cycles 20,40,60,80,100,200,...)

```
    50  R: 54.204  Charge:     193.62   Peaks:  1.71  Sym: 99.75   Score:    ---
    60  R: 54.156  Charge:     191.96   Peaks:  1.85  Sym: 99.92   Score:    ---
    70  R: 54.125  Charge:     191.66   Peaks:  1.91  Sym: 99.92   Score:    ---
    80  R: 54.105  Charge:     191.06   Peaks:  2.05  Sym: 99.95   Score:    ---
    90  R: 54.088  Charge:     189.33   Peaks:  2.13  Sym: 99.95   Score:    ---
   100  R: 53.941  Charge:     189.39   Peaks:  2.14  Sym:100.28   Score:    ---
   200  R: 54.002  Charge:     185.84   Peaks:  2.61  Sym: 99.93   Score:    ---
   300  R: 54.252  Charge:     184.61   Peaks:  2.89  Sym:100.01   Score:    ---
   400  R: 54.230  Charge:     182.47   Peaks:  3.10  Sym: 99.82   Score:    ---
   500  R: 54.276  Charge:     181.97   Peaks:  3.46  Sym: 99.84   Score:    ---
   600  R: 54.245  Charge:     181.30   Peaks:  3.60  Sym:100.06   Score:    ---
   700  R: 54.274  Charge:     181.21   Peaks:  3.70  Sym: 99.68   Score:    ---
   800  R: 54.130  Charge:     181.05   Peaks:  3.79  Sym: 99.75   Score:    ---
   900  R: 54.266  Charge:     179.57   Peaks:  3.84  Sym: 97.90   Score:    ---
  1000  R: 54.173  Charge:     180.57   Peaks:  3.98  Sym:100.07   Score:    ---
  1300  R: 50.447  Charge:     147.23   Peaks: 10.17  Sym: 61.69   Score:    ---
Calculation successfully converged after  1300 cycles.

    50 cycles of noise suppression follow:
    10  R: 34.521  Charge:       0.00   Peaks: 39.24
    20  R: 34.084  Charge:       0.00   Peaks: 38.55
    30  R: 34.035  Charge:       0.00   Peaks: 38.42
    40  R: 34.024  Charge:       0.00   Peaks: 38.39
    50  R: 34.018  Charge:       0.00   Peaks: 38.39


Checking the density for symmetry:

Symmetry operations compatible with the lattice and centering:
                              Symmetry operation               agreement factor
      2_1(0,0,1):            -x1          -x2       1/2+x3     0.085
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      2_1(1,0,0):        1/2+x1           -x2          -x3     0.107
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      2_1(0,1,0):            -x1       1/2+x2          -x3     0.169
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
        m(0,1,0):             x1          -x2           x3    85.503    XXXXXXX
              -1:            -x1          -x2          -x3    85.538    XXXXXXX
        m(1,0,0):            -x1           x2           x3    89.723    XXXXX
        m(0,0,1):             x1           x2          -x3    93.811    XXX
        2(0,1,0):            -x1           x2          -x3    94.784    XXX
        b(0,0,1):             x1       1/2+x2          -x3    95.341    XX
        n(0,1,0):        1/2+x1           -x2       1/2+x3    95.408    XX
        2(1,0,0):             x1          -x2          -x3    95.807    XX
        2(0,0,1):            -x1          -x2           x3    96.723    XX
        n(0,0,1):        1/2+x1       1/2+x2          -x3    96.946    XX
        c(0,1,0):             x1          -x2       1/2+x3    97.955    X
        a(0,0,1):        1/2+x1           x2          -x3   101.371    X
        n(1,0,0):            -x1       1/2+x2       1/2+x3   101.633    X
        b(1,0,0):            -x1       1/2+x2           x3   102.172    X
        c(1,0,0):            -x1           x2       1/2+x3   102.610    X
        a(0,1,0):        1/2+x1           -x2           x3   103.925    X


*************************************************
Space group derived from the symmetry operations:
*************************************************
    HM symbol:      P212121
    Hall symbol:    p 2ac 2ab
    Fingerprint:    3300223}040qW3 (0,3/4,1/2)
    Symmetry operations:
               1:             x1           x2           x3
      2_1(0,0,1):        1/2-x1           -x2       1/2+x3
      2_1(1,0,0):        1/2+x1        1/2-x2          -x3
      2_1(0,1,0):            -x1       1/2+x2       1/2-x3

Searching for the origin of the space group:
Agreement factors of individual generators:
Number smb agreement
   2   21       0.09
   3   21       0.11

Overall agreement factor:    0.12

End of the calculation: 18.JAN 2012, 10:58:19
Superflip version: 09/05/11 14:22

         ***********  SUPERFLIP procedure finished  **********
```

Commentaire: Convergence is detected at cycle 1300 (Sym<75, the default sym-threshold value).

Commentaire: Independent control on the quality of the map obtained by CF: the symmetry is derived from the P1 map (eventually, presence of potential higher crystallographic symmetry)

Commentaire: The P1 map is now constrained to obey the input XL symmetry properties: the agreement score is very good << 5-10)

```
      Input file for SUPERFLIP   ......................   mfm.inflip
      Input hkl-amplitude file for SUPERFLIP  ........   mfm.hkl
      SUPERFLIP logfile in  ........................   mfm.sflog
      Best CF density map FT{Enorm; PHIcf}  ..........   mfm.map
      Output HKL file with CF phased reflections .....   mfm-phased.hkl
      Output MTZ file with CF phased reflections .....   mfm.mtz
        containing h k l,  Fobs amplitudes, Ecf=Enorm and phases PHIcf
```

Commentaire: this file

Commentaire: electron-density map in CCP4 format, symmetry P212121 (*but CCP4 header with P1 symmetry)*

```
=================================================================
 Using Charge flipping phased diffraction data for model building

 Automated protein model building with ARP/wARP (version 7.x):
 example with 2anv model:
   2*146 residues and 2anv.seq the corresponding protomer sequence file

 Setup the proper environment for ARP/wARP and run the command line:
$warpbin/auto_tracing.sh   datafile mfm.mtz     residues 153    \
 fp Fobs sigfp SIGFP phibest PHIcfi   seqin 1mfm.seq  buildingcycles 5

=================================================================
```

Commentaire: test the 2 phase sets PHIcf and PHIcfi for the correct hand

```
# setup PHENIX environment
$ phenix.get_cc_mtz_pdb mfm.mtz 1MFM.pdb labin="FP=Fobs PHIB=PHIcf"
#                       get_cc_mtz_pdb
#
# Get correlation between atoms in a PDB file and map
# offsetting the PDB file by allowed origin shifts

Correlation in region of model:  0.159 ...overall:  0.154
overall CC:  0.154
local CC:  0.159


$ phenix.get_cc_mtz_pdb mfm.mtz 1MFM.pdb labin="FP=Fobs PHIB=PHIcfi"
#                       get_cc_mtz_pdb
#
# Get correlation between atoms in a PDB file and map
# offsetting the PDB file by allowed origin shifts
....
Offset PDB file is in offset.pdb

Correlation in region of model:  0.823 ...overall:  0.816
overall CC:  0.816
local CC:  0.823

# display Charge Flipping map and model
$ coot --pdb offset.pdb --data mfm.mtz
```

Commentaire: The CC score is poor: the phase set used (PHIcf) corresponds to the wrong enantiomer

Commentaire: The CC score is good and corresponds to the correct phase set with PHIcfi label.