```
$ fliprot 2anv-sf.cif name=anv SG=5

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

Now converting 2anv-sf.cif file to MTZ format

--------------------  Crystal data ---------------------
cifin file  or           .......  2anv-sf.cif
mtzin file               .......  anv_fromcif.mtz
label for amplitude or I .......  FP
generic name             .......  anv
dmin resolution limit    .......  1.038 A
dmax resolution limit    .......  30.0 A
unit cell parameters     .......  134.0130 50.4150 46.5870 90.0000 103.7980 90.0000
SG symmetry number       .......  5

----------------  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
--------------------------------------------------

Preparing input hkl file for SUPERFLIP using observed amplitude


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

The input file anv.inflip was succesfully read.
Start of the calculation: 18.JAN 2012, 14:46:51
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:         255     2255     5937    11977    19628    29271    40808    54252
Total refl. in shell:        335     2301     6170    11990    19628    29352    40915    54328
Coverage in shell:         76.1%    98.0%    96.2%    99.9%   100.0%    99.7%    99.7%    99.9%
Commulative coverage:      76.1%    95.2%    95.9%    98.2%    99.1%    99.4%    99.5%    99.6%

Resolution (sin(th)/l):    0.450    0.482
Resolution (d_min):        1.111    1.038
Obs. refl. in shell:       69709    52253
Total refl. in shell:      69804    53060
Coverage in shell:         99.9%    98.5%
Commulative coverage:      99.7%    99.5%

...successfully finished.

Starting iteration:

Estimated delta:  0.0025
Random seed: 144655584

Current k_ed =    1.30000  (absolute delta =   0.00320)
   10  R: 52.485  Charge:     214.87   Peaks:  1.00  Sym:100.00   Score:    ---
   20  R: 52.412  Charge:     212.27   Peaks:  1.21  Sym: 99.18   Score:    ---
   30  R: 52.362  Charge:     209.86   Peaks:  1.37  Sym: 99.18   Score:    ---
   40  R: 52.399  Charge:     208.34   Peaks:  1.54  Sym: 99.09   Score:    ---
   50  R: 52.289  Charge:     206.35   Peaks:  1.82  Sym: 99.09   Score:    ---
   60  R: 52.118  Charge:     204.23   Peaks:  2.27  Sym: 99.36   Score:    ---
   70  R: 52.291  Charge:     200.65   Peaks:  3.42  Sym: 99.36   Score:    ---
   80  R: 52.257  Charge:     196.32   Peaks:  4.99  Sym: 93.41   Score:    ---
   90  R: 52.157  Charge:     194.18   Peaks:  6.51  Sym: 93.41   Score:    ---
  100  R: 52.021  Charge:     191.20   Peaks:  7.64  Sym: 91.11   Score:    ---
  200  R: 51.724  Charge:     181.58   Peaks: 13.83  Sym: 83.74   Score:    ---
  300  R: 49.186  Charge:     156.86   Peaks: 21.84  Sym: 61.84   Score:    ---
  400  R: 49.114  Charge:     156.91   Peaks: 21.94  Sym: 61.84   Score:    ---

Calculation successfully converged after   400 cycles.
```

Commentaire: input command using all default parameters except SG (space-group information not present in the CIF file).

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,...

Commentaire: Convergence is detected at cycle 400 (Sym<75, the default sym-threshold value); 100 additional cycles are added.

```
    50 cycles of noise suppression follow:
   10  R: 34.262  Charge:       0.00   Peaks:128.77
   20  R: 33.453  Charge:       0.00   Peaks:125.28
   30  R: 33.321  Charge:       0.00   Peaks:123.73
   40  R: 33.281  Charge:       0.00   Peaks:123.19
   50  R: 33.265  Charge:       0.00   Peaks:122.98
```

Commentaire: 50 cycles of LDE density modification are added to improve the solution

```
Checking the density for symmetry:

Centering vectors:
  0.000  0.000  0.000
  0.500  0.500  0.000

Symmetry operations compatible with the lattice and centering:
                          Symmetry operation             agreement factor
       2(0,1,0):          -x1          x2          -x3    0.048    XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
       m(0,1,0):           x1         -x2           x3   63.582    XXXXXXXXXXXXXXXXX
            -1:           -x1         -x2          -x3   63.642    XXXXXXXXXXXXXXXXX
       c(0,1,0):           x1          -x2       1/2+x3  100.247    X
```

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

```
************************************************
Space group derived from the symmetry operations:
************************************************
    HM symbol:      C2
    Hall symbol:    c 2y
    Fingerprint:    33121060qW0 (0,0,0)
    Centering vectors:
      0.000  0.000  0.000
      0.500  0.500  0.000
    Symmetry operations:
             1:           x1          x2          x3
       2(0,1,0):          -x1          x2          -x3

Searching for the origin of the space group:
Agreement factors of individual generators:
Number smb agreement
   2   2        0.05

Overall agreement factor:    0.05

End of the calculation: 18.JAN 2012, 14:49:54
Superflip version: 09/05/11 14:22
```

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

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

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

Commentaire: this file

Commentaire: eletron-density map in CCP4 format, symmetry C2 (*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 anv.mtz  residues 292   fp FP sigfp SIGFP phibest PHIcfi  \
 seqin 2anv.seq   cgr 2   buildingcycles 5

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

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

```
#setup PHENIX environment:
$ phenix.get_cc_mtz_pdb anv.mtz 2ANV.pdb labin="FP=FP 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:  0.228 ...overall:  0.219
overall CC:  0.219
local CC:  0.228
```

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

```
$ phenix.get_cc_mtz_pdb anv.mtz 2ANV.pdb labin="FP=FP 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:  0.814 ...overall:  0.803
overall CC:  0.803
local CC:  0.814

# Display the Charge flipping map and the reference model
$ coot --pdb offset.pdb  --data anv.mtz
```

Commentaire: The CC is good: the correct phases in the anv.mtz file correspond to PHIcfi label.