Supplementary Materials.

Example of input files and output file in the refinement of DL-Ala-Met dipeptide.

- Reflection Intensities available from IUCR journals website at publication:
Guillot *et al*. *Acta Cryst.* (2001). B**57**, 567-578 [doi:10.1107/S0108768101007212]

Input File “mopro.tab”

```
!----------------- Carbon ---------------------------------------------
CHEM C
CORE WAVE 1s2
VALE 4. WAVE 1s0 2s2 2p2
MONO 0. SLAT 2 0.
DIPO    SLAT 2 3.
QUAD    SLAT 2 3.
OCTA    SLAT 3 3.
HEXA    SLAT 4 3.
! ANOM use asf_Kissel.dat

!---------- Nitrogen -------------
CHEM N
CORE WAVE 1s2
VALE 5. WAVE 1s0 2s2 2p3
MONO 0. SLAT 2 3.8
DIPO    SLAT 2 3.8
QUAD    SLAT 2 3.8
OCTA    SLAT 3 3.8
HEXA    SLAT 4 3.8
!ANOM  use asf_Kissel.dat

!----------------- Hydrogen ---------
CHEM H
CORE WAVE 1s0
VALE 1. WAVE 1s1
MONO 0. SLAT 1 1.
DIPO    SLAT 1 2.26
QUAD    SLAT 2 2.26
ANOM  0.0  0.0

!----------------- Oxygen -----------
CHEM O
CORE WAVE 1s2
VALE 6. WAVE 2s2 2p4
MONO 0. SLAT 2 1.
DIPO    SLAT 2 4.5
QUAD    SLAT 2 4.5
OCTA    SLAT 3 4.5
HEXA    SLAT 4 4.5
!ANOM use asf_Kissel.dat


!------------ Sulfur ------------
CHEM S
CORE WAVE 1s2 2s2 2p6
VALE 6. WAVE 3s2 3p4
MONO 0. SLAT 4 1.
DIPO    SLAT 4 4.1
QUAD    SLAT 4 4.1
OCTA    SLAT 6 4.1
HEXA    SLAT 8 4.1
!ANOM  use asf_Kissel.dat
```

FILE "CONSTRAIN"

```
AVEPLM  ALA  H1  H2  H3
AVEPLM  ALA  HB1  HB2  HB3
AVEPLM  MET  HB1  HB2
AVEPLM  MET  HG1  HG2
AVEPLM  MET  HE1  HE2  HE3
AVEPLM  ALL  HA
AVEPLM  ALA  H1   MET  H0

AVEPLM  ALL  CA
AVEPLM  MET  OT1  OT2

SYMPLM  3m  MET  CE
SYMPLM  3m  ALA  NT
SYMPLM  3m  ALA  CB
SYMPLM  mymz  MET  CT
SYMPLM  mxmy  MET  CB
SYMPLM  mxmy  ALL  CA
SYMPLM  mxmy  MET  SD
SYMPLM  mz  MET  CG
SYMPLM  mz  MET  N
SYMPLM  mz  MET  OT1
SYMPLM  mz  MET  OT2
SYMPLM  mz  ALA  C
SYMPLM  mz  ALA  O
CONANG  AXHHH  MET   CE SD  HE1  HE2  HE3
CONANG  AXHHH  ALA   CB CA  HB1  HB2  HB3
CONANG  AXHHH  ALA   NT CA  H1   H2   H3
CONANG  AXYZH  ALA   CA C   NT   CB   HA
CONANG  AXYZH  MET   CA C   NT   CB   HA
CONANG  AXYH   ---   N  CA  H0   C
CONANG  AXYHH  MET   CG CB  SD   HG1  HG2
CONANG  AXYHH  MET   CB CA  CG   HB1  HB2
```

FILE "RESTRAIN"

```
KAPVAL   H           0.001
KAPVAL   C O N  S    0.001
RIGIDB  ALL BON  0.001
RIGIDB  ALL ANG  0.004
PLANAR  4   ++2  C  O  N  H0   0.01

DISTAN  H1  1  NT   1  1.033   0.01
DISTAN  H2  1  NT   1  1.033   0.01
DISTAN  H3  1  NT   1  1.033   0.01
DISTAN  ALA  HB1  CB   1.059   0.01
DISTAN  ALA  HB2  CB   1.059   0.01
DISTAN  ALA  HB3  CB   1.059   0.01
DISTAN  ALL   HA  CA   1.099   0.01
DISTAN  ALL   N   H0   1.009   0.01
DISTAN  MET  HB1  CB   1.083   0.01
DISTAN  MET  HB2  CB   1.083   0.01
DISTAN  MET  HG1  CG   1.083   0.01
DISTAN  MET  HG2  CG   1.083   0.01
DISTAN  MET  HE1  CE   1.059   0.01
DISTAN  MET  HE2  CE   1.059   0.01
DISTAN  MET  HE3  CE   1.059   0.01

ANGLER  H1 1  NT 1  H2 1  109.5   2.
ANGLER  H2 1  NT 1  H3 1  109.5   2.
ANGLER  H3 1  NT 1  H1 1  109.5   2.
ANGLER  MET  HE1  CE  HE3   109.5   2.
ANGLER  MET  HE2  CE  HE1   109.5   2.
ANGLER  MET  HE2  CE  HE3   109.5   2.

SIMVAL   MET  OT1  OT2  0.02
SIMVAL   MET  CA   ALA  CA   0.02
SIMPLM   MET  CE   ALA  CB   0.02
SIMKAP   ALL  CA     0.02
```

FILE alamet.17 (molecular parameters file)

```
! MOPRO.3      17/09/2004     alamet.17  am.Ihkl
!  RF  factor =  4.796  %        RI  factor =  3.279%
! wR2F factor =  2.293  %       wR2I factor =  4.276%
! g.o.f. =   1.657  Nobs=    11196  Nfree=        0


CELL 13.096   5.343  15.926  90.000 108.560  90.000   0.559

SYMM    2  P   CENTRO
 X , Y,  Z
 -X , 1/2+Y,  1/2-Z

SCALE    1     1.86625

FMULT     1.00000

UOVER     0.00000

SOLVT     0.00000     0.00000

EXTIN  0.00000


DUMMY    0

KAPPA   18
  0.997616  0.957872         !  # 1   NT    ALA   1        1x
  1.182632  1.089413         !  # 2   H1    ALA   1        3x
  1.004958  1.031170         !  # 3   CA    ALA   1        2x
  1.164468  1.019748         !  # 4   HA    ALA   1        2x
  1.003445  0.950545         !  # 5   CB    ALA   1        1x
  1.157067  1.089907         !  # 6   HB1   ALA   1        6x
  1.012128  0.998906         !  # 7   C     ALA   1        1x
  1.006920  1.055804         !  # 8   O     ALA   1        1x
  1.002698  0.979914         !  # 9   N     MET   2        1x
  1.173289  1.075498         !  #10   H0    MET   2        1x
  1.008866  0.987624         !  #11   CT    MET   2        1x
  1.006003  1.011691         !  #12   OT1   MET   2        1x
  1.006001  0.866173         !  #13   OT2   MET   2        1x
  1.000899  1.003057         !  #14   CB    MET   2        1x
  1.158692  1.152659         !  #15   HB1   MET   2        4x
  1.006283  0.962734         !  #16   CG    MET   2        1x
  1.007159  1.026934         !  #17   SD    MET   2        1x
  1.016088  0.976515         !  #18   CE    MET   2        1x

ATOMS   30

ATOM     1  NT    ALA    1  0.427395  0.049973  0.613829  1.0 1 N
 ZX  CA   H1          OCT  K1    V0   M0   Q0
UANI  0.012855  0.010159  0.009568  -.000229  0.005238  -.000548
  5.442  0.     0.     0.     -.056  -.045  0.     0.     0.     0.
  0.160  0.     0.     0.     0.     0.147  0.

ATOM     2  H1    ALA    1  0.412275  0.234717  0.594817  1.0 1 H
 ZX  NT   CA          DIP  K2    V0   M0   Q0
UISO  0.016015
  0.738  0.     0.     0.     0.122
```

```
ATOM     3  H2    ALA    1  0.507063  0.021174  0.650709  1.0 1 H
 ZX  NT   CA          DIP  K2    V1_H1   M0   Q0
UISO  0.016068
  0.738  0.     0.     0.     0.122

ATOM     4  H3    ALA    1  0.417026 -0.047982  0.555781  1.0 1 H
 ZX  NT   CA          DIP  K2    V1_H1   M0   Q0
UISO  0.016969
  0.738  0.     0.     0.     0.122

ATOM     5  CA    ALA    1  0.354123 -0.047046  0.660375  1.0 1 C
mZX  CB   C           OCT  K3    V0   M0   Q0
UANI  0.013031  0.010060  0.008517  -.000898  0.004525  -.000558
  4.194  0.     0.     0.     0.024  0.017  0.     0.     0.023  0.
  0.006  0.     0.     0.252  0.     0.     0.

ATOM     6  HA    ALA    1  0.374115 -0.245225  0.675533  1.0 1 H
 ZX  CA   NT          DIP  K4    V2_HA   M0   Q0
UISO  0.013150
  0.857  0.     0.     0.     0.152

ATOM     7  CB    ALA    1  0.237763 -0.027485  0.599633  1.0 1 C
 ZX  CA   HB1         OCT  K5    V0   M0   Q0
UANI  0.012708  0.023634  0.012676  -.001939  0.003855  -.003857
  4.245  0.     0.     0.     -.040  0.002  0.     0.     0.     0.
  0.201  0.     0.     0.     0.     0.154  0.

ATOM     8  HB1   ALA    1  0.183911 -0.078047  0.634237  1.0 1 H
 ZX  CB   CA          DIP  K6    V0   M0   Q0
UISO  0.025159
  0.880  0.     0.     0.     0.090

ATOM     9  HB2   ALA    1  0.226694 -0.145976  0.544134  1.0 1 H
 ZX  CB   CA          DIP  K6    V1_HB1   M0   Q0
UISO  0.024349
  0.880  0.     0.     0.     0.090

ATOM    10  HB3   ALA    1  0.220759  0.160634  0.578957  1.0 1 H
 ZX  CB   CA          DIP  K6    V1_HB1   M0   Q0
UISO  0.024392
  0.880  0.     0.     0.     0.090

ATOM    11  C     ALA    1  0.367965  0.106310  0.744109  1.0 1 C
 XY  O   2_N          OCT  K7    V0   M0   Q0
UANI  0.013478  0.009803  0.007761  -.000746  0.004393  0.000002
  3.963  0.     0.072  0.026  0.     -.212  0.   0.   0.043  -.022
  0.     -.006  0.021  0.     0.     0.251  -.042

ATOM    12  O     ALA    1  0.390380  0.332262  0.747483  1.0 1 O
 XY  C   2_N          OCT  K8    V0   M0   Q0
UANI  0.021275  0.010127  0.010600  -.003503  0.006313  -.000957
  6.130  0.     -.066  0.011  0.     -.036  0.   0.   -.018  -.015
  0.     -.002  -.013  0.     0.     0.028  -.002

ATOM    13  N     MET    2  0.347616 -0.020193  0.809614  1.0 1 N
mXY  1_C   CA          OCT  K9    V0   M0   Q0
UANI  0.017137  0.009890  0.008737  -.001026  0.006241  -.000148
  5.273  0.     0.012  -.010  0.     0.007  0.   0.   0.027  -.009
  0.     0.022  -.019  0.     0.     -.150  0.008

ATOM    14  H0    MET    2  0.339968 -0.208036  0.804984  1.0 1 H
```

```
 ZX  N   1_C          DIP  K10   V0   M1_H1   Q0
UISO  0.021778
  0.798  0.     0.     0.     0.122

ATOM    15  CA    MET    2  0.345400  0.098131  0.891398  1.0 1 C
mZX  CB   CT          OCT  K3    V1_CA   M0   Q0
UANI  0.013276  0.009490  0.008377  -.000718  0.004572  0.000014
  4.194  0.     0.     0.     0.024  0.017  0.     0.    0.023  0.
  0.006  0.     0.     0.252  0.     0.     0.

ATOM    16  HA    MET    2  0.406790  0.245856  0.911402  1.0 1 H
 ZX  CA   N           DIP  K4    V0   M0   Q0
UISO  0.012697
  0.857  0.     0.     0.     0.152

ATOM    17  CT    MET    2  0.375351 -0.095659  0.966537  1.0 1 C
mXY  OT1   OT2        OCT  K11   V0   M0   Q0
UANI  0.012635  0.008928  0.007970  -.000819  0.003875  -.000194
  4.071  0.     0.068  0.     0.     -.248  0.   0.    -.097  0.
  0.     -.008  0.     0.     0.     -.334  0.

ATOM    18  OT1   MET    2  0.382669 -0.019327  1.042819  1.0 1 O
 XY  CT   OT2         OCT  K12   V0   M0   Q0
UANI  0.024143  0.010915  0.008443  -.001057  0.006199  -.000789
  6.161  0.     -.062  -.016  0.     -.027  0.   0.   -.058  0.011
  0.     -.013  -.017  0.     0.     0.025  0.001

ATOM    19  OT2   MET    2  0.389000 -0.319190  0.947533  1.0 1 O
 XY  CT   OT1         OCT  K13   V2_OT1   M0   Q0
UANI  0.019221  0.009258  0.011281  0.000602  0.006341  -.000110
  6.161  0.     -.062  -.016  0.     -.027  0.   0.   -.058  0.011
  0.     -.013  -.017  0.     0.     0.025  0.001

ATOM    20  CB    MET    2  0.235370  0.218244  0.880899  1.0 1 C
mZX  CA   CG          OCT  K14   V0   M0   Q0
UANI  0.014041  0.011495  0.011914  0.000753  0.004584  0.000390
  4.333  0.     0.     0.     0.010  0.003  0.   0.   0.001  0.
  -.020  0.     0.     0.290  0.     0.     0.

ATOM    21  HB1   MET    2  0.214969  0.344354  0.823998  1.0 1 H
 ZX  CB   CA          DIP  K15   V0   M0   Q0
UISO  0.015230
  0.831  0.     0.     0.     0.074

ATOM    22  HB2   MET    2  0.243717  0.330061  0.940109  1.0 1 H
 ZX  CB   CA          DIP  K15   V2_HB1   M0   Q0
UISO  0.015742
  0.831  0.     0.     0.     0.074

ATOM    23  CG    MET    2  0.145930  0.026576  0.869949  1.0 1 C
mZX  CB   SD          OCT  K16   V0   M0   Q0
UANI  0.013292  0.014131  0.019634  0.000080  0.004853  0.000710
  4.145  0.     -.011  -.012  0.     0.034  0.   0.   -.030  0.025
  0.     0.012  -.042  0.     0.     -.026  -.010

ATOM    24  HG1   MET    2  0.165283 -0.092307  0.925506  1.0 1 H
 ZX  CG   CB          DIP  K15   V0   M2_HB1   Q0
UISO  0.020194
  0.958  0.     0.     0.     0.074

ATOM    25  HG2   MET    2  0.132166 -0.079067  0.812272  1.0 1 H
```

```
 ZX  CG   CB          DIP  K15   V2_HG1   M0   Q0
UISO  0.019623
  0.958  0.     0.     0.     0.074

ATOM    26  SD    MET    2  0.020941  0.184471  0.861972  1.0 1 S
mZX  CG   CE          HEX  K17   V0   M0   Q0
UANI  0.015168  0.018258  0.031337  0.002188  0.010193  0.003353
  6.120  0.     0.     0.     0.039  0.047  0.   0.   -.106  0.
  -.103  0.     0.     0.190  0.     0.     0.
  -.160  0.     0.     0.098  0.     0.     0.     0.039  0.

ATOM    27  CE    MET    2 -0.059655 -0.085636  0.866673  1.0 1 C
 ZX  SD   HE1         OCT  K18   V0   M0   Q0
UANI  0.017564  0.025008  0.031568  -.003707  0.008855  0.001608
  3.811  0.     0.     0.     -.064  -.038  0.     0.     0.     0.
  0.152  0.     0.     0.     0.     0.110  0.

ATOM    28  HE1   MET    2 -0.055525 -0.219137  0.821564  1.0 1 H
 ZX  CE   SD          DIP  K6    V0   M1_HB1   Q0
UISO  0.036975
  0.936  0.     0.     0.     0.090

ATOM    29  HE2   MET    2 -0.140861 -0.029749  0.854863  1.0 1 H
 ZX  CE   SD          DIP  K6    V2_HE1   M0   Q0
UISO  0.038173
  0.936  0.     0.     0.     0.090

ATOM    30  HE3   MET    2 -0.031745 -0.173169  0.928202  1.0 1 H
 ZX  CE   SD          DIP  K6    V2_HE1   M0   Q0
UISO  0.038055
  0.936  0.     0.     0.     0.090

ANHAR    1    3
          26       SD              2
-6.39E-06 1.29E-04 1.44E-05-4.65E-05 1.99E-04 1.01E-04 1.47E-04-
1.78E-04
-5.11E-04-5.54E-04


STOP
```

FILE mopro.inp

```
FILE   PARA   alamet.17
FILE   DATA   am.Ihkl

FILE   CONS   ./CONSTRAIN
FILE   REST   RESTRAIN
FILE   TABL   ~/LibMoPro/mopro.tab
FILE   WAVE   ~/LibMoPro/WAVEF
FILE   ANOM   ~/LibMoPro/asf_Kissel.dat

VERB SHELL 10  DELF 6  SHIFT 0. CGC  AXES
VERB  CORR   0.9   SIGC 0.
HKLI  I      ! input = intensities
HKLR  F      ! refine versus F

SELE  {  XYZ  NOH    ! select  variables to refine
REFI  LS  1      ! perform 1 cycles of least squares

WRIT DIST           ! analyze distances
WRIT PDB   alamet.17.pdb
STOP
```

FILE mopro.out

```
     -------------------------------------------
     |--> Applying : FILE   PARA   alamet.17   |
     -------------------------------------------


=====================================================================
================== Parameters input from file : alamet.17
=====================================================================

---> Cell parameters
 a           =     13.096 A
 b           =      5.343 A
 c           =     15.926 A
 Alpha       =     90.000 deg.
 Beta        =    108.560 deg.
 Gamma       =     90.000 deg.
 Cell volume =   1056.415 A3
 Wavelength  =    0.55900 A

---> Unit Cell content = H64 C32 N8 O12 S4

---> Crystal Symmetry
 Card No   1 /  2  =  X , Y,  Z
 Card No   2 /  2  =  -X , 1/2+Y,  1/2-Z
 The structure is centrosymmetric
 Lattice mode =  P
 Multiplicity =  2

---> Atomic parameters
 Number of atoms                                    :       30
 Number of atoms with isotropic thermal motion      :       16
 Number of atoms with anisotropic thermal motion    :       14
 Number of anharmonically vibrating atoms           :        1
 Highest order of Gram-Charlier coefficients        :        3
 Number of coefficients per atom (see mopro.check)  :       10
 Number of atoms with U converted from iso to aniso :        0
 Number of dummy atoms                              :        0
 Number of coeff. for the polynomial scale factor   :        1
 Number of kappa sets                               :       18
 The maximal number of multipoles per atoms is      :       37
 Total number of Parameters  (refined or not)       :     1552
 Disordered solvent modeling method                 : Exponential
but not applied :                         Ksol and Bsol are zero
 Total number of Valence Electrons                  :    81.99

=====================================================================

     -----------------------------------------
     |--> Applying : FILE   DATA   am.Ihkl   |
     -----------------------------------------

     ----------------------------------------------
     |--> Applying : FILE   CONS   ../CONSTRAIN   |
     ----------------------------------------------

     -----------------------------------------
     |--> Applying : FILE   REST   RESTRAIN   |
     -----------------------------------------
```

```
     -----------------------------------------------------
     |--> Applying : FILE   TABL   ~/LibMoPro/mopro.tab   |
     -----------------------------------------------------

     ---------------------------------------------------
     |--> Applying : FILE   WAVE   ~/LibMoPro/WAVEF   |
     ---------------------------------------------------

     -------------------------------------------------------------
     |--> Applying : FILE   ANOM   ~/LibMoPro/asf_Kissel.dat   |
     -------------------------------------------------------------

     ----------------------------------------------------------------
     |--> Applying : VERB SHELL 10  DELF 6  SHIFT 0. CGC  AXES   |
     ----------------------------------------------------------------

     ----------------------------------------------
     |--> Applying : VERB  CORR   0.7   SIGC 0.   |
     ----------------------------------------------
Print correlations larger            >   0.70


     ----------------------------
     |--> Applying : HKLI  I   |
     ----------------------------
Input reflections are (Ihkl/Fhkl)   : Ihkl

     ----------------------------
     |--> Applying : HKLR  F   |
     ----------------------------
Refinement versus Fhkl Structure Factors

     ----------------------------------
     |--> Applying : RESO  0.4  0.7   |
     ----------------------------------
 Resolution range
  Direct     :   0.400 -   0.700 A
  Reciprocal :   0.714 -   1.250 A-1

     --------------------------------------
     |--> Applying : SELE  {  XYZ  NOH   |
     --------------------------------------

     -------------------------------
     |--> Applying : REFI  LS  1   |
     -------------------------------

=====================================================================
================== Scattering factors from file
'~/LibMoPro/mopro.tab'
=====================================================================


---> List of   5 atom types :
        atom type     Nb of occurences
        ------------------------------
           [N]               2
           [H]              16
           [C]               8
           [O]               3
           [S]               1
```

```
-----------------------------------------------------------
 Chemical type  [N]
-----------------------------------------------------------

 [N] Core
    Orbital  : 1s --- Pop. =  2.

 [N] Slater function (r^nl)exp(-zr)
            Pval    P00    Dip    Qua    Oct    Hex    32P
    nl =      -3      2      2      2      3      4      0
    z  =   1.000  3.800  3.800  3.800  3.800  3.800  0.000

 [N] Valence --> monopole Pval
    Orbital  : 2s --- Pop. =  2.
    Orbital  : 2p --- Pop. =  3.

  Missing 'ANOM' for chemical [N]. Using values from Kissel (1995)
 [N] Anomalous Scattering Amplitudes  f' =  0.003(e)  f'' =
0.002(e)

-----------------------------------------------------------
 Chemical type  [H]
-----------------------------------------------------------

 [H] Core

 [H] Anomalous scattering amplitudes  f' =  0.000(e)  f'' =
0.000(e)

 [H] Slater function (r^nl)exp(-zr)
            Pval    P00    Dip    Qua    Oct    Hex    32P
    nl =      -3      1      1      2      0      0      0
    z  =   1.000  1.000  2.260  2.260  1.000  1.000  0.000

 [H] Valence --> monopole Pval
    Orbital  : 1s --- Pop. =  1.

-----------------------------------------------------------
 Chemical type  [C]
-----------------------------------------------------------

 [C] Core
    Orbital  : 1s --- Pop. =  2.

 [C] Slater function (r^nl)exp(-zr)
            Pval    P00    Dip    Qua    Oct    Hex    32P
    nl =      -3      2      2      2      3      4      0
    z  =   1.000  3.000  3.000  3.000  3.000  3.000  0.000

 [C] Valence --> monopole Pval
    Orbital  : 2s --- Pop. =  2.
    Orbital  : 2p --- Pop. =  2.

  Missing 'ANOM' for chemical [C]. Using values from Kissel (1995)
 [C] Anomalous Scattering Amplitudes  f' =  0.001(e)  f'' =
0.001(e)

-----------------------------------------------------------
 Chemical type  [O]
-----------------------------------------------------------
```

```
 [O] Core
    Orbital  : 1s --- Pop. =  2.

 [O] Slater function (r^nl)exp(-zr)
            Pval    P00    Dip    Qua    Oct    Hex    32P
    nl =      -3      2      2      2      3      4      0
    z  =   1.000  4.500  4.500  4.500  4.500  4.500  0.000

 [O] Valence --> monopole Pval
    Orbital  : 2s --- Pop. =  2.
    Orbital  : 2p --- Pop. =  4.

  Missing 'ANOM' for chemical [O]. Using values from Kissel (1995)
 [O] Anomalous Scattering Amplitudes  f' =  0.006(e)  f'' =
0.004(e)

-------------------------------------------------------------
 Chemical type  [S]
-------------------------------------------------------------

 [S] Core
    Orbital  : 1s --- Pop. =  2.
    Orbital  : 2s --- Pop. =  2.
    Orbital  : 2p --- Pop. =  6.

 [S] Slater function (r^nl)exp(-zr)
            Pval    P00    Dip    Qua    Oct    Hex    32P
    nl =      -3      4      4      4      6      8      0
    z  =   1.000  4.100  4.100  4.100  4.100  4.100  0.000

 [S] Valence --> monopole Pval
    Orbital  : 3s --- Pop. =  2.
    Orbital  : 3p --- Pop. =  4.

  Missing 'ANOM' for chemical [S]. Using values from Kissel (1995)
 [S] Anomalous Scattering Amplitudes  f' =  0.083(e)  f'' =
0.077(e)

 Constraining Equivalent Atoms to have same Charge Density
Parameters
           3  equivalencies

=====================================================================
================== Refined parameters selection :
=====================================================================

 NOH: hydrogen  atoms not refined
 XYZ: refining           42  positional parameters

 Constraining          14  Atoms to have Zero
 Multipoles Antisymmetric /Z /Y    INSTRUCTIONs

=====================================================================
================== Diffraction data from file 'am.Ihkl'
=====================================================================

  Format of input reflections (I/F)      :      I
  Total number of reflections read       :  11533
  Number of free reflections             :      0
  Overall resolution range               :  7.615 - 0.431 Angstrom
```

```
  Overall  sinTheta/Lambda range         :  0.066 - 1.161 A-1
  hmin =    0 hmax =   29
  kmin =    0 kmax =   12
  lmin =  -35 lmax =   33


=================================================================
================== Refinement Step No :   1
=================================================================

---> Step options summary
 Parameters to refine selection from file   : {  XYZ  NOH
 Nb Cycle(s) of least squares refinement    :        1
 Number of variables                        :       42
 Number of observations used                :     8572
 Refinement against (I/F)                   :    F
 Application of restrains in refinement     :  Yes, as asked
 Working resolution range (min-max A-1)     : 0.714 - 1.161
 I/sigmaI cutoff                            :      0.0
 Number of resolution shells                :       10
 Parameters shifts printed if (shift/s.u.)  >      0.0
 Weighting scheme             :  sig^2 = (a*sig^2 + b*Io^2)*D^c
  (a,b,c) coefficients                      :  1.000  0.00  0.00

================================================================


================================================================
==================  CYCLE :   1 / 1
================================================================

(%)  RF    wR2F   RI  wR2I  gof_F  gof_Ffree  RF_fr  wR2F_fr Nobs
>>  7.588  4.136  6.746 7.320 1.378 0.000    0.000   0.000   8572

PARAMETERS CORRELATION LARGER THAN:  0.7000
param1 param2 matrix correlation
 19    20     605  -0.740461   X    CA MET  2 &   Y   CA MET 2

Shifts summary: -->   <|shift/s.u.|> :    0.129
    --> MAX(|shift/s.u.|) :    0.926 for      Y    SD    MET  2

-----------------------------------------------------------------
PARAMETER        OLD VALUE    SHIFT    NEW VALUE  S.U.  SHIFT/S.U.
-----------------------------------------------------------------


 X    NT ALA 1   0.427395   0.000002   0.427397   0.000011    0.194
 Y    NT ALA 1   0.049973   0.000003   0.049976   0.000023    0.143
 Z    NT ALA 1   0.613829  -0.000001   0.613828   0.000008   -0.124

 X    CA ALA 1   0.354123   0.000002   0.354125   0.000026    0.093
 Y    CA ALA 1  -0.047046   0.000001  -0.047045   0.000028    0.025
 Z    CA ALA 1   0.660375  -0.000001   0.660374   0.000022   -0.050

 X    CB ALA 1   0.237763   0.000000   0.237763   0.000016   -0.011
 Y    CB ALA 1  -0.027485   0.000001  -0.027484   0.000022    0.054
 Z    CB ALA 1   0.599633   0.000000   0.599633   0.000010   -0.030

 X    C  ALA 1   0.367965  -0.000001   0.367964   0.000027   -0.029
 Y    C  ALA 1   0.106310  -0.000007   0.106303   0.000063   -0.107
```

```
 Z    C  ALA 1   0.744109   0.000000   0.744109   0.000022    0.015

 X    O  ALA 1   0.390380  -0.000002   0.390378   0.000030   -0.066
 Y    O  ALA 1   0.332262  -0.000028   0.332234   0.000059   -0.472
 Z    O  ALA 1   0.747483  -0.000001   0.747482   0.000022   -0.037

 X    N  MET 2   0.347616  -0.000001   0.347615   0.000028   -0.037
 Y    N  MET 2  -0.020193   0.000001  -0.020192   0.000024    0.038
 Z    N  MET 2   0.809614  -0.000002   0.809612   0.000022   -0.071

 X    CA MET 2   0.345400   0.000000   0.345400   0.000021   -0.010
 Y    CA MET 2   0.098131   0.000001   0.098132   0.000047    0.024
 Z    CA MET 2   0.891398  -0.000004   0.891394   0.000021   -0.183

 X    CT MET 2   0.375351   0.000000   0.375351   0.000027   -0.003
 Y    CT MET 2  -0.095659   0.000003  -0.095656   0.000060    0.048
 Z    CT MET 2   0.966537   0.000000   0.966537   0.000022   -0.019

 X    OT1MET 2   0.382669   0.000000   0.382669   0.000032   -0.009
 Y    OT1MET 2  -0.019327  -0.000008  -0.019335   0.000061   -0.132
 Z    OT1MET 2   1.042819  -0.000003   1.042816   0.000021   -0.141

 X    OT2MET 2   0.389000   0.000001   0.389001   0.000028    0.046
 Y    OT2MET 2  -0.319190  -0.000046  -0.319236   0.000057   -0.818
 Z    OT2MET 2   0.947533  -0.000008   0.947525   0.000022   -0.358

 X    CB MET 2   0.235370   0.000000   0.235370   0.000029    0.000
 Y    CB MET 2   0.218244   0.000000   0.218243   0.000030   -0.017
 Z    CB MET 2   0.880899   0.000001   0.880900   0.000008    0.078

 X    CG MET 2   0.145930   0.000002   0.145932   0.000033    0.063
 Y    CG MET 2   0.026576   0.000001   0.026577   0.000082    0.013
 Z    CG MET 2   0.869949   0.000000   0.869949   0.000034   -0.006

 X    SD MET 2   0.020941   0.000006   0.020947   0.000011    0.576
 Y    SD MET 2   0.184471  -0.000027   0.184444   0.000029   -0.926
 Z    SD MET 2   0.861972   0.000003   0.861975   0.000013    0.225

 X    CE MET 2  -0.059655   0.000002  -0.059653   0.000047    0.035
 Y    CE MET 2  -0.085636  -0.000010  -0.085646   0.000136   -0.072
 Z    CE MET 2   0.866673  -0.000001   0.866672   0.000055   -0.018



=====================================================================
---> Step No    1 CPU time profile  :
=====================================================================
     Pre-cycle computations                :     0.9243 s
 Cycle No   1
     Fcalc, derivatives and normal matrix :     1.3205 s
     Mimimization (CG/LS)                 :     0.0010 s

     ------------------------------
     |--> Applying : WRIT  DIST   |
     ------------------------------

ANALYSIS OF BOND DISTANCES
 "." indicates a coordinate xyz was NOT refined
```

```
 "+" indicates a coordinate xyz was     refined
  . => its sigma is considered as zero

 If RESTRAINs are applied in the latest cycle
 they are taken into account to compute the standard deviations

ATOM1                ATOM2              DIST     sigDIST     xyz xyz
NT    ALA    1  --  H1    ALA    1   1.032969   0.000176   +++ ...
NT    ALA    1  --  H2    ALA    1   1.032985   0.000176   +++ ...
NT    ALA    1  --  H3    ALA    1   1.032992   0.000176   +++ ...
NT    ALA    1  --  CA    ALA    1   1.480482   0.000598   +++ +++
CA    ALA    1  --  HA    ALA    1   1.098998   0.000190   +++ ...
CA    ALA    1  --  CB    ALA    1   1.526598   0.000679   +++ +++
CA    ALA    1  --  C     ALA    1   1.526013   0.000801   +++ +++
CB    ALA    1  --  HB1   ALA    1   1.059008   0.000186   +++ ...
CB    ALA    1  --  HB2   ALA    1   1.059008   0.000186   +++ ...
CB    ALA    1  --  HB3   ALA    1   1.059051   0.000190   +++ ...
C     ALA    1  --  O     ALA    1   1.239441   0.000719   +++ +++
C     ALA    1  --  N     MET    2   1.339053   0.000697   +++ +++
N     MET    2  --  H0    MET    2   1.008998   0.000179   +++ ...
N     MET    2  --  CA    MET    2   1.456354   0.000710   +++ +++
CA    MET    2  --  HA    MET    2   1.098994   0.000190   +++ ...
CA    MET    2  --  CT    MET    2   1.535984   0.000818   +++ +++
CA    MET    2  --  CB    MET    2   1.537143   0.000799   +++ +++
CT    MET    2  --  OT1   MET    2   1.255851   0.000715   +++ +++
CT    MET    2  --  OT2   MET    2   1.259019   0.000717   +++ +++
CB    MET    2  --  HB1   MET    2   1.092016   0.000191   +++ ...
CB    MET    2  --  HB2   MET    2   1.091995   0.000191   +++ ...
CB    MET    2  --  CG    MET    2   1.523481   0.000926   +++ +++
CG    MET    2  --  HG1   MET    2   1.052538   0.000694   +++ ...
CG    MET    2  --  HG2   MET    2   1.043764   0.000714   +++ ...
CG    MET    2  --  SD    MET    2   1.809526   0.000804   +++ +++
SD    MET    2  --  CE    MET    2   1.803482   0.001167   +++ +++
CE    MET    2  --  HE1   MET    2   1.025889   0.001142   +++ ...
CE    MET    2  --  HE2   MET    2   1.062197   0.000877   +++ ...
CE    MET    2  --  HE3   MET    2   1.041404   0.001143   +++ ...
-----------------------------------------------

     ------------------------
     |--> Applying : STOP   |
     ------------------------

=====================================================================
================== End  MoPro job        :  17/09/2004  18:14:13
================== Total CPU time needed :       0 mn    2.3190 s

================== Writing parameter file : alamet.18
=====================================================================
```