UNRES

protarch package

A package for protein structure prediction based on the thermodynamic hypothesis.

- The UNRES/CSA program for global conformational search with the CSA method at the united-residue level.

- CLUSTER cluster analysis of the united-residue conformations obtained from the UNRES/CSA program.

- PHOENIX - construction of all-atom backbone from the united-residue chain.

CTC's Velocity Windows Cluster

- connect to the login nodes on Velocity (ctclogin1 or ctclogin2) with Terminal Server or telnet
- Cluster CoNTroller System (CCS)

ccq	shows jobs currently running and scheduled
ccrm	removes a running or queued job
ccsubmit	submit a batch or interactive batch job file
cctypes	lists the various cluster resources and their availability
ccusage	lists the various cluster nodes and their associated status and jobs
getccid	returns the job Id associated with the particular node it is executed on
ccrelease	removes a running job based on the job ID associated with the node it is executed on
ccpasswd	allows users to change the NT cluster password from a telnet session

Running UNRES on TC clusters

`ccsubmit i.bat`

i.bat

```
REM CCS account = czarek
REM CCS type = batch
REM CCS nodes = 1
REM CCS requirements = 1@cbweb
REM CCS minutes = 1440

set workdir=\users\czarek\WORKSHOP\ala19_ene

h:
cd %workdir%
time /T >log
date /T >>log
call unres_env.bat GB ala19_ene %workdir%

h:\users\jarekp\unres\bin\unres_ifl_oldscp.exe 1>> log 2>err
time /T >>log
date /T >>log
ccrelease
```

unres_env.bat

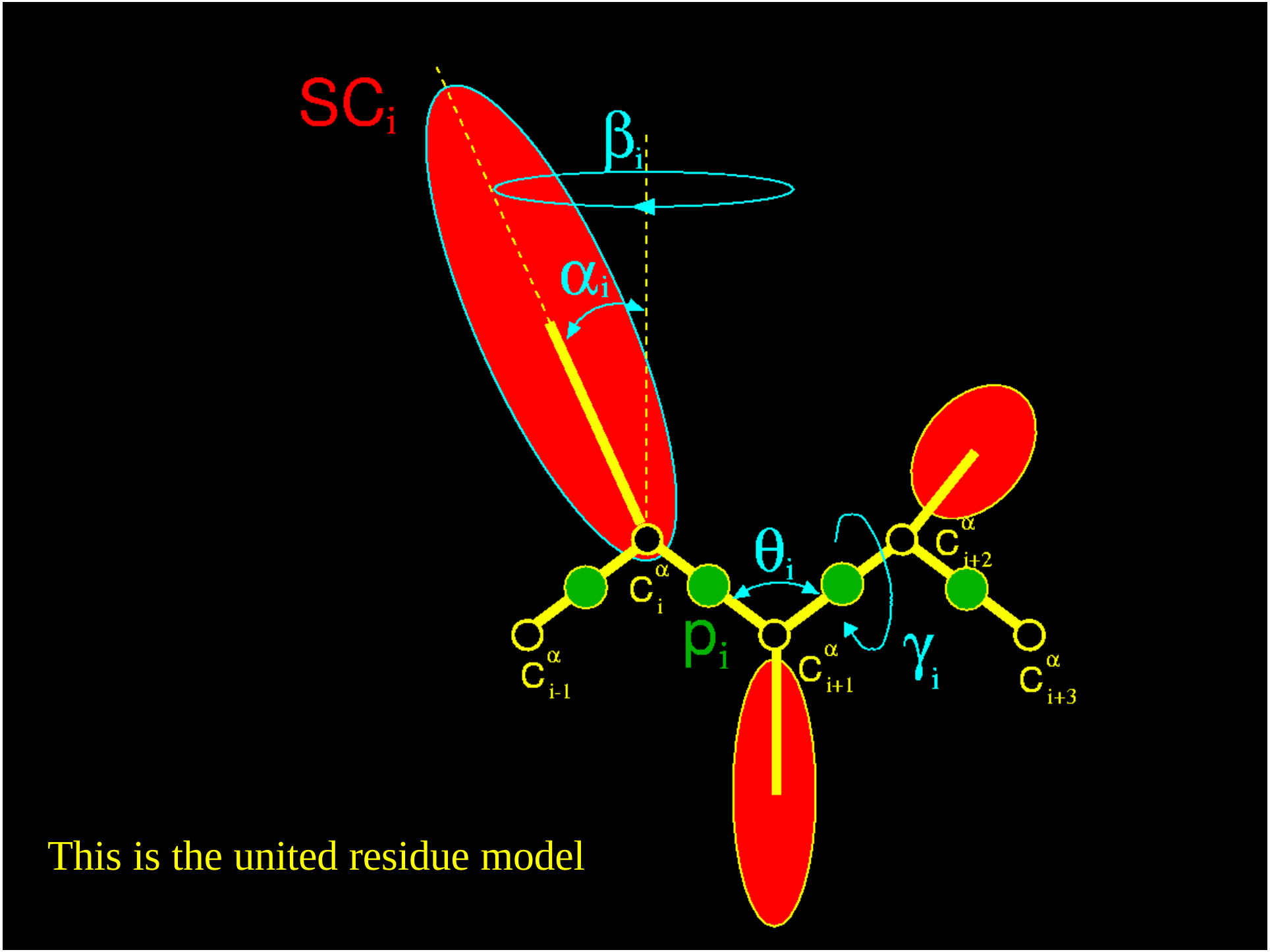
```
set DD=h:\users\jarekp\UNRES\PARAM
set POT=%1
set PREFIX=%2
set THETPAR=%DD%\thetaml.5parm
set ROTPAR=%DD%\scgauss.parm
set TORPAR=%DD%\torsion_ecepp.parm
set TORDPAR=%DD%\torsion_double_abinitio.parm
set ELEPAR=%DD%\electr.parm
set SIDEPAR=%DD%\scinter_%1.parm
set SCPPAR=%DD%\scp.parm
set FOURIER=%DD%\fourier_GAP.parm
set PATTERN=%DD%\patterns.cart
set SECPREDFIL=%2.spred
h:
cd %3
del /q env
set > env
```

Energy calculation for UNRES model of

Ac-Ala19-NHMe

```
Test - polyalanine
SEED=-4239865 PDBOUT ENERGY
WSC=1.0000 WSCP=1.43178 WELEC=0.41501 WANG=0.37790 WSCLOC=0.12880 WTOR=1.00000 &
WTORD=0.0000 WCORRH=2.50526 WCORR5=0.23873 WCORR6=0.76327 WEL_LOC=2.97687      &
WTURN3=0.09261 WTURN4=0.79171 WTURN6=0.01074 CUTOFF=7.00000 WCORR4=0.00000
21
 Gly Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala
 Gly
 0
 0
   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000
   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000
   90.0000   90.0000   90.0000
   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000
   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000
   47.0000   47.0000
  130.0000  130.0000  130.0000  130.00001 130.0000  130.0000  130.0000  130.0000
  130.0000  130.0000  130.0000  130.00001 130.0000  130.0000  130.0000  130.0000
  130.0000  130.0000  130.0000
  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000
  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000
  -76.0000  -76.0000  -76.0000
```

ala19_ene.inp



This is the united residue model

```
EVDW=     -4.532343E+01 WEIGHT=    1.000000D+00 (SC-SC)
EVDW2=     8.815677E+01 WEIGHT=    1.431780D+00 (SC-p)
EES=      -4.616870E+01 WEIGHT=    4.150100D-01 (p-p)
EBE=      -5.070653E+01 WEIGHT=    3.779000D-01 (bending)
ESC=      -5.416198E+01 WEIGHT=    1.288000D-01 (SC local)
ETORS=     1.763547E+01 WEIGHT=    1.000000D+00 (torsional)
ETORSD=   -3.279115E+00 WEIGHT=    0.000000D+00 (double torsional)
EHBP=      0.000000E+00 WEIGHT=    1.000000D+00 (SS bridges & dist. c
ECORR4=   -2.731991E+01 WEIGHT=    2.505260D+00 (multi-body)
ECORR5=    6.530331E+01 WEIGHT=    2.387300D-01 (multi-body)
ECORR6=   -5.996005E+01 WEIGHT=    7.632700D-01 (multi-body)
EELLO=    -4.858590E+00 WEIGHT=    2.976870D+00 (electrostatic-local)
ETURN3=    2.081856E+01 WEIGHT=    9.261000D-02 (turns, 3rd order)
ETURN4=   -1.011848E+01 WEIGHT=    7.917100D-01 (turns, 4th order)
ETURN6=   -2.075488E+00 WEIGHT=    1.074000D-02 (turns, 6th order)
EDIHC=     0.000000E+00 (dihedral angle constraints)
ESS=       0.000000E+00 (disulfide-bridge intrinsic energy)
ETOT=     -6.595329E+01 (total)
```

ala19_ene.out_GB000

Energy minimization for UNRES model of Ac-Ala19-NHMe

```
Test - polyalanine
SEED=-4239865 PDBOUT MINIMIZE
MAXMIN=2000 MAXFUN=5000
WSC=1.0000 WSCP=1.43178 WELEC=0.41501 WANG=0.37790 WSCLOC=0.12880 WTOR=1.00000 &
WTORD=0.0000 WCORRH=2.50526 WCORR5=0.23873 WCORR6=0.76327 WEL_LOC=2.97687      &
WTURN3=0.09261 WTURN4=0.79171 WTURN6=0.01074 CUTOFF=7.00000 WCORR4=0.00000
21
 Gly Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala Ala
 Gly
 0
 0
   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000
   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000   90.0000
   90.0000   90.0000   90.0000
   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000
   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000   47.0000
   47.0000   47.0000
  130.0000  130.0000  130.0000  130.00001 130.0000  130.0000  130.0000  130.0000
  130.0000  130.0000  130.0000  130.00001 130.0000  130.0000  130.0000  130.0000
  130.0000  130.0000  130.0000
  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000
  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000  -76.0000
  -76.0000  -76.0000  -76.0000
```

ala19_min.inp

```
EVDW=     -4.758043E+01 WEIGHT=    1.000000D+00 (SC-SC)
EVDW2=     9.825882E+01 WEIGHT=    1.431780D+00 (SC-p)
EES=      -4.761318E+01 WEIGHT=    4.150100D-01 (p-p)
EBE=      -4.534415E+01 WEIGHT=    3.779000D-01 (bending)
ESC=      -4.891917E+01 WEIGHT=    1.288000D-01 (SC local)
ETORS=     1.715670E+01 WEIGHT=    1.000000D+00 (torsional)
ETORSD=   -2.958534E+00 WEIGHT=    0.000000D+00 (double torsional)
EHBP=      0.000000E+00 WEIGHT=    1.000000D+00 (SS bridges & dist.
ECORR4=   -3.120866E+01 WEIGHT=    2.505260D+00 (multi-body)
ECORR5=    7.357923E+01 WEIGHT=    2.387300D-01 (multi-body)
ECORR6=   -7.118953E+01 WEIGHT=    7.632700D-01 (multi-body)
EELLO=    -5.400176E+00 WEIGHT=    2.976870D+00 (electrostatic-local)
ETURN3=    2.116925E+01 WEIGHT=    9.261000D-02 (turns, 3rd order)
ETURN4=   -1.086067E+01 WEIGHT=    7.917100D-01 (turns, 4th order)
ETURN6=   -2.314775E+00 WEIGHT=    1.074000D-02 (turns, 6th order)
EDIHC=     0.000000E+00 (dihedral angle constraints)
ESS=       0.000000E+00 (disulfide-bridge intrinsic energy)
ETOT=     -7.063059E+01 (total)
....
SUMSL return code:  4
# of energy evaluations:                  66
```

ala19_min.out_GB000

Energy minimization of the experimental structure read from the pdb file

```
minimization
SEED=-3059743 MINIMIZE PDBSTART PDBOUT PDBREF
MAXMIN=2000 MAXFUN=5000
WSC=1.0000 WSCP=1.43178 WELEC=0.41501 WANG=0.37790 WSCLOC=0.12880 WTOR=1.00000 &
WTORD=0.0000 WCORRH=2.50526 WCORR5=0.23873 WCORR6=0.76327 WEL_LOC=2.97687      &
WTURN3=0.09261 WTURN4=0.79171 WTURN6=0.01074 CUTOFF=7.00000 WCORR4=0.00000
1igd.pdb
0
0
```

min.inp

```
regular
SEED=-3059743 MINIMIZE PDBSTART PDBOUT PDBREF SOFTREG
MAXMIN=2000 MAXFUN=5000
WSC=1.0000 WSCP=1.43178 WELEC=0.41501 WANG=0.37790 WSCLOC=0.12880 WTOR=1.00000 &
WTORD=0.0000 WCORRH=2.50526 WCORR5=0.23873 WCORR6=0.76327 WEL_LOC=2.97687      &
WTURN3=0.09261 WTURN4=0.79171 WTURN6=0.01074 CUTOFF=7.00000 WCORR4=0.00000
1igd.pdb
0
0
```

regular.inp

Prediction of the structure of 1FSD protein using UNRES/CSA

```
1FSD
SEED=-3059743 CSA MINIMIZE
MAXMIN=2000 MAXFUN=5000
NCONF=50 NSTMAX=1000  N1=3 N2=0 N3=2 N4=1 N6=2 IS1=3 IS2=20 NSEED=20          &
NTOTAL=20000 CUT1=2.0 CUT2=5.0 ESTOP=-3000.0 IRESTART=0                       &
NBANKTM=1000 DELE=10.0 DIFCUT=720.0 IREF=0 RMSCUT=4.0
WSC=1.0000 WSCP=1.43178 WELEC=0.41501 WANG=0.37790 WSCLOC=0.12880 WTOR=1.00000 &
WTORD=0.0000 WCORRH=2.50526 WCORR5=0.23873 WCORR6=0.76327 WEL_LOC=2.97687     &
WTURN3=0.09261 WTURN4=0.79171 WTURN6=0.01074 CUTOFF=7.00000 WCORR4=0.00000
30
 D   GLN GLN TYR THR ALA LYS ILE LYS GLY ARG THR PHE ARG ASN GLU LYS GLU LEU ARG
 ASP PHE ILE GLU LYS PHE LYS GLY ARG D
 0
 0
```

1fsd.inp

ii.bat

```
REM CCS account = czarek
REM CCS type = batch
REM CCS nodes = 2
REM CCS requirements = 2@cbweb
REM CCS minutes = 1440

set workdir=\users\czarek\WORKSHOP\1fsd

h:
cd %workdir%
time /T >log
date /T >>log
call MachineMaker.bat >> log
call unres_env.bat GB 1fsd %workdir%
set MPI_COMM=TCP
mpirun -np 4 unres.bat  %workdir%  1>> log 2>err
time /T >>log
date /T >>log
ccrelease
```

unres.bat

```
h:

cd %1

h:\users\jarekp\unres\bin\unres_ifl_oldscp.exe
```

```
 1 0      50  2331.8   1  50  -3.58261E+01   8.80402E+42     34697  50  50  50
 1 0     209  2314.8   6  37  -4.20168E+01  -2.76164E+01    101675  46  50  80
 1 0     369  2297.9  46  26  -4.65300E+01  -3.14259E+01    175540  47  50  99
 1 0     529  2281.1  46  34  -5.35659E+01  -3.58054E+01    258251  45  50  95
 1 0     689  2264.5  46  10  -5.35659E+01  -3.89710E+01    341640  40  50  42
 1 0     849  2247.9   4  31  -5.37838E+01  -4.13682E+01    423101  34  50  69
 1 0    1012  2231.5  19  37  -5.45203E+01  -4.21675E+01    500618  34  50  75
jlee =  1:       0.0       0.0       0.0       0.0 E = -54.520   1012    500618
```

1fsd.CSA.history

```
Calling FEEDIN NCONF          50
  Time for first bank min.   66.2408298132941
make_var : nseed=          20 ntry=         180
....
Nonsetup time           139.41 sec, Eval/s =    480.42
Time for iter    1      139.41 sec, Eval/s =    480.42
 UPDATING          179
  4 e  160    1 etot  -1.4517E+01 mv   6   0
  4 e  235    2 etot  -1.4931E+01 mv   6   0
  4 e  108    4 etot  -3.5725E+01 mv   6   0
  8 e  392    7 etot  -2.1030E+01 mv   6   0
 -1 e    1    8 etot   2.7251E+20 mv   6   0
  4 e  578    6 etot  -3.7523E+01 mv   6   0 f  50
  4 e  720    5 etot  -4.0318E+01 mv   6   0 f  49
  4 e  388    9 etot  -3.1336E+01 mv   6   0 c   9
  4 e  807   10 etot  -3.0392E+01 mv   6   0 f  47
```

1fsd.out_GB000

```
....
## N0 total=  20 close=   5 far=   0 %acc 25.0
## N1 total=  60 close=  13 far=   1 %acc 23.3
## N2 total=   0 close=   0 far=   0 %acc  0.0
## N3 total=  40 close=   8 far=   4 %acc 30.0
## N4 total=  20 close=   0 far=   1 %acc  5.0
## N5 total=   0 close=   0 far=   0 %acc  0.0
## N6 total=  40 close=   9 far=   0 %acc 22.5
## N7 total=   0 close=   0 far=   0 %acc  0.0
## N8 total=   0 close=   0 far=   0 %acc  0.0
....
### Total stats:
### N0 total=   119 close=  37 far=   0 %acc 31.1
### N1 total=   360 close=  74 far=  18 %acc 25.6
### N2 total=     0 close=   0 far=   0 %acc  0.0
### N3 total=   238 close=  34 far=  50 %acc 35.3
### N4 total=   100 close=   2 far=  24 %acc 26.0
### N5 total=     0 close=   0 far=   0 %acc  0.0
### N6 total=   262 close=  57 far=  31 %acc 33.6
### N7 total=     0 close=   0 far=   0 %acc  0.0
### N8 total=     0 close=   0 far=   0 %acc  0.0
 End of RUN, master time     1090.16953619476       sec
 Total eval/s    427.383984353752
```

1fsd.out_GB000 cont.

Cluster analysis of the conformations obtained in the CSA run

`unres_clust.bat tree 1fsd`

```
clustering 1fsd
NRES=30  NCUT=3 CUTOFF= 5.0 -4.0 3.0                                    &
PLOT_TREE MOL2OUT=0 PDBOUT=3  ECUT=990.0
 D   GLN GLN TYR THR ALA LYS ILE LYS GLY ARG THR PHE ARG ASN GLU LYS GLU LEU ARG
 ASP PHE ILE GLU LYS PHE LYS GLY ARG D
 0
 0
```

tree.inp

```
AT CUTOFF:   4.00000


THERE ARE   32 FAMILIES OF CONFORMATIONS

FAMILY    1 CONTAINS   12 CONFORMATION(S):
  33 -5.9516E+01   1 -5.3443E+01  10 -5.2416E+01  17 -5.2209E+01  46 -5.1749E+01
  23 -5.0626E+01   8 -5.0128E+01  48 -5.0016E+01  35 -4.7062E+01  44 -4.6178E+01
  12 -4.4515E+01  21 -4.1802E+01


Max. distance in the family:     8.1; average distance in the family:     5.4

FAMILY    2 CONTAINS    1 CONFORMATION(S):
   5 -5.5033E+01


Max. distance in the family:     0.0; average distance in the family:     0.0
```

1fsd_clust.out

Construction of the full-atom model of the lowest-energy UNRES

`phoenix2.exe 1fsd@012.pdb`

```
REMARK GM 12 e    445787 m   1000                                ENERGY    -5.95159E+01
ATOM      1  CA  GLN     1       3.800   0.000   0.000
ATOM      2  CB  GLN     1       4.750   1.377   1.490
ATOM      3  CA  GLN     2       3.939  -3.797   0.000
ATOM      4  CB  GLN     2       2.707  -5.296   1.120
.....
ATOM     52  CB  GLY    27      14.314 -21.502   4.996
ATOM     53  CA  ARG    28      12.765 -22.183   8.398
ATOM     54  CB  ARG    28      11.630 -19.597   7.329
```

1fsd@012.pdb