MolMech

In the current version of the program, the PDB file with coordinates of atoms in a protein in the input data. The coordinates may be retrieved from the file or PDB database. For computation, indicate the chain identifier, given in the PDB file.

The program automatically prepares the file with topology of the molecule, containing AMBER force field parameters. The program uses this file in further calculations of molecular mechanical minimization. A standard AMBER and/or user topology database of individual residues is used for creating this topology file. AMBER parameters file is used for determining the constants of potential energy function, such as equilibrium bond lengths, angles, dihedral angles, their force constants, non-bonded 6-12 parameters, and H-bond 10-12 parameters.

Minimization stops after 50 iterations.

The output data are the coordinates of the atoms of protein chain after minimization in PDB format.

Output example:

```
HEADER    SoftBerry molecular mechanic Ver. 1.0
REMARK   1
REMARK   1 Charge modification is NOT performed.
REMARK   1 NO periodic boundaries are applied.
REMARK   1 Non-bonded interactions evaluated normally.
REMARK   1 Energy is reported in Kcal/mol
REMARK   1 Complete interaction is calculated.
REMARK   1 NB pairlist generated in residue-residue basis.
REMARK   1 No pair list will be generated.
REMARK   1 NB list updated every 10 steps.
REMARK   1 Buffer region updates every 1 steps.
REMARK   1 Constant dielectric function used.
REMARK   1 Solvent pointer = 142.
REMARK   1 No water model chosen.
REMARK   1 NB cutoff distance =     8.0000 Angstroms.
REMARK   1 1,4 non-bonds divided by     2.0000.
REMARK   1 1,4 electrostatics divided by     2.0000.
REMARK   1 The dielectric constant =     1.0000.
REMARK   1 The buffer cutoff is    8.00000 Angstroms.
REMARK   1 CAP Option is inactivated.
REMARK   1
REMARK   1 The number of degrees of freedom = 6426.
REMARK   1 INITIAL CONDITIONS OF SYSTEM:
REMARK   1
REMARK   1 Potential Energy = -4643.602515
REMARK   1 Non-bond         = -784.604532
REMARK   1 H-bond           = 0.000000
REMARK   1 Electrostatic    = -10490.096084
REMARK   1 Bond             = 183.712294
REMARK   1 Angle            = 715.484007
REMARK   1 Dihedral         = 557.877658
REMARK   1 1,4 Non-bonded   = 721.197306
REMARK   1 1,4 Electrostatic= 4452.826836
REMARK   1
REMARK   1 MINIMIZATION TERMINATED  : Exceeded maximum number of cycles
REMARK   1 Number of function calls 102
REMARK   1 Number of iterations 50
REMARK   1
REMARK   1 Potential Energy = -6031.148428
REMARK   1 Non-bond         = -1078.280106
```

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REMARK   1 H-bond           = 0.000000
REMARK   1 Electrostatic    = -10870.756945
REMARK   1 Bond             = 38.980831
REMARK   1 Angle            = 364.506930
REMARK   1 Dihedral         = 569.815489
REMARK   1 1,4 Non-bonded   = 499.520121
REMARK   1 1,4 Electrostatic= 4445.065252
REMARK   1
ATOM      1  N   VAL     1       7.357  18.204   5.000   0.058  0.00
ATOM      2  H1  VAL     1       7.744  18.600   5.855   0.227  0.00
ATOM      3  H2  VAL     1       6.358  18.336   4.957   0.227  0.00
ATOM      4  H3  VAL     1       7.576  17.220   4.974   0.227  0.00
ATOM      5  CA  VAL     1       7.948  18.857   3.812  -0.005  0.00
ATOM      6  HA  VAL     1       7.513  18.373   2.927   0.109  0.00
ATOM      7  CB  VAL     1       7.562  20.374   3.761   0.320  0.00
ATOM      8  HB  VAL     1       8.205  20.922   4.460  -0.022  0.00
ATOM      9  CG1 VAL     1       7.734  20.963   2.351  -0.313  0.00
ATOM     10  HG1 VAL     1       7.200  20.370   1.614   0.073  0.00
ATOM     11  HG1 VAL     1       7.348  21.971   2.334   0.073  0.00
ATOM     12  HG1 VAL     1       8.777  21.031   2.074   0.073  0.00
ATOM     13  CG2 VAL     1       6.091  20.612   4.182  -0.313  0.00
ATOM     14  HG2 VAL     1       5.914  20.395   5.230   0.073  0.00
ATOM     15  HG2 VAL     1       5.837  21.655   4.045   0.073  0.00
ATOM     16  HG2 VAL     1       5.401  20.033   3.576   0.073  0.00
ATOM     17  C   VAL     1       9.470  18.591   3.816   0.616  0.00
ATOM     18  O   VAL     1       9.994  18.012   4.791  -0.572  0.00
ATOM     19  N   LEU     2      10.152  18.988   2.739  -0.416  0.00
ATOM     20  H   LEU     2       9.702  19.420   1.936   0.272  0.00
ATOM     21  CA  LEU     2      11.603  19.008   2.683  -0.052  0.00
ATOM     22  HA  LEU     2      11.983  18.097   3.120   0.092  0.00
ATOM     23  CB  LEU     2      12.095  19.097   1.232  -0.110  0.00
ATOM     24  HB2 LEU     2      11.708  20.020   0.810   0.046  0.00
…..
…..
ATOM   2114  CD2 TYR   140      -4.256   9.053 -10.416  -0.191  0.00
ATOM   2115  HD2 TYR   140      -5.071   8.446 -10.050   0.170  0.00
ATOM   2116  C   TYR   140      -7.480  12.287 -10.110   0.597  0.00
ATOM   2117  O   TYR   140      -8.121  11.618 -10.920  -0.568  0.00
ATOM   2118  N   ARG   141      -8.048  12.955  -9.114  -0.348  0.00
ATOM   2119  H   ARG   141      -7.526  13.520  -8.446   0.276  0.00
ATOM   2120  CA  ARG   141      -9.462  13.123  -8.845  -0.307  0.00
ATOM   2121  HA  ARG   141      -9.978  13.465  -9.741   0.145  0.00
ATOM   2122  CB  ARG   141     -10.109  11.835  -8.298  -0.037  0.00
ATOM   2123  HB2 ARG   141     -11.111  12.088  -7.947   0.037  0.00
ATOM   2124  HB3 ARG   141     -10.206  11.103  -9.099   0.037  0.00
ATOM   2125  CG  ARG   141      -9.316  11.209  -7.137   0.074  0.00
ATOM   2126  HG2 ARG   141      -8.389  10.775  -7.516   0.018  0.00
ATOM   2127  HG3 ARG   141      -9.057  11.977  -6.410   0.018  0.00
ATOM   2128  CD  ARG   141     -10.113  10.122  -6.411   0.111  0.00
ATOM   2129  HD2 ARG   141     -11.122  10.491  -6.222   0.047  0.00
ATOM   2130  HD3 ARG   141     -10.167   9.231  -7.040   0.047  0.00
ATOM   2131  NE  ARG   141      -9.476   9.806  -5.122  -0.556  0.00
ATOM   2132  HE  ARG   141      -8.628  10.338  -4.986   0.348  0.00
ATOM   2133  CZ  ARG   141      -9.989   9.061  -4.137   0.837  0.00
ATOM   2134  NH1 ARG   141     -11.125   8.390  -4.322  -0.874  0.00
ATOM   2135  HH1 ARG   141     -11.567   7.834  -3.606   0.449  0.00
ATOM   2136  HH1 ARG   141     -11.600   8.467  -5.211   0.449  0.00
ATOM   2137  NH2 ARG   141      -9.357   8.998  -2.966  -0.874  0.00
ATOM   2138  HH2 ARG   141      -9.719   8.469  -2.187   0.449  0.00
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ATOM   2139  HH2 ARG   141      -8.518   9.540  -2.806   0.449  0.00
ATOM   2140  C   ARG   141      -9.530  14.235  -7.814   0.856  0.00
ATOM   2141  O   ARG   141      -8.516  14.373  -7.084  -0.826  0.00
ATOM   2142  OXT ARG   141     -10.586  14.879  -7.753  -0.826  0.00
```

Parameters:

Input	
PDB structure	Input filename of protein structure (file in PDB format) (http://www.umass.edu/microbio/rasmol/pdb.htm).
Protein chain ID	Protein chain ID.