mol_go.top

```
#define GO_VIRT

#include "martini_v3.0.0_go.itp"

#include "mol_go.itp"

#include "martini_v3.0.0_solvents_v1.itp"
#include "martini_v3.0.0_ions_v1.itp"

[ system ]
<title>

[ molecules ]
mol        1
W       2042
NA        17
CL        15
```

martini_v3.0.0_go.itp

```
[ defaults ]
;nb-func  comb rule
1               2 ;
; nbfunc: 1 = LJ, 2 = Buckingham
; comb-rule: only used if this a pair is not explicitly
listed in section [ nonbond_params ]

[ atomtypes ]
; type   m      q        ptype   V     W
P6      72.0  0.000        A    0.0   0.0
...
; std. MARTINI beads here

#ifdef GO_VIRT
#include "atomtypes_go.itp"
#endif

[ nonbond_params ]
; ai    aj  func       σ_ij                    ε_ij
P6    P6  1  4.700000e-01  4.990000e+00
...

#ifdef GO_VIRT
#include "nonbond_params_go.itp"
#endif
```

mol_go.itp

```
[ moleculetype ]
; name                nexcl
  mol                   1

[ atoms ]
; nr atomtype resid  resname atomname
charge group  q[e] m[u]
1      Q5         1  GLY  BB     1  1
...

#include "mol_atoms_go.itp"

[ position_restraints ], [ bonds ]
[ constraints ], [ angles ], [ dihedrals ], etc.

[ exclusions ]
; triangle blocks: ring side chains
; ndx ndx ndx ...

#include "mol_exclusions_go.itp"

[ virtual_sitesn ]
#include "mol_virtual_sitesn_go.itp"
```

atomtypes_go.itp

```
#ifdef GO_VIRT
#include "atomtypes_go.itp"
#endif
```

nonbond_params_go.itp

```
#ifdef GO_VIRT
#include "mol_nonbond_params_go.itp"
#endif
```

mol_atoms_go.itp

```
; virtual sites
123 mol_A1        1 GLY VWA 123   0.0
…
165 mol_B1        1 GLY VWB 165   0.0
…
207 mol_C1        1 GLY VWC 207   0.0
…
244 mol_D1        1 GLY VWD 244   0.0
…
; nr atomtype resid  resname atomname
charge group  q[e] m[u]
```

mol_virtual_sitesn_go.itp

```
; ndx   fucnt   >=1 constructing indices
 123 1   1
 …
; ndx of Vsite  -  BB particles' ndx, i.e Go Vsite is
exactly at the position of BB particle
```

mol_atomtypes_go.itp

```
; protein BB virtual particles
; INTRA particles
mol_A1 0.0 0.000   A   0.0   0.0
...
mol_B1 0.0 0.000   A   0.0   0.0
...
; INTER particles
mol_C3 0.0 0.000   A   0.0   0.0
...
mol_D3 0.0 0.000   A   0.0   0.0
...
; type     m      q   ptype  V    W
```

mol_nonbond_params_go.itp

```
; OV + symmetric rCSU contacts
; INTRA section: A-B pairs (+/- go_eps_intra)
mol_A1  mol_A5    1  0.5329   12.0000
mol_B1  mol_B5    1  0.5329  -11.9999
…
; INTER section: C (go_eps_inter)
mol_C1  mol_C51  1  0.4900   6.0000
…
; INTER section: D (-go_eps_BB)
mol_D1  mol_D51  1  0.4700  -6.4499
…
; ai    aj  func       σ_ij                    ε_ij
```

mol_exclusions_go.itp

```
; [ exclusions for intra BB sites ]
; atomnr atomnr  -  resnr resnr
  1          8          ;  1          5
 ...
; [ exclusions for intra VWB sites ]
 165       169        ;  1          5
 ...
; [ exclusions for inter VWC sites ]
 207       243        ;  1          51
 ...
; [ exclusions for inter VWD sites ]
 244       280        ;  1          51
 ...
```