

(A)

;;; LEUCINE

[moleculetype]

; molname nrexcl

LEU 1

[atoms]

;id type resnr residu atom cgnr charge

1 P5 1 LEU BB 1 0

2 C1 1 LEU SC1 2 0

[bonds]

; i j funct length force.c.

1 2 1 0.33 7500

(B)

RESIdue LEU

GROUP

ATOM BB type=F5 charge=0.000 END

ATOM SC1 type=LC1 charge=0.000 END

BOND BB SC1

END