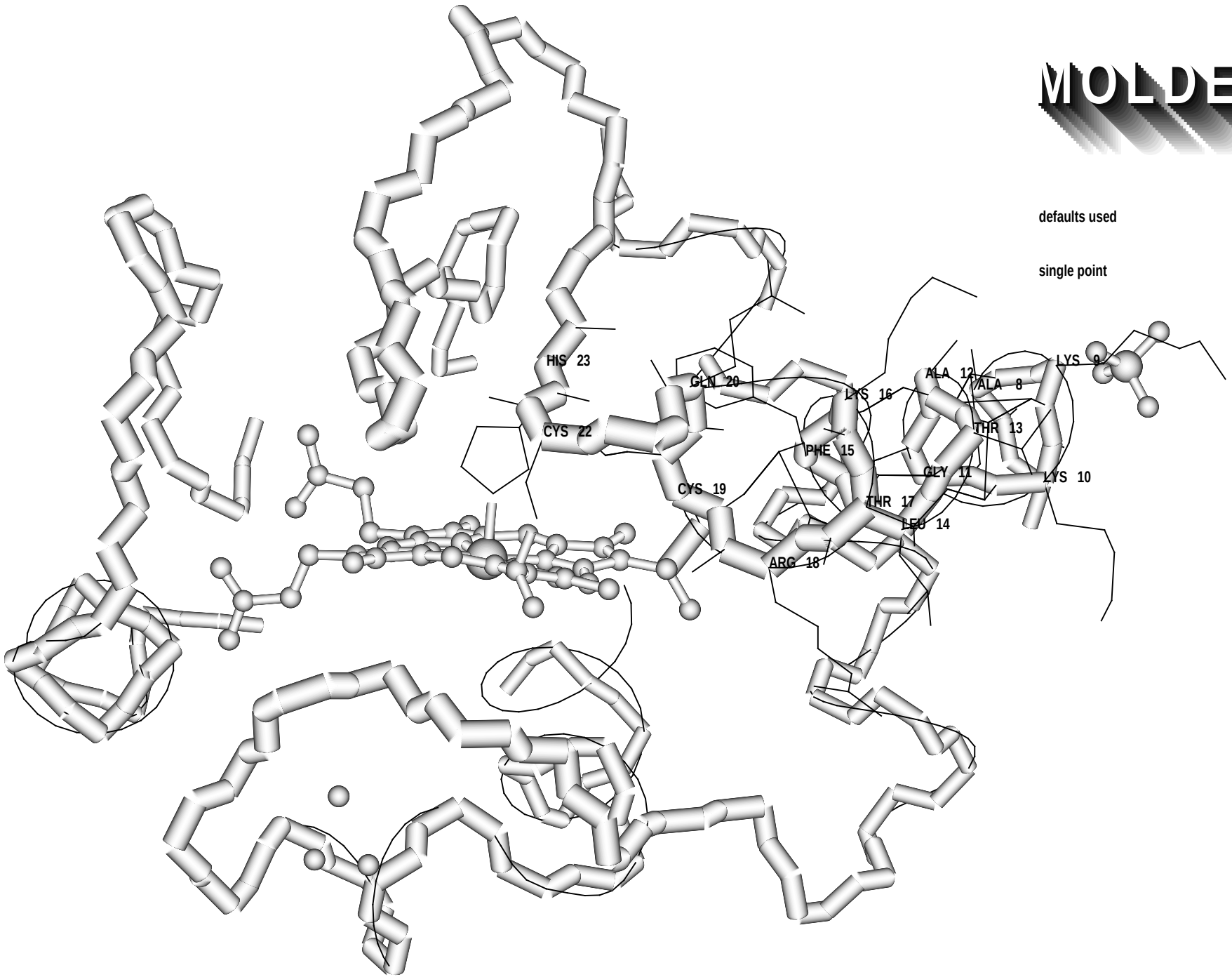
MOLDEN
defaults used
single point
HIS 23
GLN 20
CYS 22
CYS 19
PHE 15
LYS 16
ALA 12
ALA 8
LYS 9
THR 13
GLY 11
LYS 10
THR 17
LEU 14
ARG 18