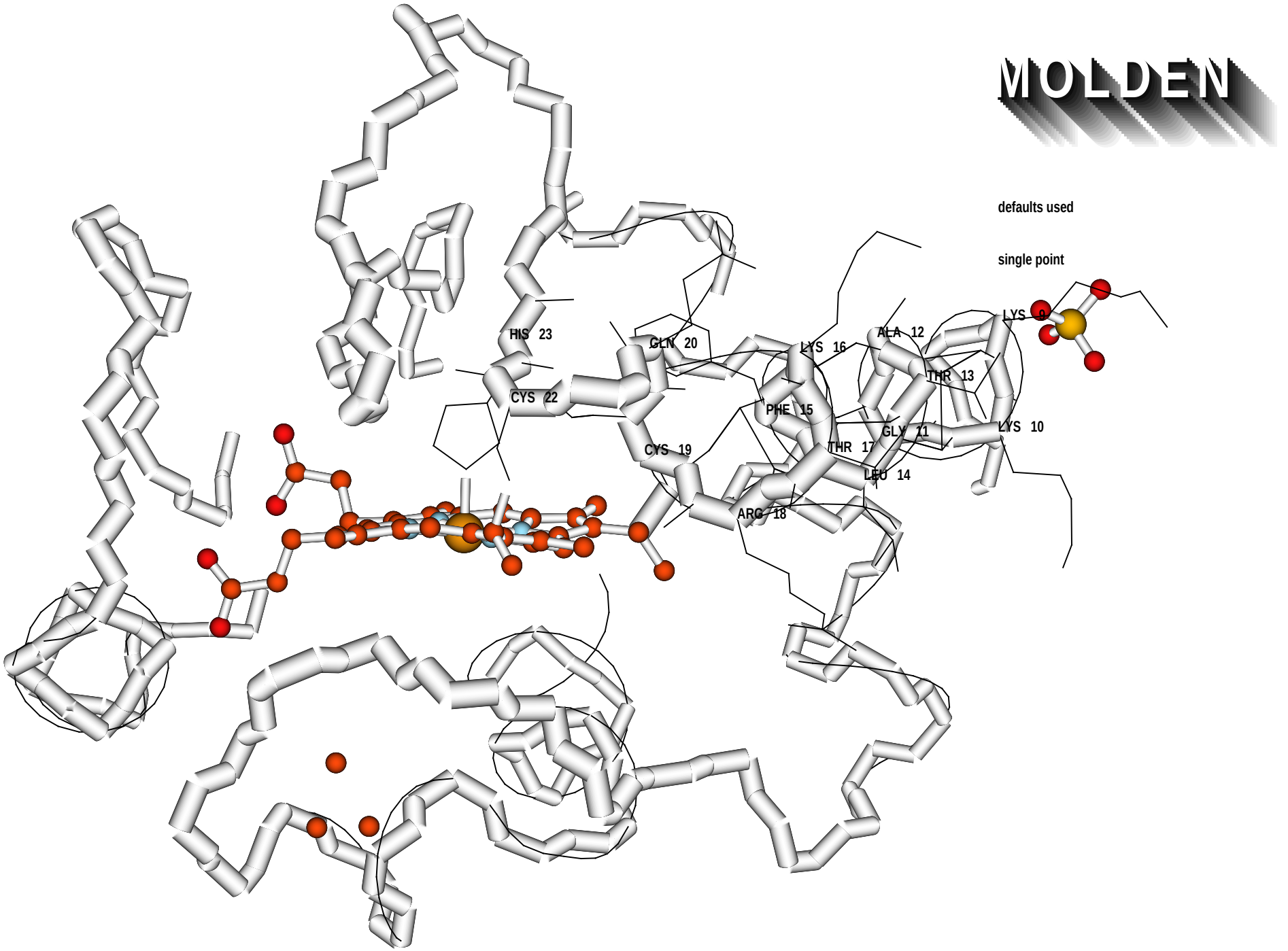
MOLDEN
defaults used
single point
HIS 23
GLN 20
LYS 16
ALA 12
LYS 9
THR 13
CYS 22
PHE 15
GLY 11
LYS 10
CYS 19
THR 17
LEU 14
ARG 18