

balabanJ  
diameter  
KierFlex  
petitjean  
petitjeanSC  
radius  
weinerPath  
weinerPol  
zagreb

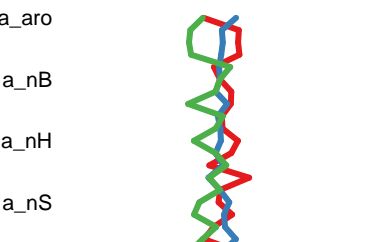



a\_aro


a\_nB

a\_nH

a\_nS

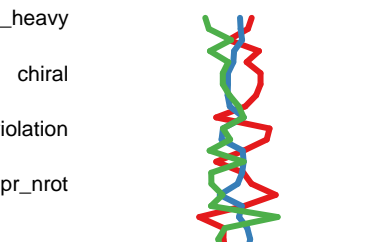


double

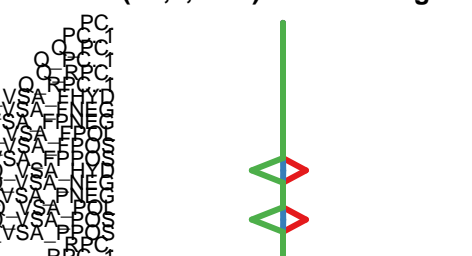


-3.0 -1.5 0.0 1.5 3.0

heavy  
chiral  
isolation  
pr\_nrot



A horizontal number line with tick marks at -3.0, -1.5, 0.0, 1.5, and 3.0.



bpol


active

a\_acc

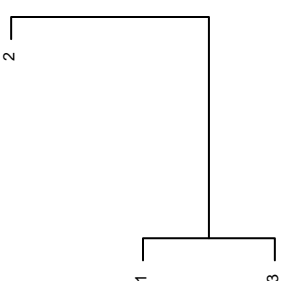
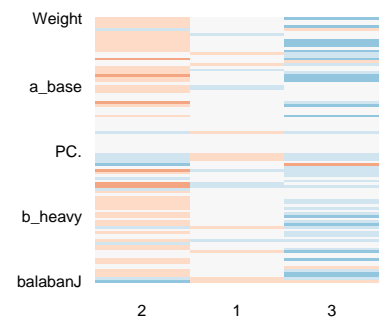
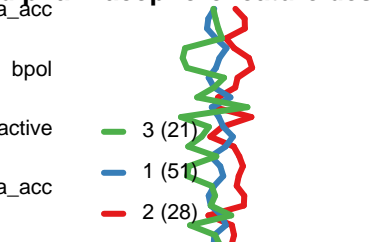
3 (21)

1 (51)

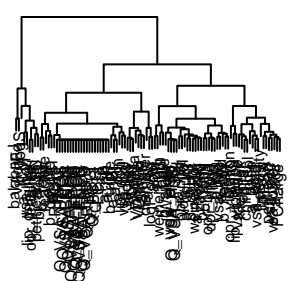
2 (28)



The diagram shows a 3D ribbon representation of the bpol active site. Three ligands are bound: a green ligand (3) with 21 atoms, a blue ligand (1) with 51 atoms, and a red ligand (2) with 28 atoms. The ligands are positioned near the active site, which is defined by the bpol protein structure.



```
dist(avg_p)
hclust (*, "complete")
```



```
dist(t(avg_p))
hclust (*, "complete")
```