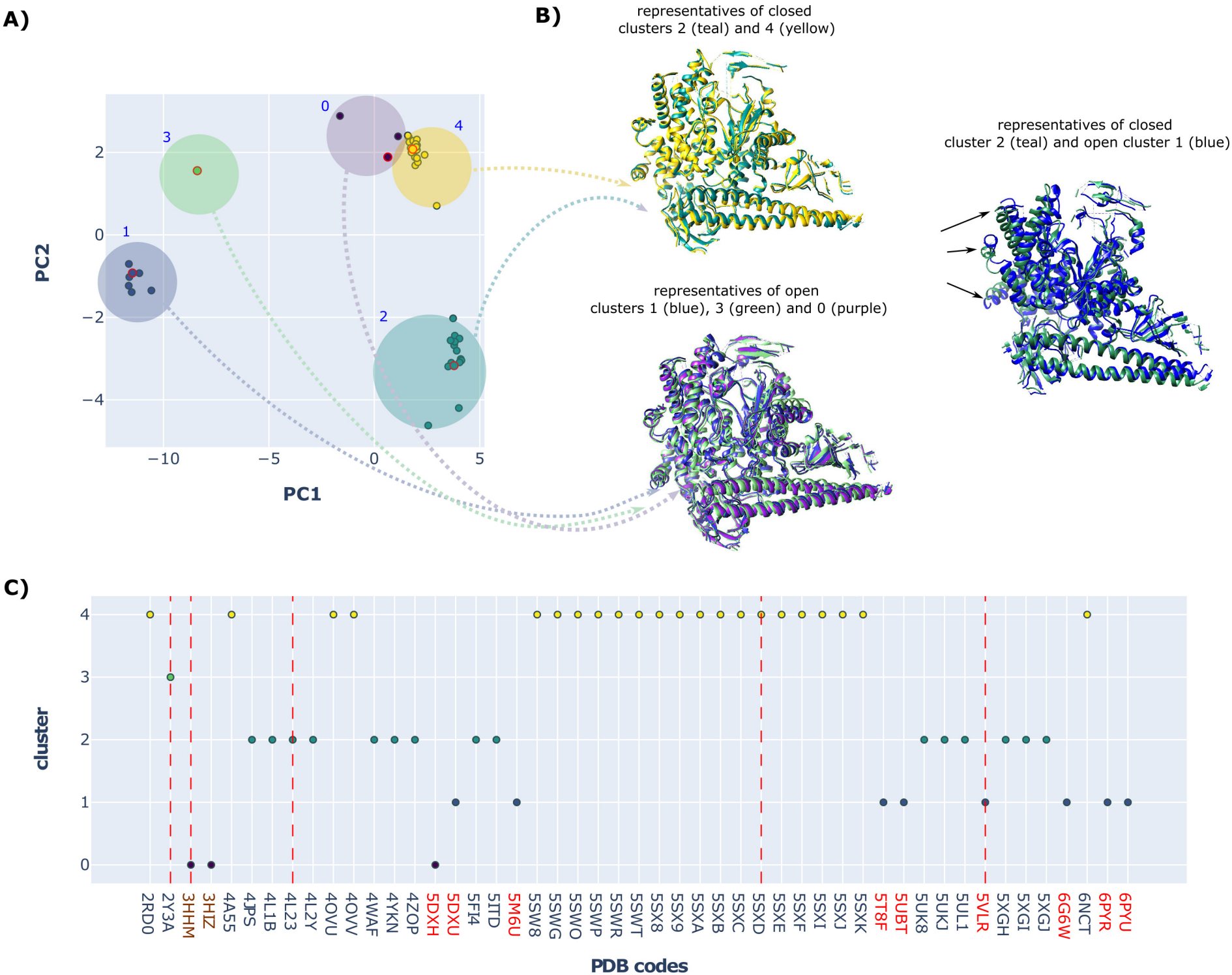
A)
B)
C)
representatives of closed
clusters 2 (teal) and 4 (yellow)
representatives of closed
cluster 2 (teal) and open cluster 1 (blue)
representatives of open
clusters 1 (blue), 3 (green) and 0 (purple)
PC1
PC2
cluster
PDB codes
2RD0
2Y3A
3HHM
3HIZ
4A55
4JPS
4L1B
4L23
4L2Y
4OVU
4OVV
4WAF
4YKN
4ZOP
5DXH
5DXU
5FI4
5ITD
5M6U
5SW8
5SWG
5SWO
5SWP
5SWR
5SWT
5SX8
5SX9
5SXA
5SXB
5SXC
5SXD
5SXE
5SXF
5SXI
5SXJ
5SXK
5T8F
5UBT
5UK8
5UKJ
5UL1
5VLR
5XGH
5XGI
5XGJ
6G6W
6NCT
6PYR
6PYU