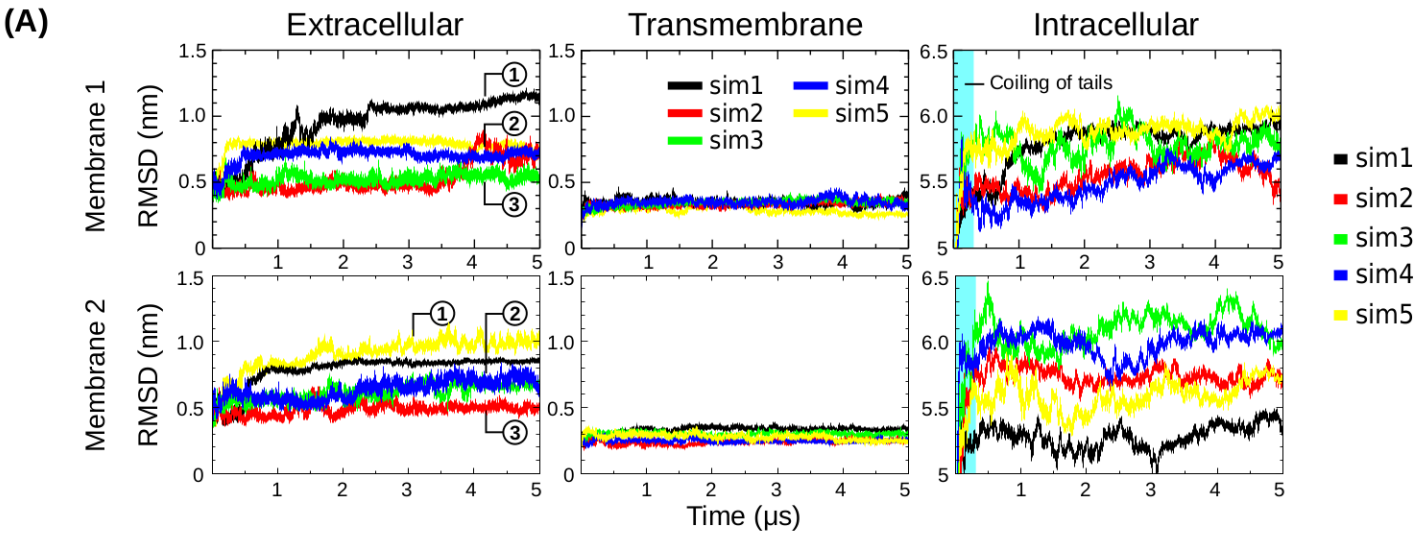
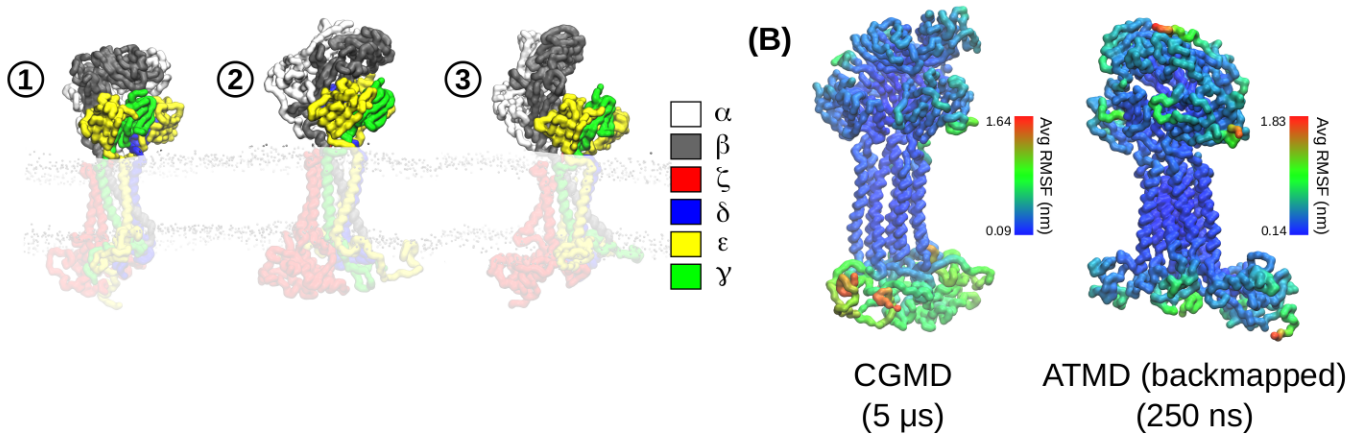
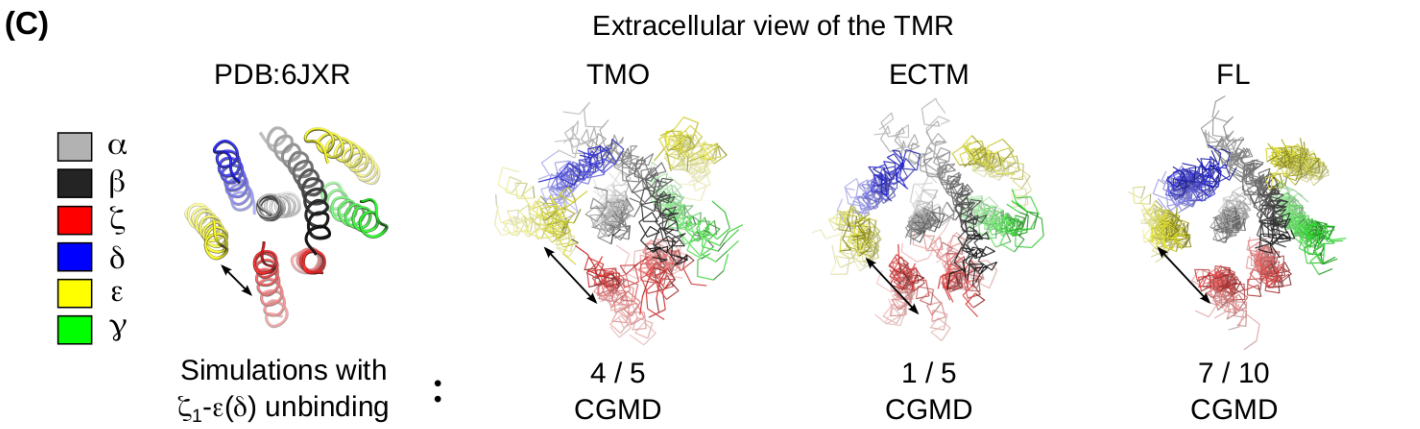
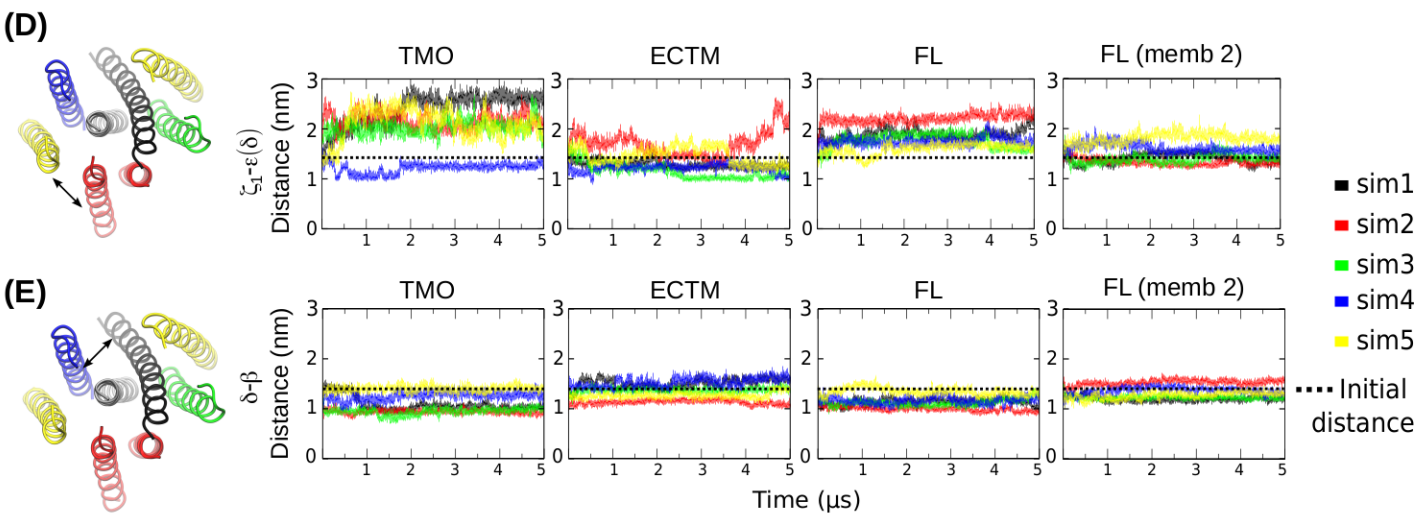

(A)
Extracellular
Transmembrane
Intracellular
Membrane 1
Membrane 2
RMSD (nm)
Coiling of tails
sim1
sim2
sim3
sim4
sim5
Time (μs)


(B)
α
β
ζ
δ
ε
γ
Avg RMSF (nm)
1.64
0.09
1.83
0.14
CGMD
(5 μs)
ATMD (backmapped)
(250 ns)


(C)
Extracellular view of the TMR
PDB:6JXR
TMO
ECTM
FL
α
β
ζ
δ
ε
γ
Simulations with
ζ1-ε(δ) unbinding
4 / 5
CGMD
1 / 5
CGMD
7 / 10
CGMD


(D)
TMO
ECTM
FL
FL (memb 2)
ζ1-ε(δ)
Distance (nm)
sim1
sim2
sim3
sim4
sim5
(E)
δ-β
Distance (nm)
Initial
distance
Time (μs)