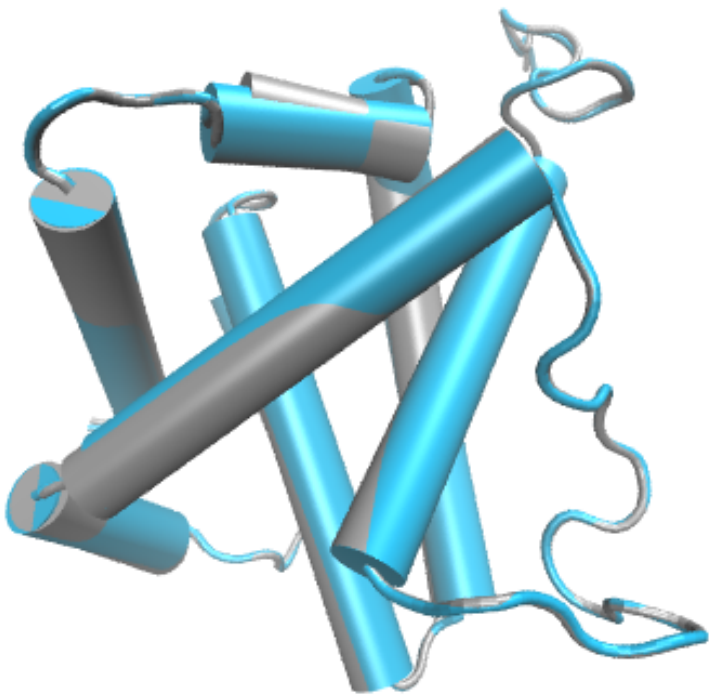
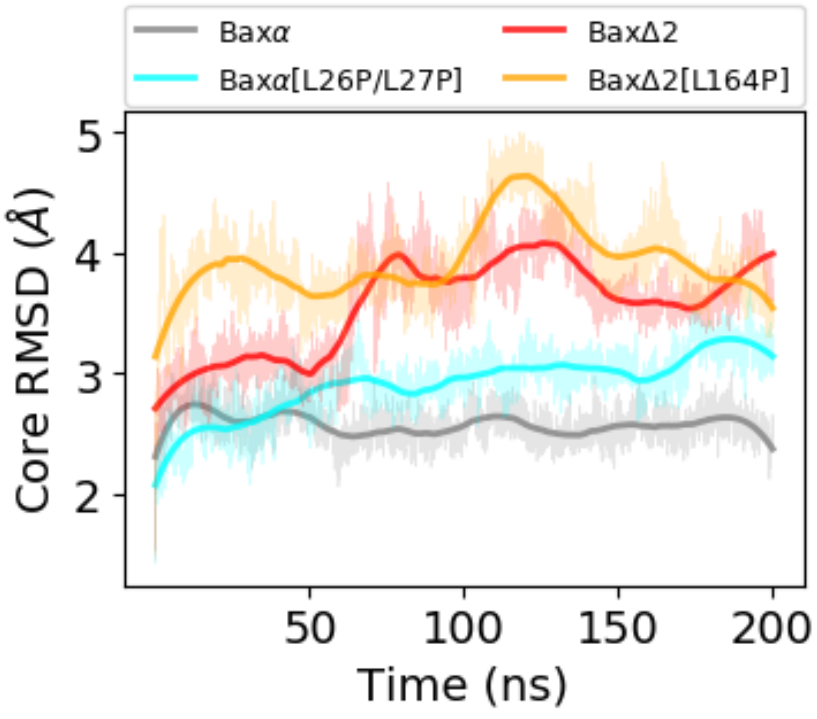
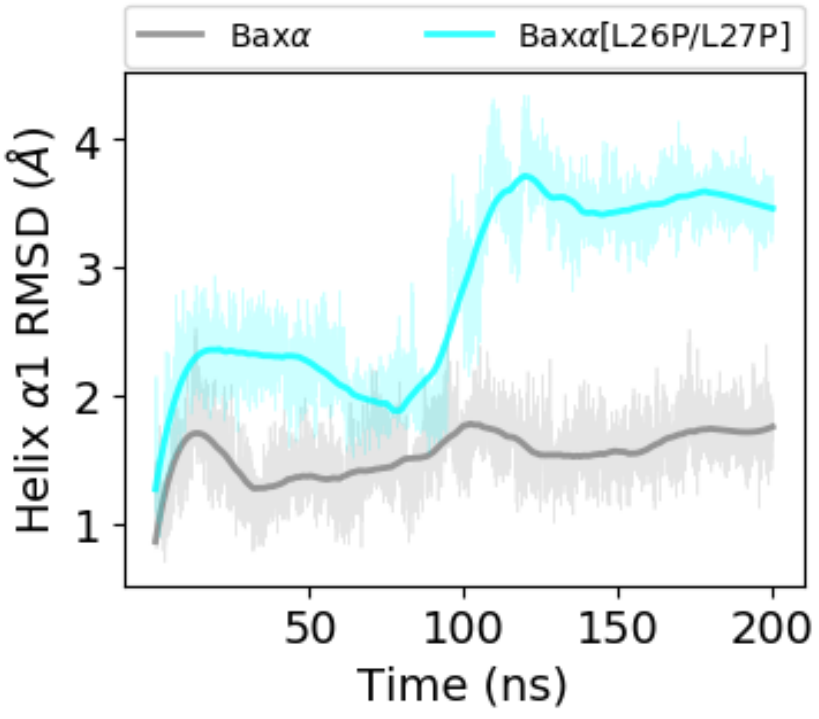
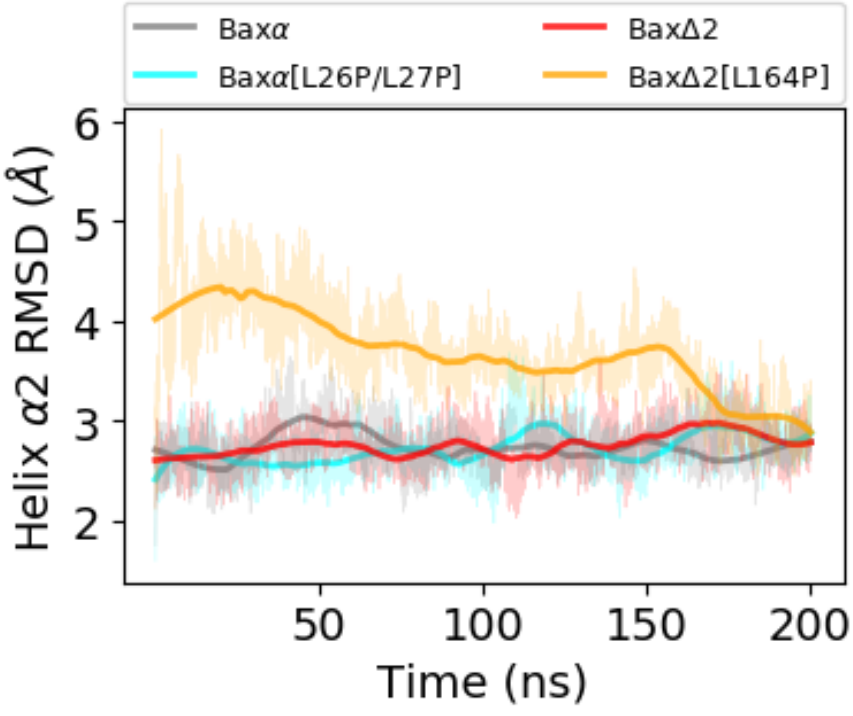


RMSD: 0.317

Fig. S2


Baxα
BaxΔ2
Baxα[L26P/L27P]
BaxΔ2[L164P]
Core RMSD (Å)
Time (ns)


Baxα
Baxα[L26P/L27P]
Helix α1 RMSD (Å)
Time (ns)


Baxα
BaxΔ2
Baxα[L26P/L27P]
BaxΔ2[L164P]
Helix α2 RMSD (Å)
Time (ns)

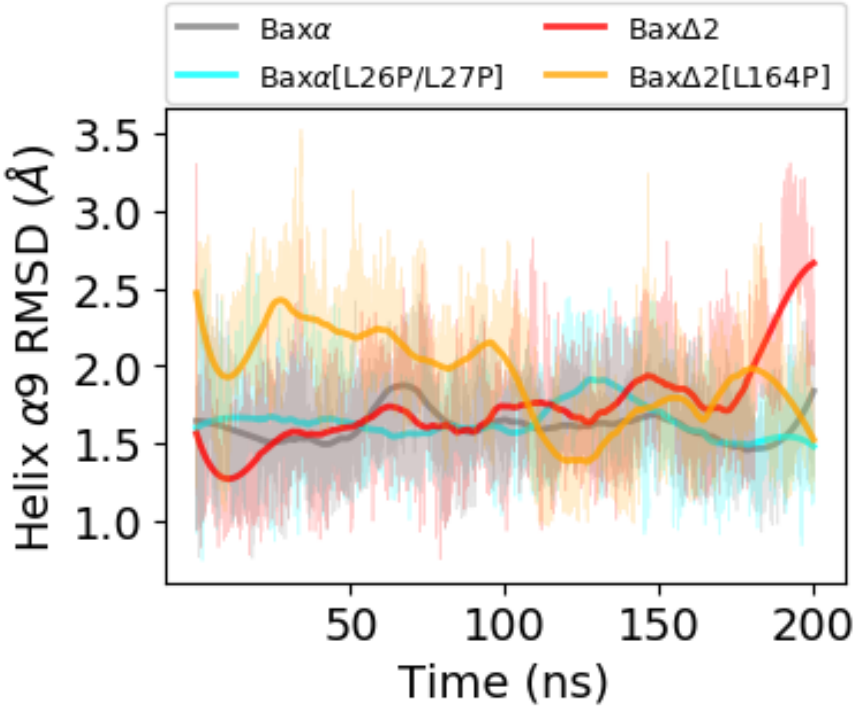
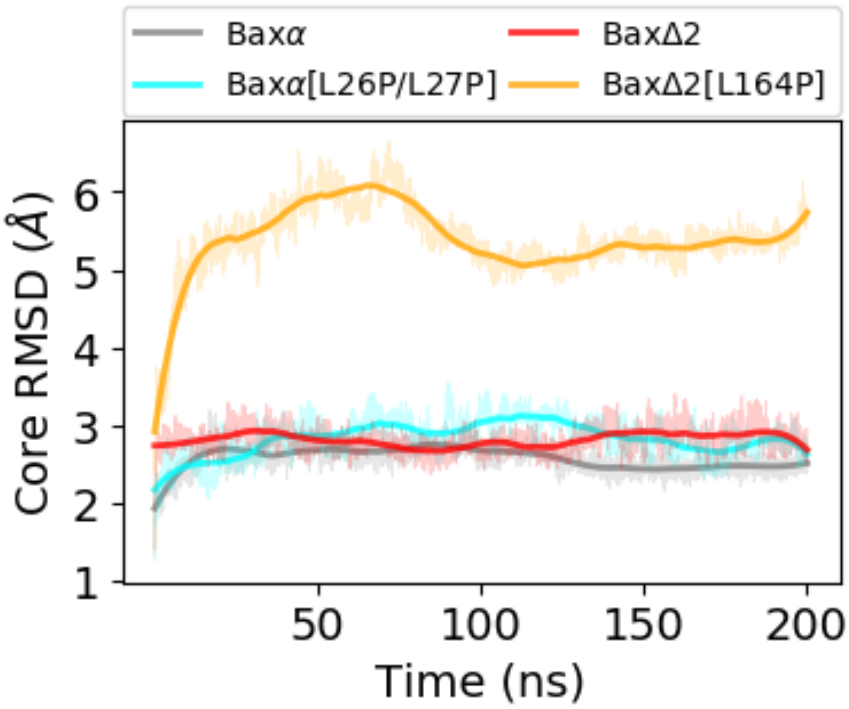
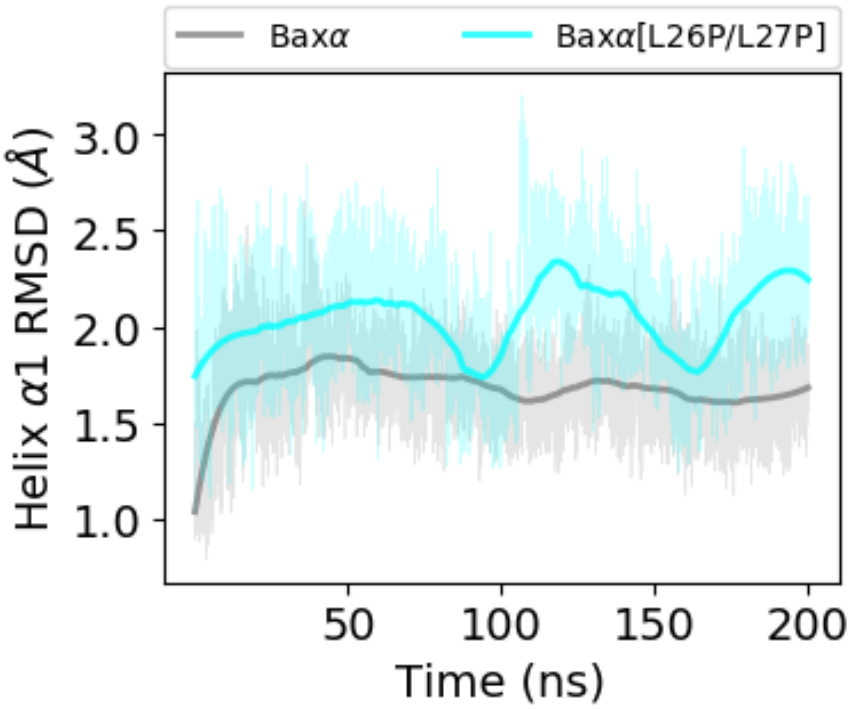
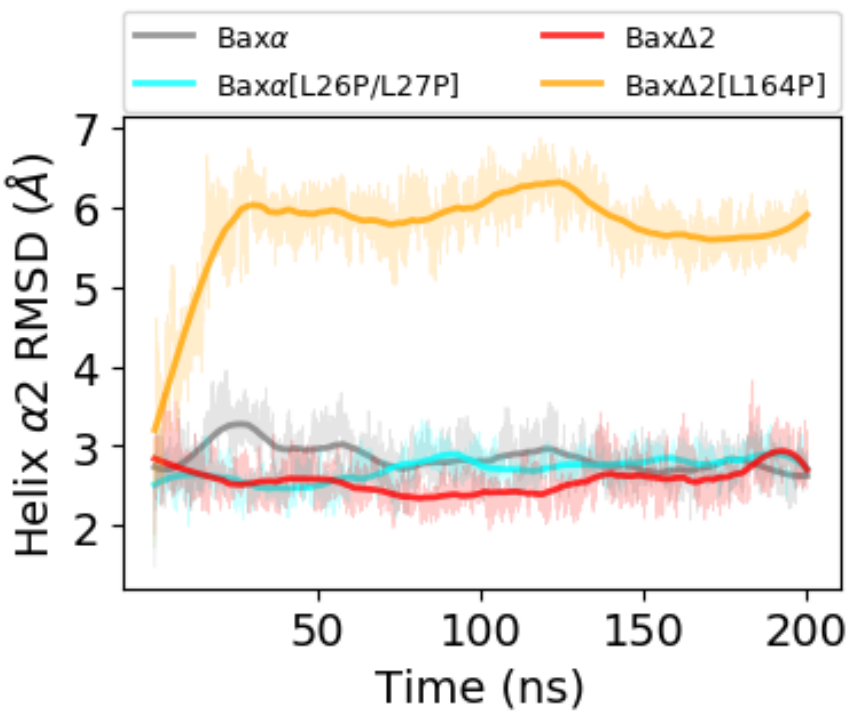

Baxα
BaxΔ2
Baxα[L26P/L27P]
BaxΔ2[L164P]
Helix α9 RMSD (Å)
Time (ns)

Fig. S3


Baxα
BaxΔ2
Baxα[L26P/L27P]
BaxΔ2[L164P]
Core RMSD (Å)
Time (ns)


Baxα
Baxα[L26P/L27P]
Helix α1 RMSD (Å)
Time (ns)


Baxα
BaxΔ2
Baxα[L26P/L27P]
BaxΔ2[L164P]
Helix α2 RMSD (Å)
Time (ns)

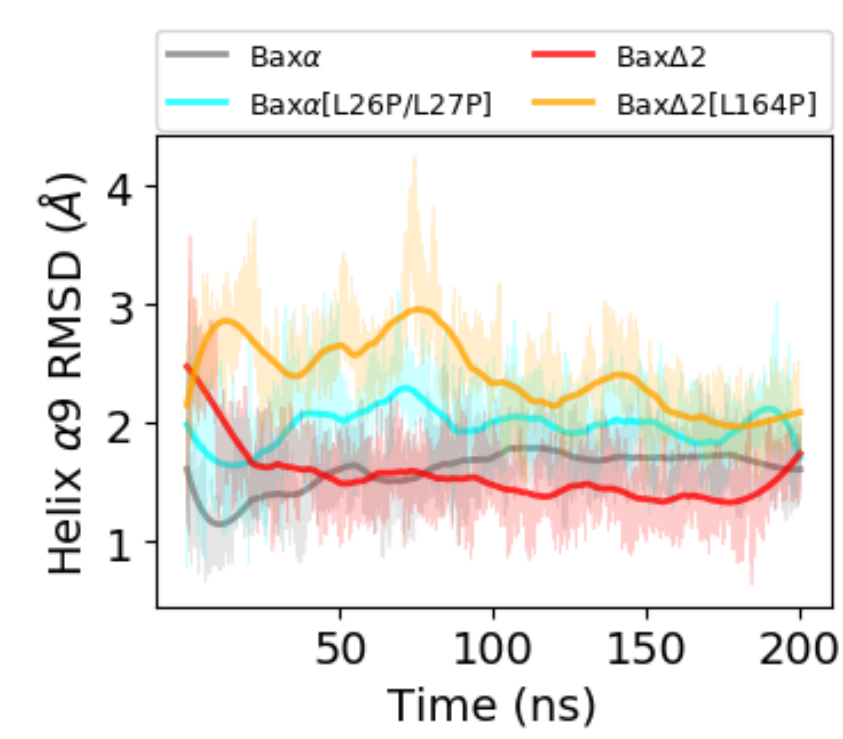
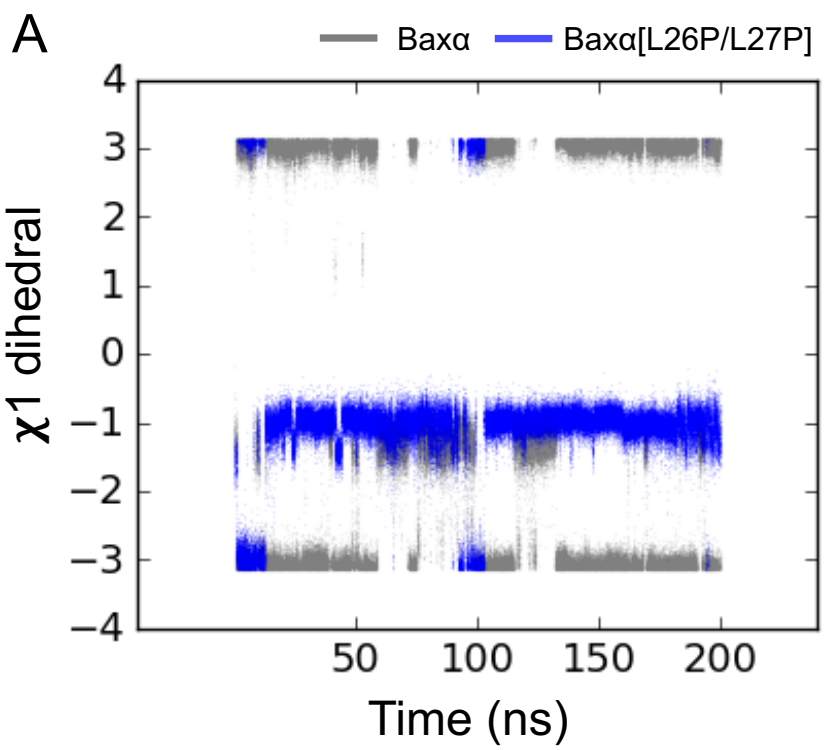
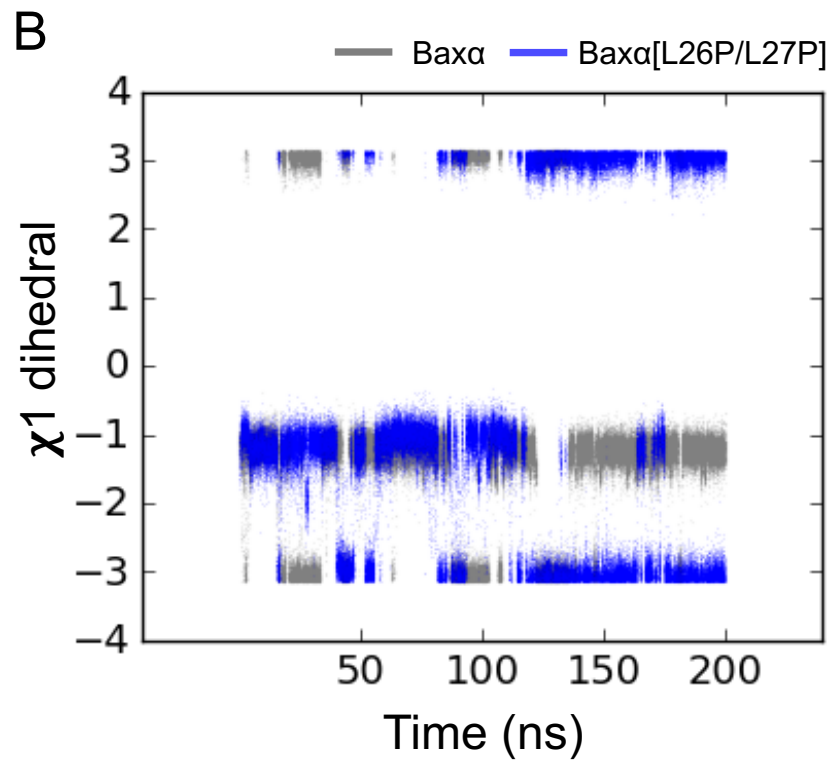

Baxα
BaxΔ2
Baxα[L26P/L27P]
BaxΔ2[L164P]
Helix α9 RMSD (Å)
Time (ns)

Fig. S4


A
Baxα
Baxα[L26P/L27P]
χ1 dihedral
4
3
2
1
0
−1
−2
−3
−4
50
100
150
200
Time (ns)


B
Baxα
Baxα[L26P/L27P]
χ1 dihedral
4
3
2
1
0
−1
−2
−3
−4
50
100
150
200
Time (ns)

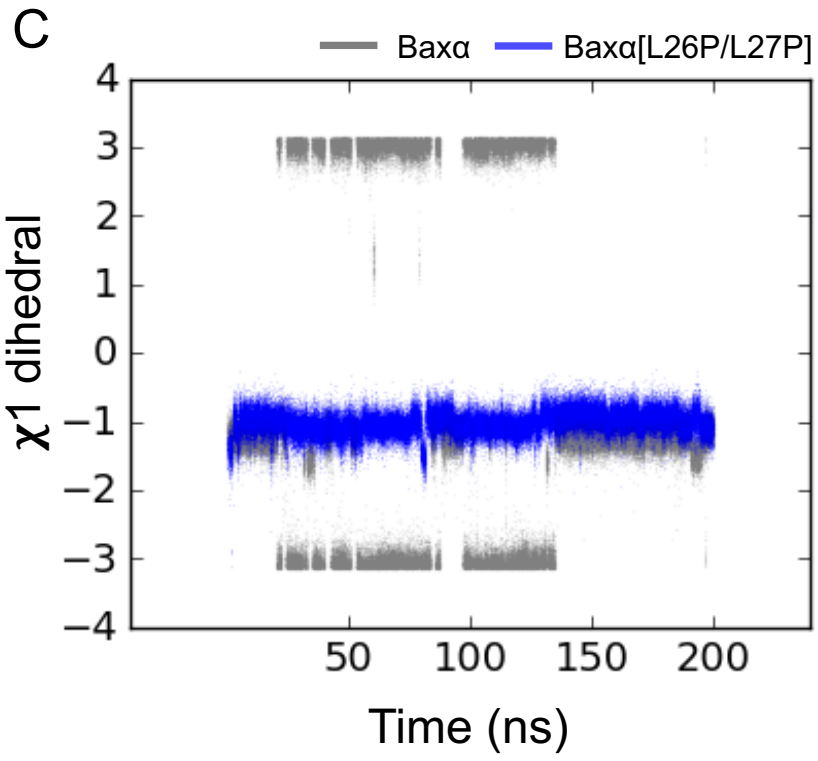
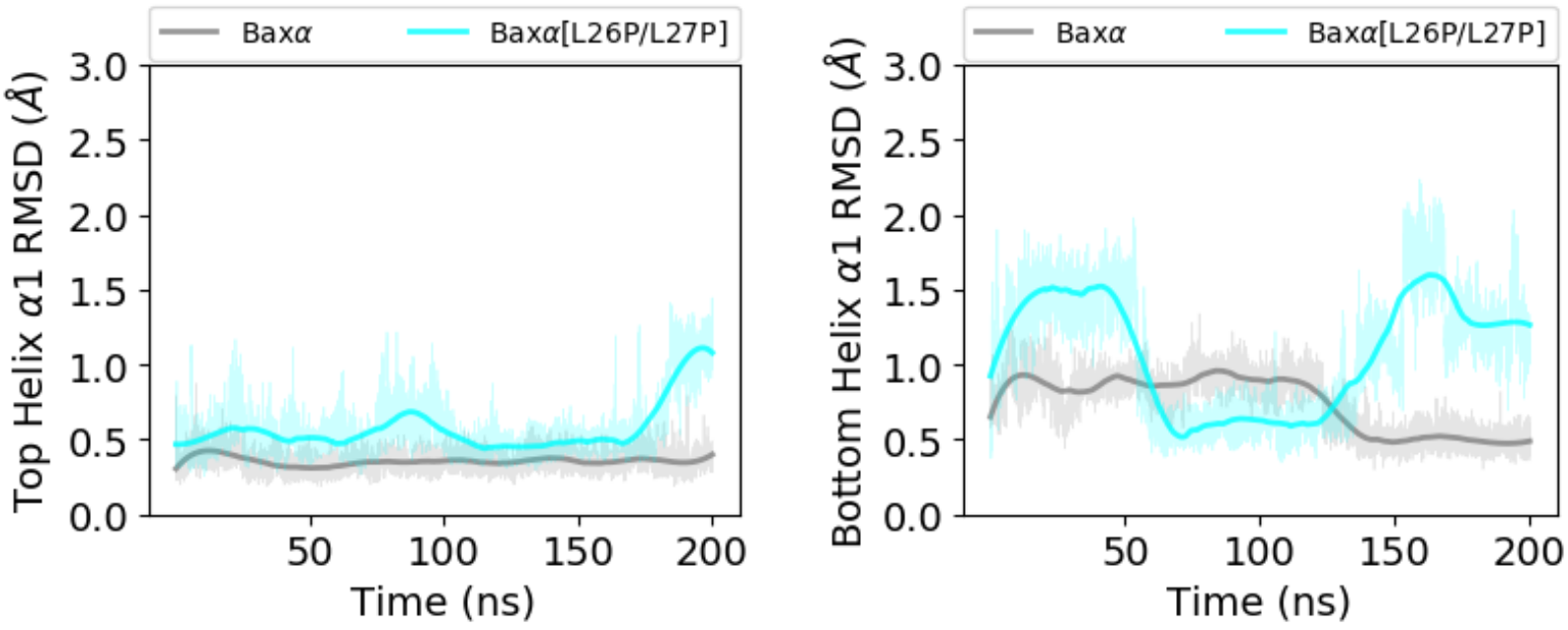
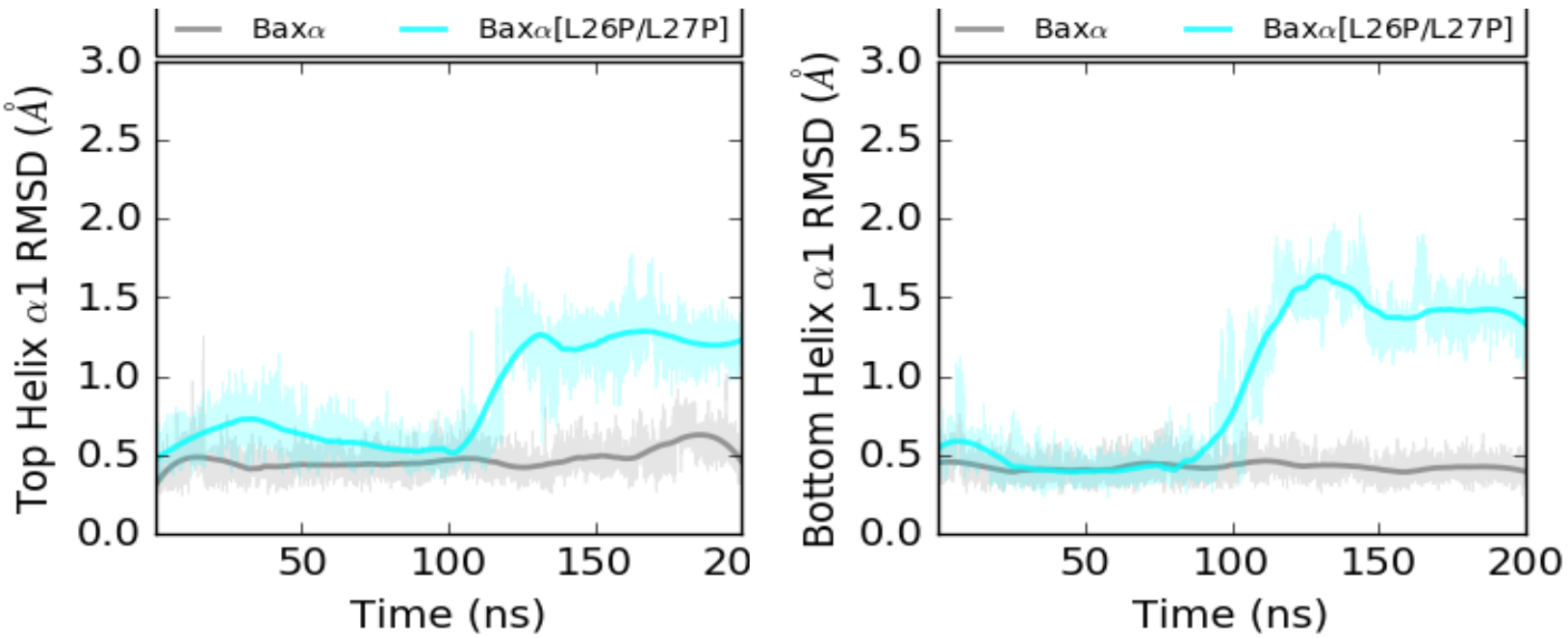

C
Baxα
Baxα[L26P/L27P]
χ1 dihedral
4
3
2
1
0
−1
−2
−3
−4
50
100
150
200
Time (ns)

Fig. S5

A


Baxα
Baxα[L26P/L27P]
Top Helix α1 RMSD (Å)
Bottom Helix α1 RMSD (Å)
Time (ns)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
50
100
150
200

B


Baxα
Baxα[L26P/L27P]
Top Helix α1 RMSD (Å)
Bottom Helix α1 RMSD (Å)
Time (ns)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
50
100
150
200

C

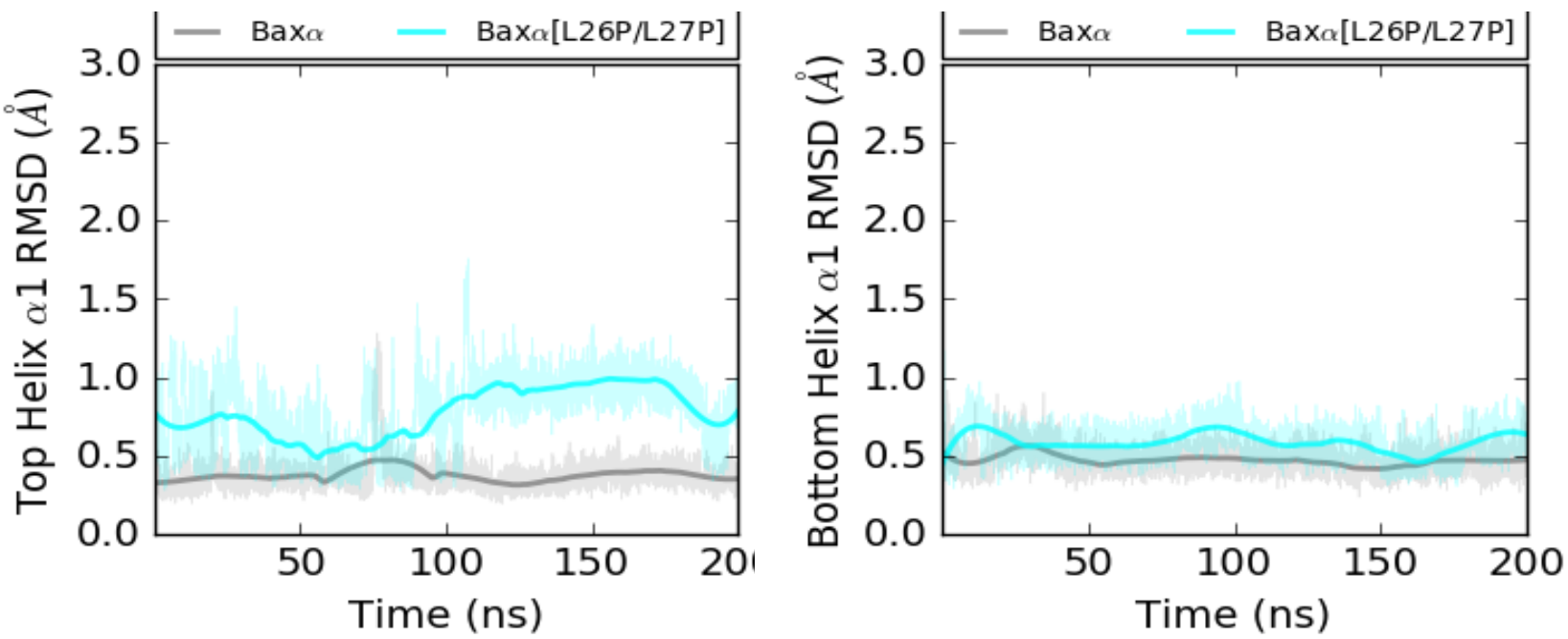

Baxα
Baxα[L26P/L27P]
Top Helix α1 RMSD (Å)
Bottom Helix α1 RMSD (Å)
Time (ns)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
50
100
150
200

Fig. S6

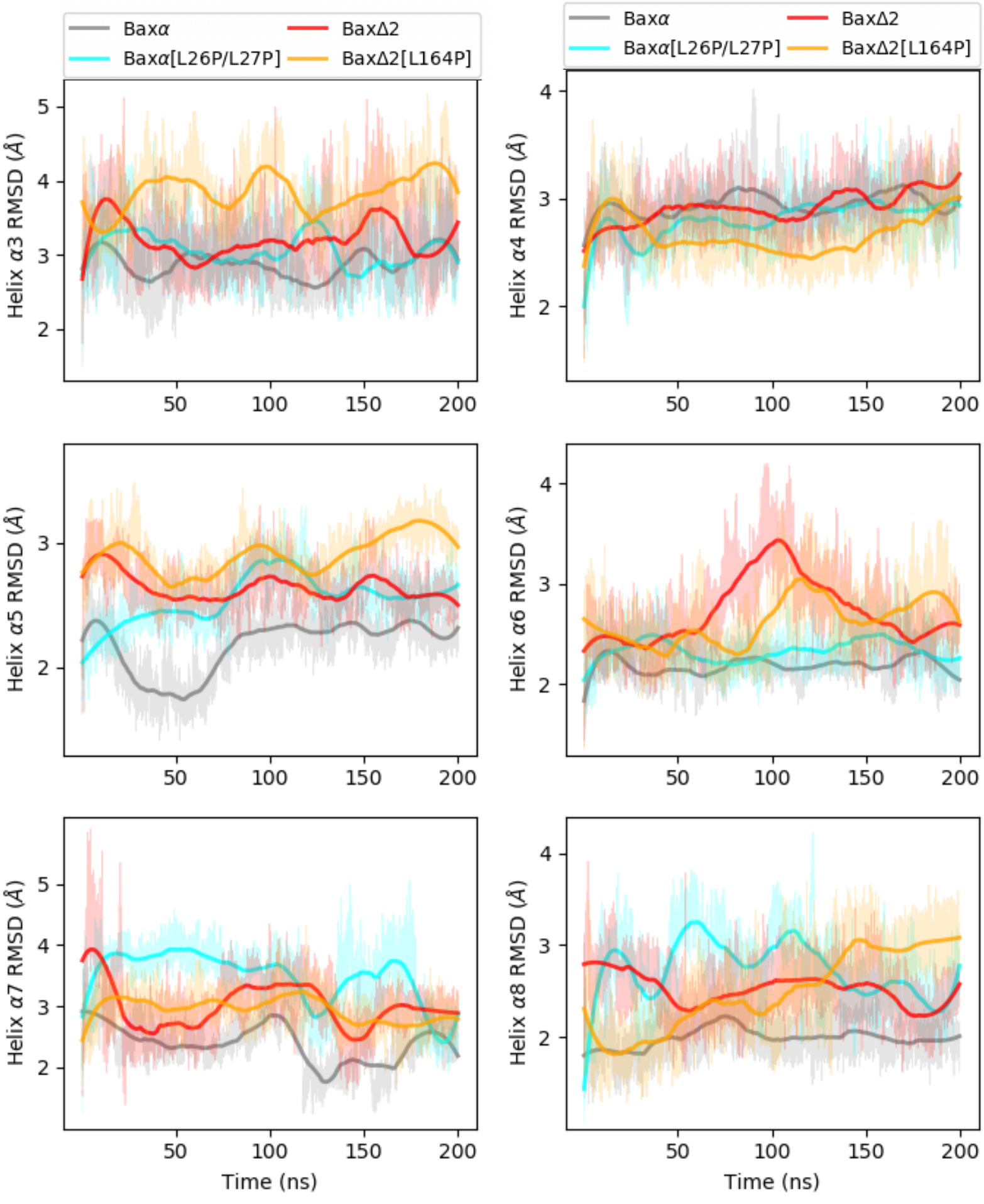

Baxα
BaxΔ2
Baxα[L26P/L27P]
BaxΔ2[L164P]
Helix α3 RMSD (Å)
Helix α4 RMSD (Å)
Helix α5 RMSD (Å)
Helix α6 RMSD (Å)
Helix α7 RMSD (Å)
Helix α8 RMSD (Å)
Time (ns)
50
100
150
200

Fig. S7

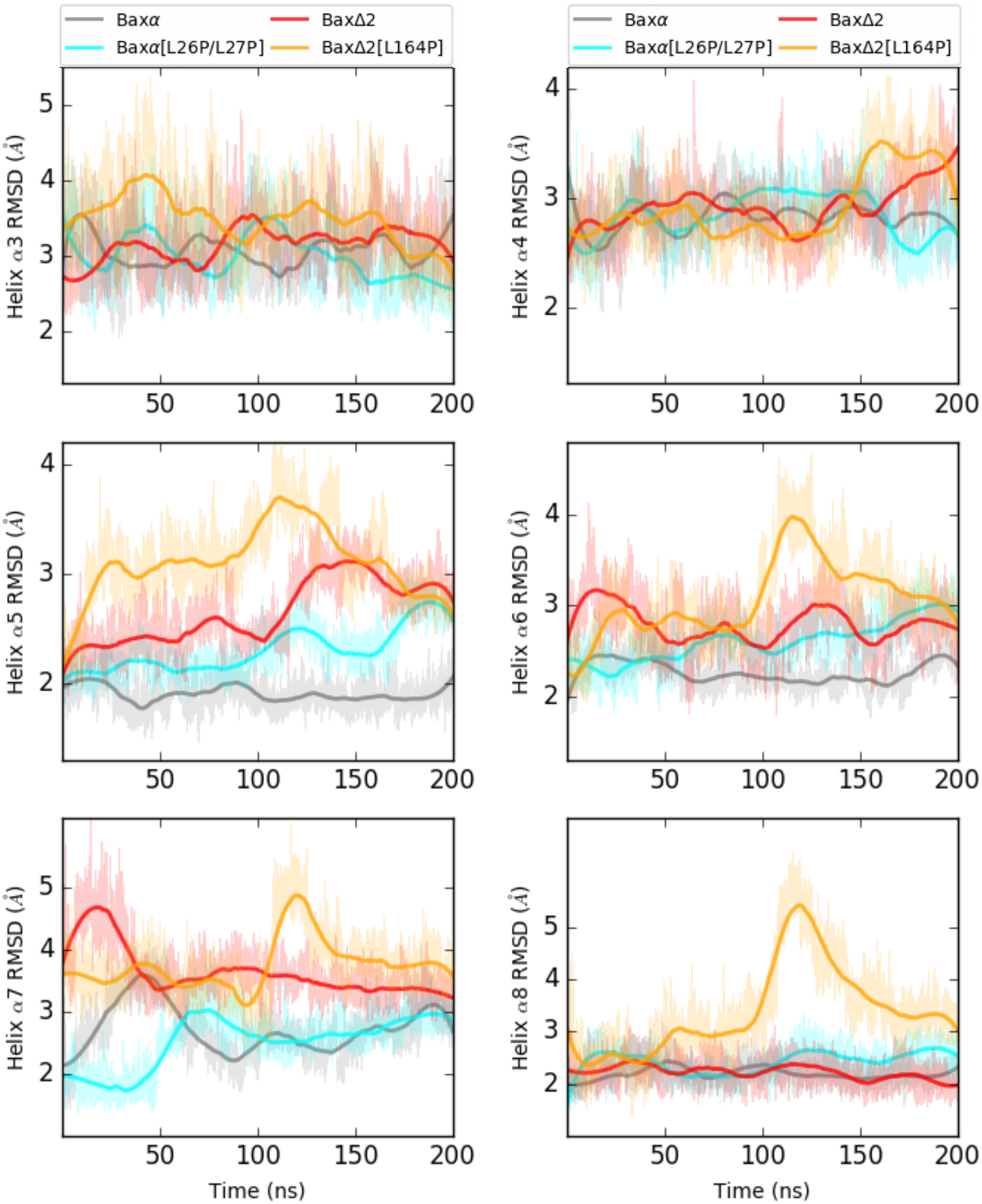

Baxα
BaxΔ2
Baxα[L26P/L27P]
BaxΔ2[L164P]
Helix α3 RMSD (Å)
Helix α4 RMSD (Å)
Helix α5 RMSD (Å)
Helix α6 RMSD (Å)
Helix α7 RMSD (Å)
Helix α8 RMSD (Å)
Time (ns)
50
100
150
200
2
3
4
5

Fig. S8

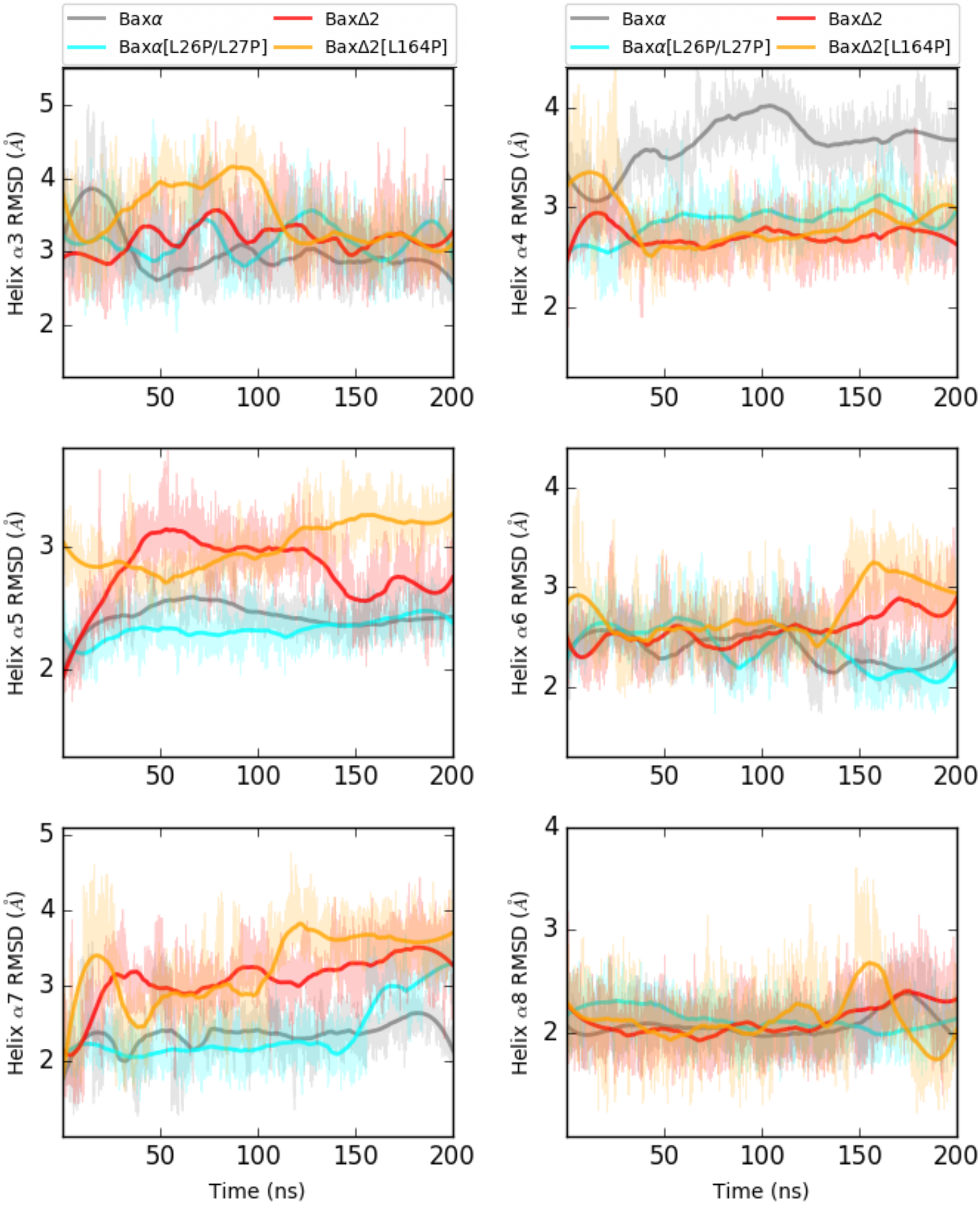
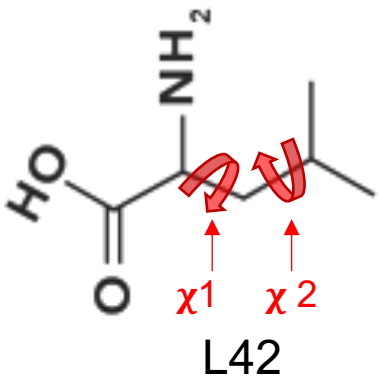
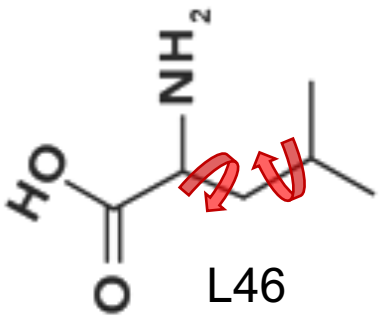

Baxα
BaxΔ2
Baxα[L26P/L27P]
BaxΔ2[L164P]
Helix α3 RMSD (Å)
Helix α4 RMSD (Å)
Helix α5 RMSD (Å)
Helix α6 RMSD (Å)
Helix α7 RMSD (Å)
Helix α8 RMSD (Å)
Time (ns)
50
100
150
200

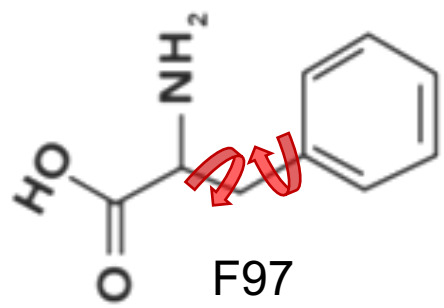
Fig. S9



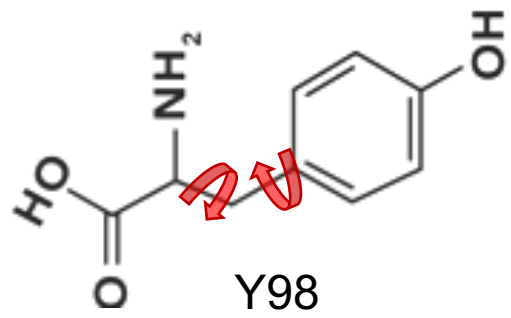
L42



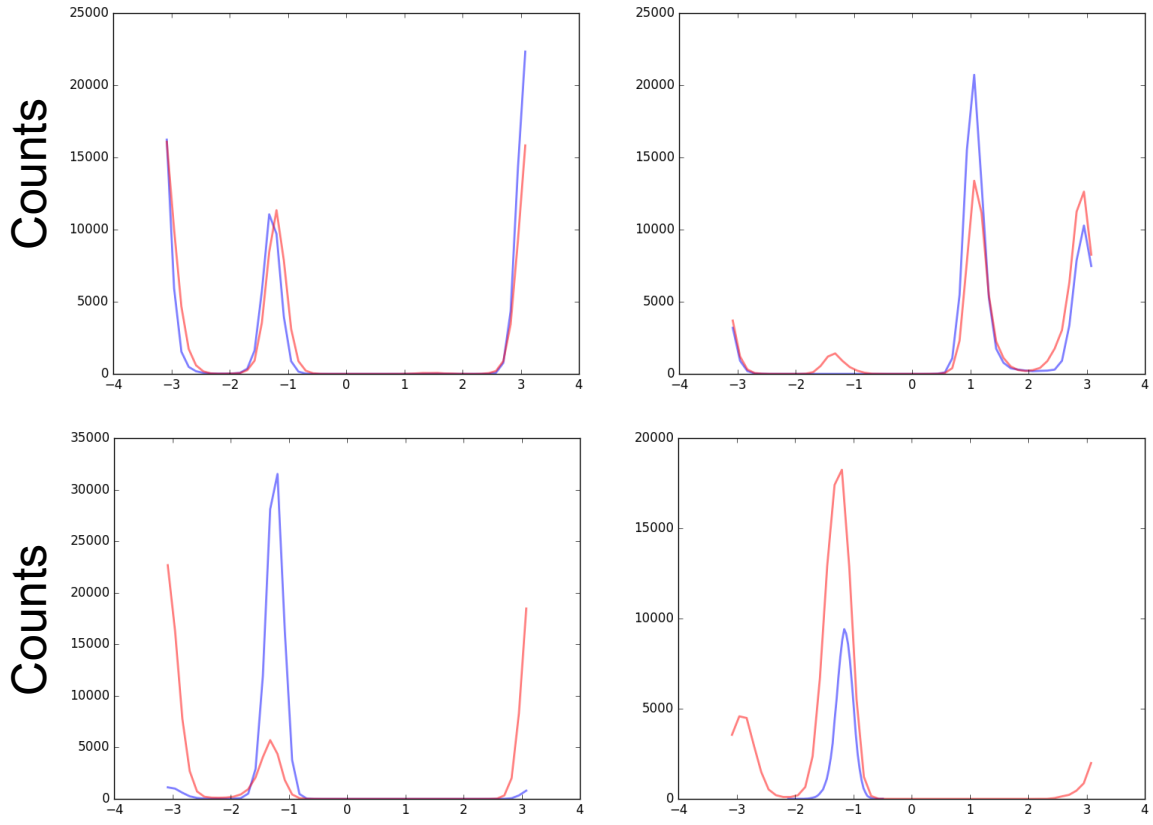
L46



F97



Y98

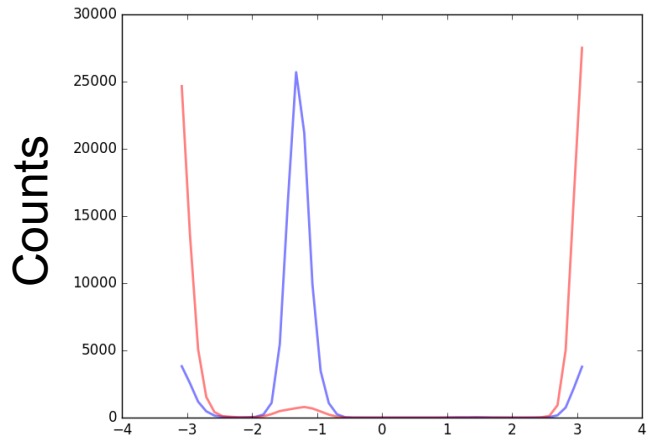


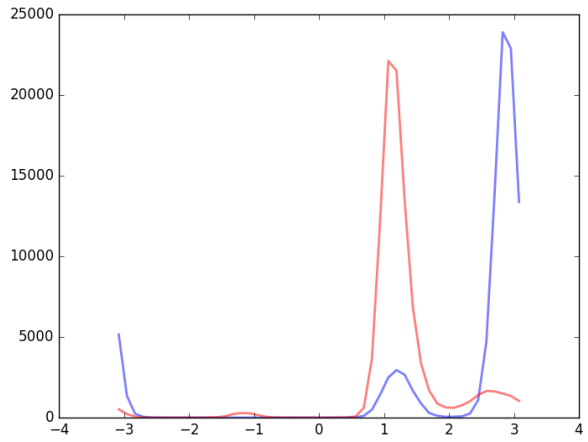
χ1 dihedral angle

χ2 dihedral angle

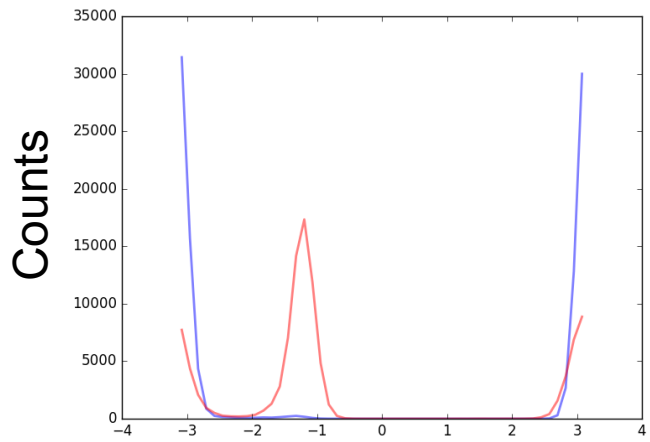
Fig. S10

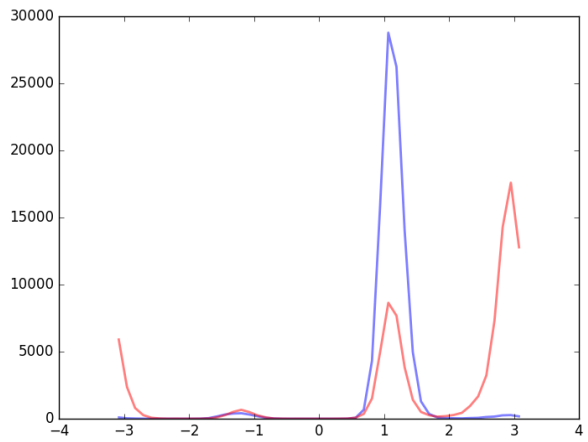
L42





L46





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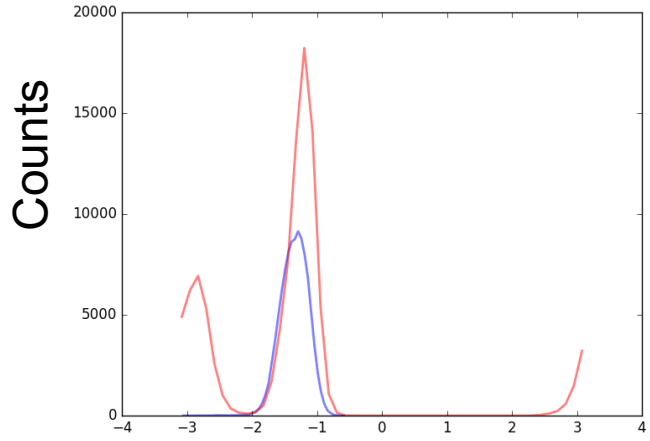
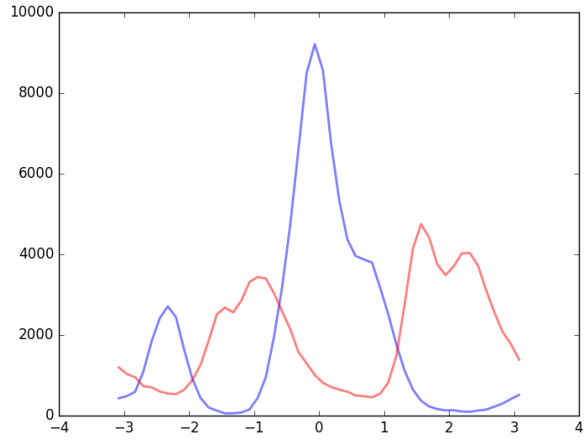
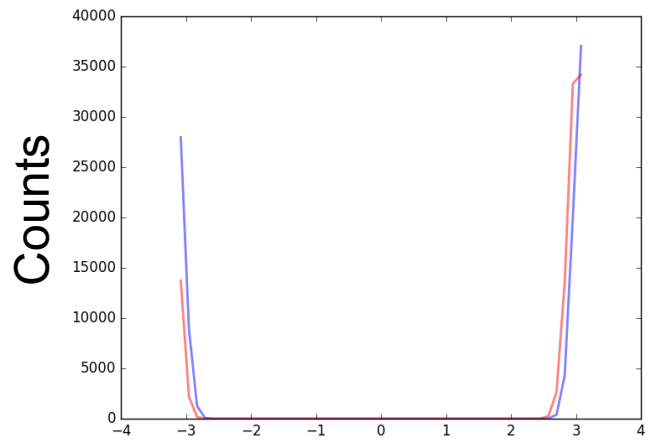




Y98



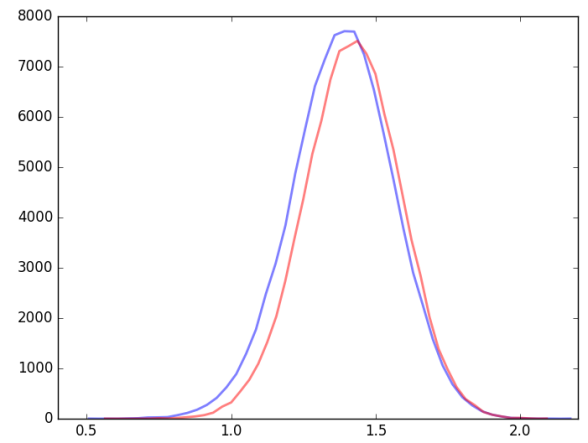
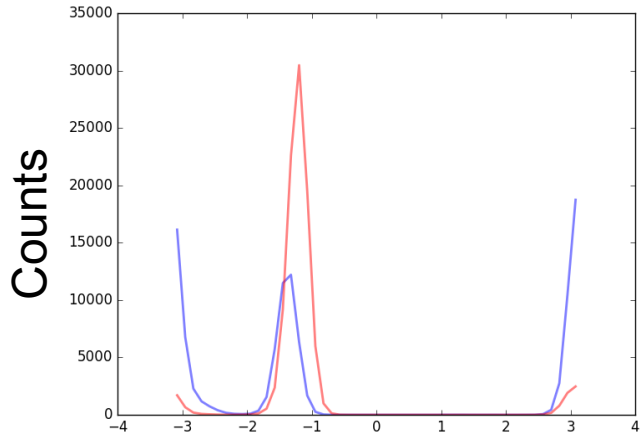
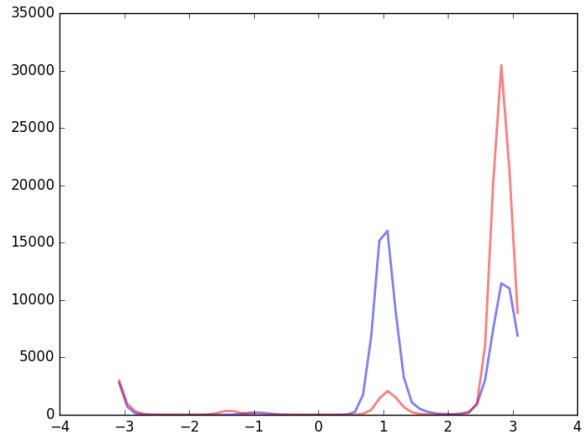


Fig. S11

L42





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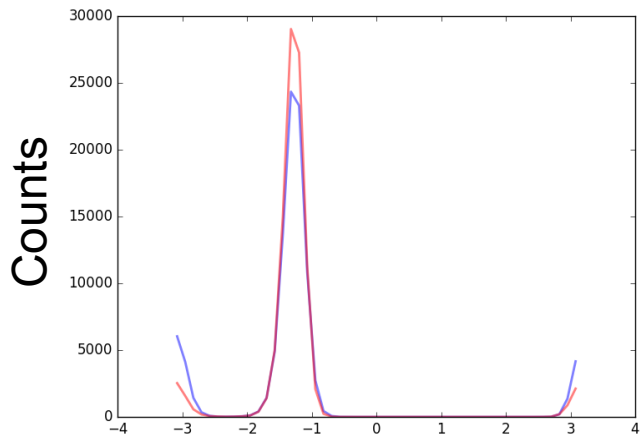
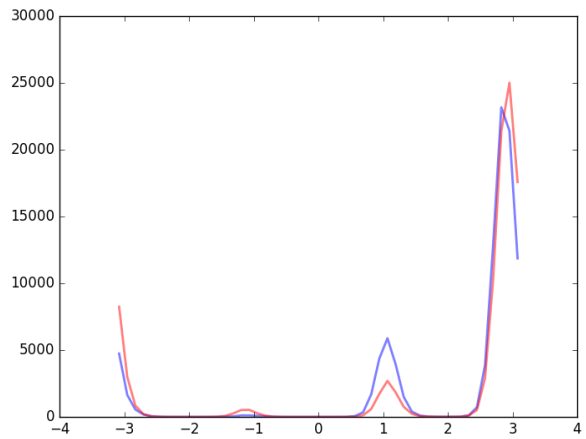
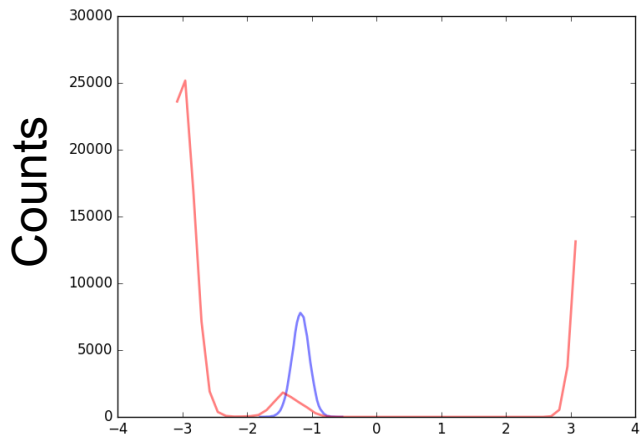
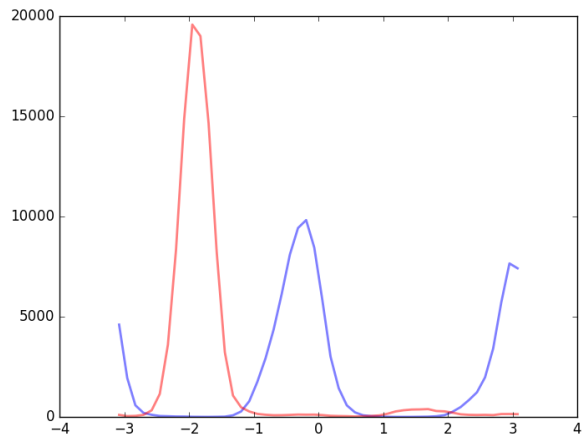


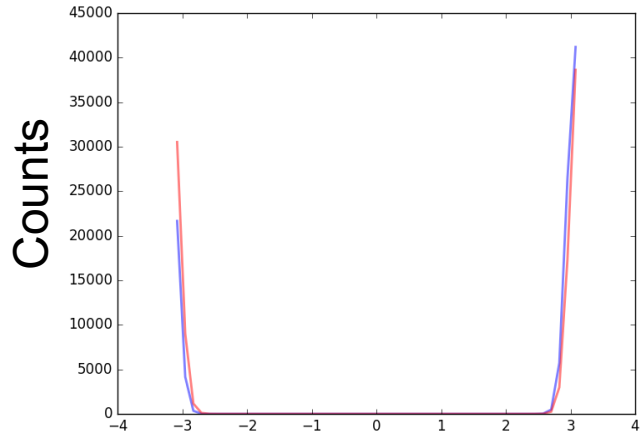


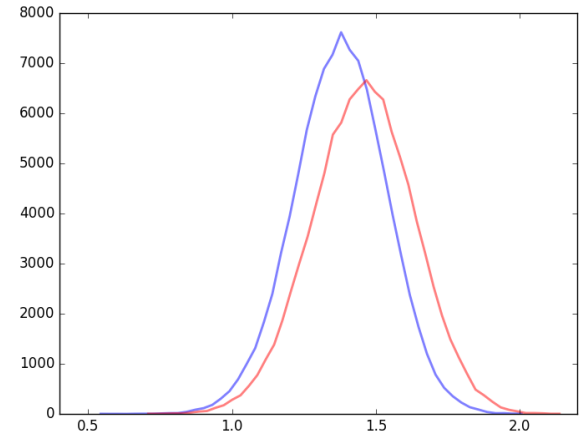
F97





Y98

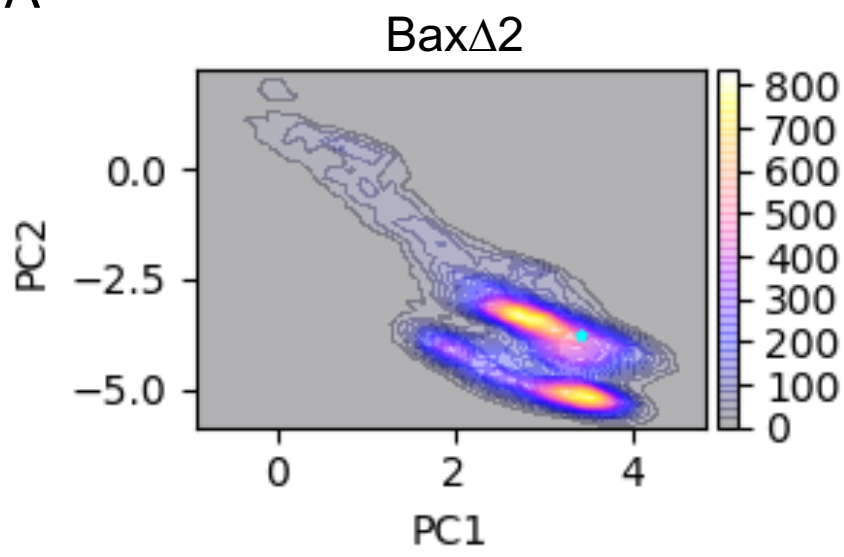


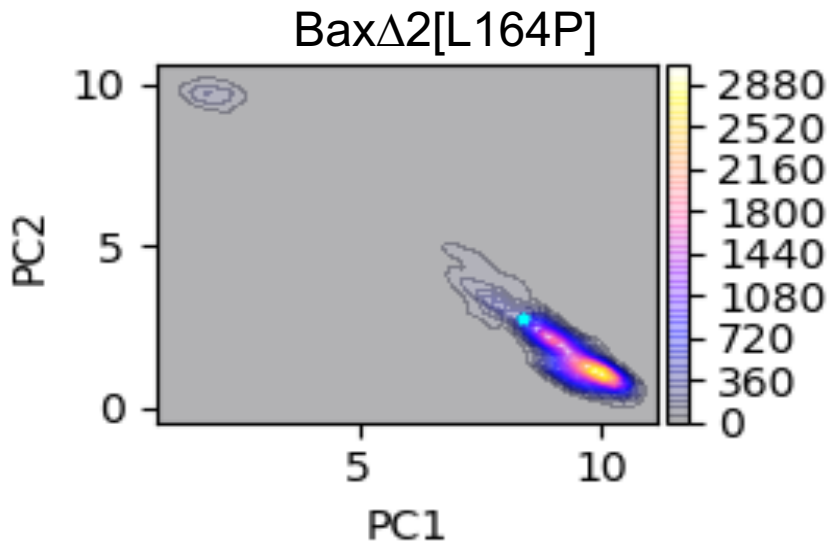


χ1 dihedral angle

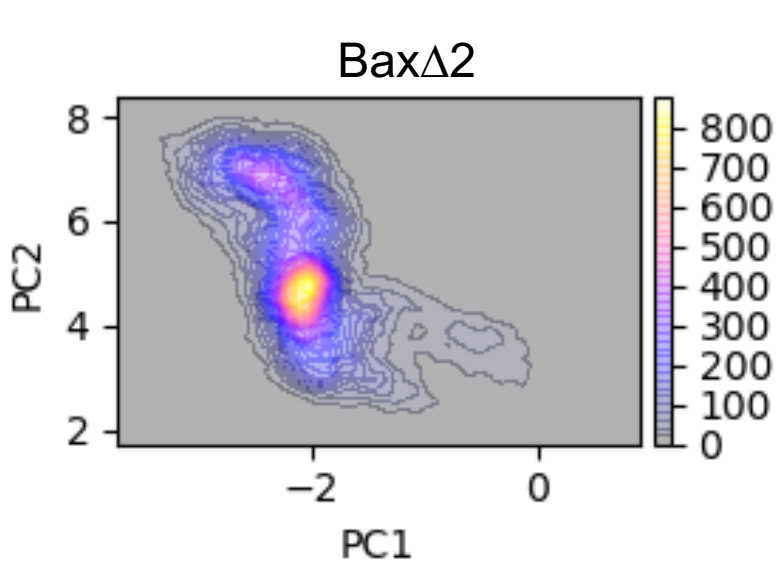
χ2 dihedral angle

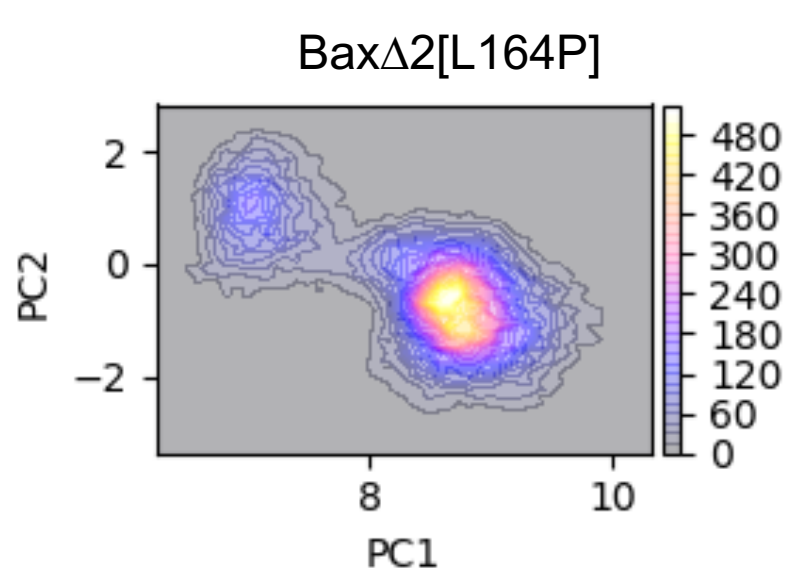
A


BaxΔ2
PC2
PC1
0.0
−2.5
−5.0
0
2
4
800
700
600
500
400
300
200
100
0

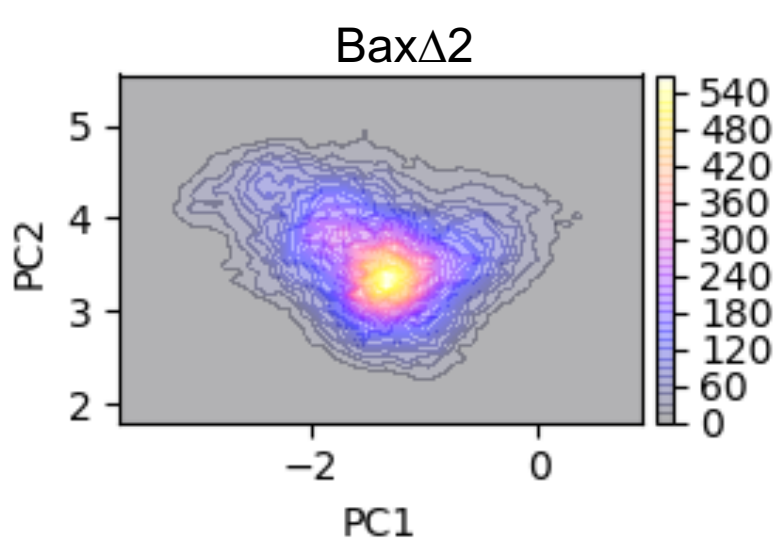

BaxΔ2[L164P]
PC2
PC1
10
5
0
5
10
2880
2520
2160
1800
1440
1080
720
360
0

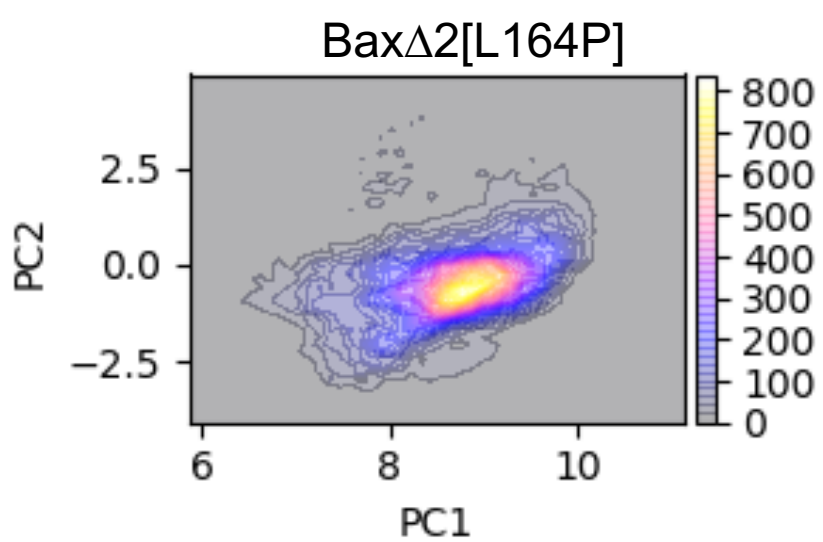
B


BaxΔ2
PC2
PC1
8
6
4
2
−2
0
800
700
600
500
400
300
200
100
0


BaxΔ2[L164P]
PC2
PC1
2
0
−2
8
10
480
420
360
300
240
180
120
60
0

C


BaxΔ2
PC2
PC1
5
4
3
2
−2
0
540
480
420
360
300
240
180
120
60
0


BaxΔ2[L164P]
PC2
PC1
2.5
0.0
−2.5
6
8
10
800
700
600
500
400
300
200
100
0

Supplementary figure legends

Fig. S1 Alignment of predicted (blue) and crystallographic (grey) structures of Baxα. The structures were aligned using VMD 1.9.0.

Fig. S2 RMSDs of backbone atoms in the core (upper left), α1 (upper right), α2 (lower left), and α9 (lower right), relative to the initial structure, during the second repetition of 200 ns of MD simulations. Coloring is by variant: Baxα (grey), Baxα[L26P/L27P] (blue), BaxΔ2 (red), and BaxΔ2[L164P] (orange). Shaded lines show RMSDs for all recorded points and solid lines are smoothed as described in section 4.4.

Fig. S3 RMSDs of backbone atoms in the core (upper left), α1 (upper right), α2 (lower left), and α9 (lower right), relative to the initial structure, during the third repetition of 200 ns of MD simulations. Coloring is by variant: Baxα (grey), Baxα[L26P/L27P] (blue), BaxΔ2 (red), and BaxΔ2[L164P] (orange). Shaded lines show RMSDs for all recorded points and solid lines are smoothed as described in section 4.4.

Fig. S4 A dihedral plot of L25. (**A)** The dihedral plot of L25 at helix α1 kink position along the simulation trajectory. Baxα (grey), Baxα[L26P/L27P] (blue). (**B**) The dihedral plot of L25 along the second (**B**) and third (**C**) repeated simulation trajectories.

Fig. S5 (A) RMSDs of backbone atoms, relative to the initial structure, of the top and bottom half of helix α1 during 200 ns of simulation. For each snapshot, the same α carbons are used for alignment and RMSD calculation. The second repeated (**B**) and third repeated (**C**) simulations. Coloring is by variant: Baxα (grey), Baxα[L26P/L27P] (blue).

Fig. S6 RMSDs of backbone atoms, relative to the initial structure, of helix α3, α4, α5, α6, α7, α8, during 200 ns of simulation are shown. Coloring is by variant: Baxα (grey), Baxα[L26P/L27P] (blue), BaxΔ2 (red), and BaxΔ2[L164P] (orange).

Fig. S7/S8 RMSDs of backbone atoms, relative to the initial structure, of helix α3, α4, α5, α6, α7, α8, during the second repeatd (**S7**) and third repeated (**S8**) simulations are shown. Coloring is by variant: Baxα (grey), Baxα[L26P/L27P] (blue), BaxΔ2 (red), and BaxΔ2[L164P] (orange).

Fig. S9 Calculation of dihedral angles. The χ1 and χ2 of Amino acids L42, L46, F97, Y98 (from top to bottom) were analyzed by using MDTraj 1.9.3. BaxΔ2 colored as blue, BaxΔ2[L164P] colored as red.

Fig. S10/S11 Calculation of dihedral angles. The χ1 and χ2 of Amino acids L42, L46, F97, Y98 (from top to bottom) in the second (**S10**) and third (**S11**) repeated simulations were analyzed by using MDTraj 1.9.3. BaxΔ2 colored as blue, BaxΔ2[L164P] colored as red.

Fig. S12 Principal component analysis (PCA). (**A**) PCA landscapes of BaxΔ2 (left) and BaxΔ2[L164P]. The blue spot pointed at the location of BaxΔ2 or BaxΔ2[L164P] docking structure which were shown in figure 7. PC, principal component. PCA landscapes of the second (**B**) and third (**C**) repeated MD simulation.