Supplemental Figures

Figure S1. Protein sequence alignment between NorM-VC and hMATE1. Identical regions are shaded in yellow, similar regions in light blue. Secondary structures are marked with cartoons. Gaps are show in dashed lines. Alignment was produced by ClustalW.

Figure S2. RMSD versus time between simulation snapshots and NorM x-ray structure (black), and hMATE1 homology model (red), after first aligning each simulation frame to the initial structures. The RMSD was taken for the Cα atoms of the protein that were embedded in the simulated membrane, and it was calculated every 50 ps of simulation time.

Figure S3. Helical tilt angles are shown versus simulation time for each of the 12 helices in both NorM (black) and hMATE1 (red). The tilt angle was calculated by fitting a line to the Cα coordinates of the membrane embedded region of each helix, and then finding the dot product of the resulting vector with the z-axis (the membrane normal direction).

Figure S4. Images of the hMATE1 homology model (a and c), and from the end of the 50 ns hMATE1 MD simulation (b and d). A side view (a and b) and a view from the extracellular side of the membrane (c and d) are shown. Coloring of the helices is from the N-terminus (blue) to the C-terminus (red). The channel profile was calculated using the program HOLE (n14). Coloring of the channel is: red (radius < 1.15 Å), green (1.15 Å < radius < 2.30 Å), and blue (radius > 2.30 Å).

Fig. S1

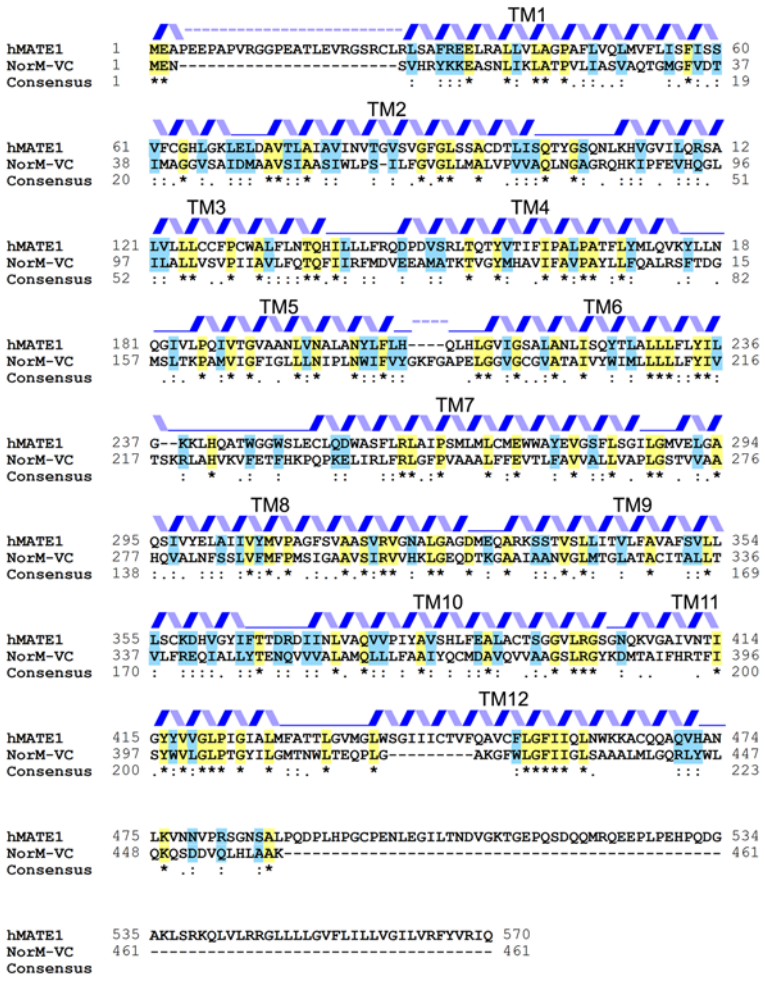
TM1
TM2
TM3
TM4
TM5
TM6
TM7
TM8
TM9
TM10
TM11
TM12
hMATE1 1 MEAPEEPAPVRGGPEATLEVRGSRCLRLSAFREELRALLVLAGPAFLVQLMVFLISFISS 60
NorM-VC 1 MEN---------- SVHRYKKEASNLIKLATPVLIASVAQTGMGFVDT 37
Consensus 1 ** : :::* *: ** *.::..: :.*:.: 19
hMATE1 61 VFCGHLGKLELDAVTLAIAVINVTGVSVGFGLSSACDTLISQTYGSQNLKHVGVILQRSA 12
NorM-VC 38 IMAGGVSAIDMAAVSIAASIWLPS-ILFGVGLLMALVPVVAQLNGAGRQHKIPFEVHQGL 96
Consensus 20 ::.* :. ::: **::* :: : : .*.** * .:::* *: . ::: . :::. 51
hMATE1 121 LVLLLCCFPCWALFLNTQHILLLFRQDPDVSRLTQTYVTIFIPALPATFLYMLQVKYLLN 18
NorM-VC 97 ILALLVSVPIIAVLFQTQFIIRFMDVEEAMATKTVGYMHAVIFAVPAYLLFQALRSFTDG 15
Consensus 52 :: ** ..* *::::**.*: :: : :: * *: .* *:** :*: .: . 82
hMATE1 181 QGIVLPQIVTGVAANLVNALANYLFLH----QLHLGVIGSALANLISQYTLALLLFLYIL 236
NorM-VC 157 MSLTKPAMVIGFIGLLLNIPLNWIFVYGKFGAPELGGVGCGVATAIVYWIMLLLLLFYIV 216
Consensus .:. * :* *. . *:* *::*:: .** :*..:*. * : : ***::**:
hMATE1 237 G--KKLHQATWGGWSLECLQDWASFLRLAIPSMLMLCMEWWAYEVGSFLSGILGMVELGA 294
NorM-VC 217 TSKRLAHVKVFETFHKPQPKELIRLFRLGFPVAAALFFEVTLFAVVALLVAPLGSTVVAA 276
Consensus : * .: : :: ::**.:* * :* : * ::* . ** . :.*
hMATE1 295 QSIVYELAIIVYMVPAGFSVAASVRVGNALGAGDMEQARKSSTVSLLITVLFAVAFSVLL 354
NorM-VC 277 HQVALNFSSLVFMFPMSIGAAVSIRVVHKLGEQDTKGAAIAANVGLMTGLATACITALLT 336
Consensus 138 :.:. ::: :*:*.* .:..*.*:** : ** * : * ::.*.*: : * ::* 169
hMATE1 355 LSCKDHVGYIFTTDRDIINLVAQVVPIYAVSHLFEALACTSGGVLRGSGNQKVGAIVNTI 414
NorM-VC 337 VLFREQIALLYTENQVVVALAMQLLLFAAIYQCMDAVQVVAAGSLRGYKDMTAIFHRTFI 396
Consensus 170 : ::::. ::* :: :: *. *:: : *: : ::*: .:.* *** : .. . * 200
hMATE1 415 GYYVVGLPIGIALMFATTLGVMGLWSGIIICTVFQAVCFLGFIIQLNWKKACQQAQVHAN 474
NorM-VC 397 SYWVLGLPTGYILGMTNWLTEQPLG---------AKGFWLGFIIGLSAAALMLGQRLYWL 447
Consensus 200 .*:*:*** * * ::. * * :***** *. ::: 223
hMATE1 475 LKVNNVPRSGNSALPQDPLHPGCPENLEGILTNDVGKTGEPQSDQQMRQEEPLPEHPQDG 534
NorM-VC 448 QKQSDDVQLHLAAK---------- 461
Consensus * .: : :*
hMATE1 535 AKLSRKQLVLRRGLLLLGVFLILLVGILVRFYVRIQ 570
NorM-VC 461 ---------- 461
Consensus

Figure S2

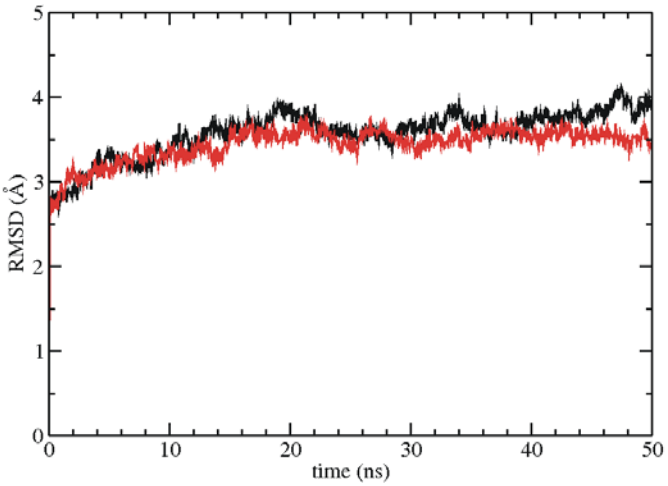

Figure S3

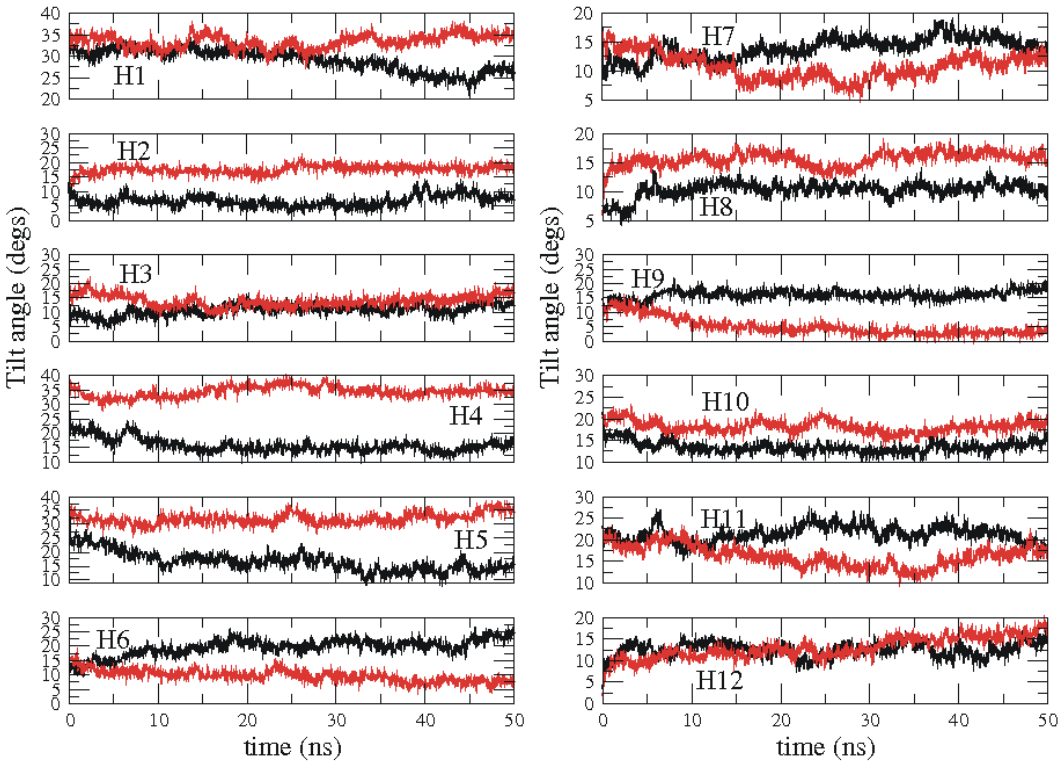
H1
H2
H3
H4
H5
H6
H7
H8
H9
H10
H11
H12
Tilt angle (degs)
Tilt angle (degs)
time (ns)
time (ns)

Figure S4