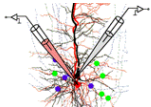


Modelling the Acetylcholine Receptor Channel



Max-Planck-Institut für medizinische Forschung

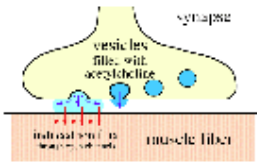


Abteilung Zellphysiologie



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Introductions to model building studies are given by [von Kitzing 92a](#) and [von Kitzing 92b](#). The details of the channel model are described by [von Kitzing 95](#).

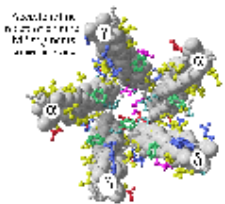
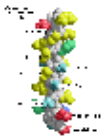


The acetylcholine receptor channel is placed at the junction between the neuronal synapse and the muscle fiber: the [neuromuscular junction](#). If the synapse becomes excited the acetylcholine filled vesicles secrete their neurotransmitter into the synaptic cleft. This neurotransmitter opens the AChR channels resulting in an ionic current through the channels. This current in turn excites the muscle fibers which then contract.

Certain amino acids in the M2-segment of the acetylcholine receptor channel strongly influence the ionic conductivity, bind to photo labels or change binding constants of certain blocking drugs. Those important amino acids are colored in the sequence alignment of the sequences. The same color code is used below for the respective atoms of the side chains in the atomic model.



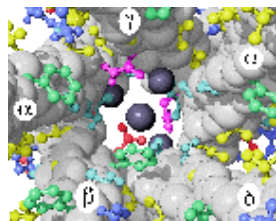
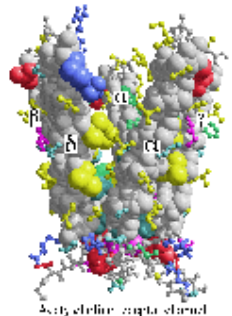
If the amino acids of the M2 segment which are assumed to line the channel pore are placed on an α -helix they all are found on one side of the helix. This led to the conclusion that the M2-segment may be α -helical. Note, here the same color coding was used as in the sequence alignment.



If the M2-segments are assumed to form contiguous α -helices, the threonine ring and the two serine rings are assumed to line the pore and close packing of the helices at the narrowest part of the channel is assumed, the resulting model is rather straight forward. Here the view from the extracellular side of the AChR pore model is presented. In this picture the backbone atoms of the putative M2 α -helix are shown as enlarged spheres in gray. The side chain atoms of the influential amino acids are given in the respective color code as in the sequence alignment. The remaining atoms are given in gray. Also

[coordinates](#) are available.

The side view of the pore model of the AChR. The subunits are indicated in the figure. The top of the figure is the extracellular side and the bottom the cytoplasmic side of the AChR pore model. The influential amino acid side chain atoms are given as enlarged spheres.



ion channel with 5 ions

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