Ion channels in crystals of gramicidin D complex with RbCl. Atomic resolution low-temperature synchrotron X-ray data, M.L. Główka, A. Olczak, J. Bojarska, M. Szczesio[a], W. L. Duax, B. M. Burkhart, W. A. Pangborn, D. A. Langs, N. Li[b], Z. Wawrzak[c],
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Gramicidin D (gD) is a naturally occurring ionophoric antibiotic produced by *Bacillus brevis*. It is active against Gram-positive species due to channel formation in their membranes. The channels are specific for monovalent cations such as Tl+, NH_4+ and alkali metals. Passage of cations through channels is vital for numerous cell functions.
Formation of helical gramicidin channels is due to the alternate D-L configuration of gramicidin pentadecapeptide. As a result, all side chains are on the same side of β-ribbons formed by pairs of antiparallel peptides. Side chains repulsion causes the ribbons to roll up into narrow cylinders.
Three types of gramicidin channels have been observed experimentally, left and right handed antiparallel double stranded β-helices (DSβH) and single-stranded head-to-head dimers. In all X-ray studies of complexed and uncomplexed gramicidin crystal structures only DSβH forms have been observed. The distribution of cations and water in the channels provides insight into the possible mechanism of cation passage. The best resolution of the available gramicidin structures until now was only 1.4 Å.
Our data are based on a crystal of rubidium chloride complex measured at 100K with synchrotron radiation. The structure was refined with anisotropic temperature factors for all non-H atoms and with many partial occupancies. The resolution is 1.14 Å and the final R of 15% was achieved. There are 7 distinct rubidium binding sites in each of the two crystallographically independent right handed antiparallel $DS\beta H_R$ dimeric unit. Occupations factors of Rb cations are between 0.11 and 0.35 and the average ion contents are 1.59 and 1.23, respectively in the two channels.
The most interesting findings are as follow:

1. Though each channel is chemically symmetrical, the distributions of rubidium binding sites in the two independent channels are not.
2. The water to cation ratio in the channel interior is four or five to one.
3. Cations are "coordinated" by delocalized π electrons of four to six carbonyl groups, that together with peptides backbone chains form the gramicidin channel walls.
4. Five or six waters separate Rb cations during their passage through the channel.
5. The passage of the cations through the channel is three-step process and the jump length is about 8 Å.