Table 1. Distance restraints[1] used at the first stages of MC simulations of the GpA_{NMR}-model in implicit membrane. The restraints were derived from the NMR-structure of the GpA dimer.[14]

Helix-1	Helix-2	Distance, Å
I77:N	L75:C	6.26
I77:O	G79:C	4.82
G79:C	I76:O	6.36
V80:C	A82:C	6.15
V80:O	G83:N	4.43
G83:O	V80:C	6.43
I85:N	V84:CA	6.84
T87:N	V84:O	6.88
I76:N	I76:N	5.53
G79:CA	I68:N	6.37
F78:O	G79:C	6.95
M81:C	V80:O	6.77
V80:O	M81:C	6.72

[1] The same values were used for lower and upper restraints.

Table 2. Packing of α-helices in the GpA dimer. Interatomic distances in models calculated *via* Monte Carlo (MC) simulations in implicit membrane (this work) and in models obtained by NMR spectroscopy in DPC micelles.[14]

Helix-1[1]	Helix-2	GpA_L[2]	GpA_{MC}[3]	$GpA_{NMR\text{-}mem}$[4]	NMR models[5]	NMR restraints[6]	
						lower	upper
V80:QHG2	G79:HN	3.90	5.99	4.51	4.55 ± 0.12	2.00	3.50
G79:HN	V80:QHG2	3.89	5.87	4.47		2.00	3.50
L75:QHD1	I76:HB	4.40	10.95	4.94	5.00 ± 0.09	2.60	3.80
I76:HB	L75:QHD1	4.44	10.86	5.14		2.60	3.80
V84:QHG2	T87:HG1	4.41	3.42	3.47	3.19 ± 0.29	1.90	2.80
T87:HG1	V84:QHG2	4.25	3.52	3.61		1.90	2.80
V84:QHG2	G83:QHA	2.49	3.80	3.24	2.96 ± 0.21	2.10	3.00
G83:QHA	V84:QHG2	2.70	3.47	3.17		2.10	3.00
T87:QHG2	I88:QHG1	6.11	2.97	4.18	3.98 ± 0.21	2.10	3.00
I88:QHG1	T87:QHG2	5.79	3.02	4.04		2.10	3.00
Average violation of distance restraints[7]		1.10	2.17	0.86	0.74 ± 0.07		

[1] The distances and restraints are given in Å.

[2] GpA_L is the hypothetical left-handed model of the dimer: results of MC simulations in implicit membrane, this work.

[3] GpA_{MC} is the right-handed model of the dimer with the interface close to that in the NMR-structure: results of MC simulations in implicit membrane, this work.

[4] $GpA_{NMR\text{-}mem}$ is the lowest-energy state found for the NMR-derived model of the dimer[14] in implicit membrane.

[5] Average interatomic distances and standard deviations calculated for 19 original NMR models (PDB code 1afo[14]).

[6] Upper and lower distance restraints measured by NMR.[14] The data are taken from the file 1afo.mr at ftp.rcsb.org.
[7] Average violation of a set of NMR distance restraints for a given structure.

Table 3. Packing of α-helices in the GpA dimer. Interatomic distances in models calculated *via* Monte Carlo (MC) simulations in implicit membrane (this work) and in models obtained by solid-state NMR spectroscopy in lipid vesicles.[15]

Helix-1[1]	Helix-2	GpA_L[2]	GpA_{MC}[3]	$GpA_{NMR\text{-}mem}$[4]	Solution NMR[5]	Solid-state NMR[6]	Restraints, solid-state NMR[7]	
							lower	upper
G79:CA	G79:C	5.06	8.46	4.78	5.26±0.44	4.10	3.80	4.40
G79:C	G79:CA	5.09	8.47	4.76			3.80	4.40
I76:C	G79:CA	7.52	8.63	5.40	5.29±0.44	4.80	4.50	5.10
G79:CA	I76:C	6.84	8.60	5.54			4.50	5.10
G83:CA	G83:C	4.14	6.58	4.61	5.16±0.30	4.30	4.00	4.60
G83:C	G83:CA	4.39	6.68	4.59			4.00	4.60
G83:CA	V80:C	6.69	6.51	4.68	4.57±0.30	4.20	3.90	4.50
V80:C	G83:CA	6.70	6.54	4.79			3.90	4.50
G79:C	V80:CG2	4.34	4.32	3.85	2.90±0.07	4.00	3.70	4.30
V80:CG2	G79:C	4.41	4.39	3.83			3.70	4.30
G83:C	V84:CG2	4.16	4.17	4.39	3.69±0.20	4.00	3.70	4.30
V84:CG2	G83:C	4.35	4.34	4.37			3.70	4.30
Average violation of distance restraints [8]		0.84	1.95	0.18	0.47±0.17	0.00		

[1] The distances and restraints are given in Å.
[2] GpA_L is the hypothetical left-handed model of the dimer: results of MC simulations in implicit membrane, this work.
[3] GpA_{MC} is the right-handed model of the dimer with the interface close to that in the NMR-structure: results of MC simulations in implicit membrane, this work.
[4] $GpA_{NMR\text{-}mem}$ is the lowest-energy state found for the NMR-derived model of the dimer[14] in implicit membrane.
[5] Average interatomic distances and standard deviations calculated for 19 NMR models (PDB code 1afo[14]).
[6] Distances in the model of Smith et al.[15]
[7] Upper and lower distance restraints were taken from.[15]
[8] Average violation of a set of NMR distance restraints for a given structure.