

Summary of structural analysis of aromatic clustering in six non-homologous integral membrane proteins

Type Protein (PDB entry)	Oligomeric state	Lipid-contacting region ^a	Lipid-inaccessible region ^d	Total	No. of aromatic pairs ^g	No. of inter- strand (helical) aromatic pairs ⁱ	No. of intra- strand (helical) aromatic pairs ^j	No. of inter- subunit aromatic pairs ^k
		No. of aromatic residues involved in aromatic pairing ^b /No. of aromatic residues ^c (^b / ^c)	No. of aromatic residues involved in aromatic pairing ^e /No. of aromatic residues ^f (^e / ^f)	No. of aromatic residues involved in aromatic pairing/No. of aromatic residues (^{b+e} / ^{c+f})				
α-helical								
KcsA (1J95)	Tetramer	4/8 (0.50)	3/3 (1.0)	7/11 (0.64)	7	2	1	4
Bacteriorhodopsin (1KME)	Monomer	6/16 (0.38)	11/16 (0.69)	17/32 (0.53)	13	6	7	
Lactose permease (2CFQ)	Monomer	15/32 (0.47)	36/44 (0.82)	51/76 (0.67)	64	39	25	
β-barrel								
OmpA ^l (1QJP)	Monomer	6/13 (0.46)	0/9 (0)	6/22 (0.27)	4	2	2	
OmpF (2OMF)	Trimer	23/33 (0.70)	7/17 (0.41)	30/50 (0.60)	28 (4 ^h)	12 (4 ^h)	8	8
BtuB (1QNE)	Monomer	28/42 (0.67)	13/30 (0.43)	41/72 (0.57)	28 (10 ^h)	23 (8 ^h)	5 (2 ^h)	

^{a-k}: per monomer

^a: for α-helical membrane proteins, aromatic residues pointing toward lipid bilayer and whose fraction of solvent-accessible area is >2.5 % (when a probe of 1.4 Å radius is used); for β-barrel proteins, aromatic residues pointing outward from the barrel

^d: for α-helical membrane proteins, all aromatic residues other than ^a, and aromatic residues, which are pointing outward and whose fraction of solvent-accessible area is <2.5 %, are classified as lipid-inaccessible residues.

^{b, c, g}: inter-centroid distance less than 7 Å

^h: aromatic pairs inside the barrel

^l: transmembrane domain only