

Supplementary data

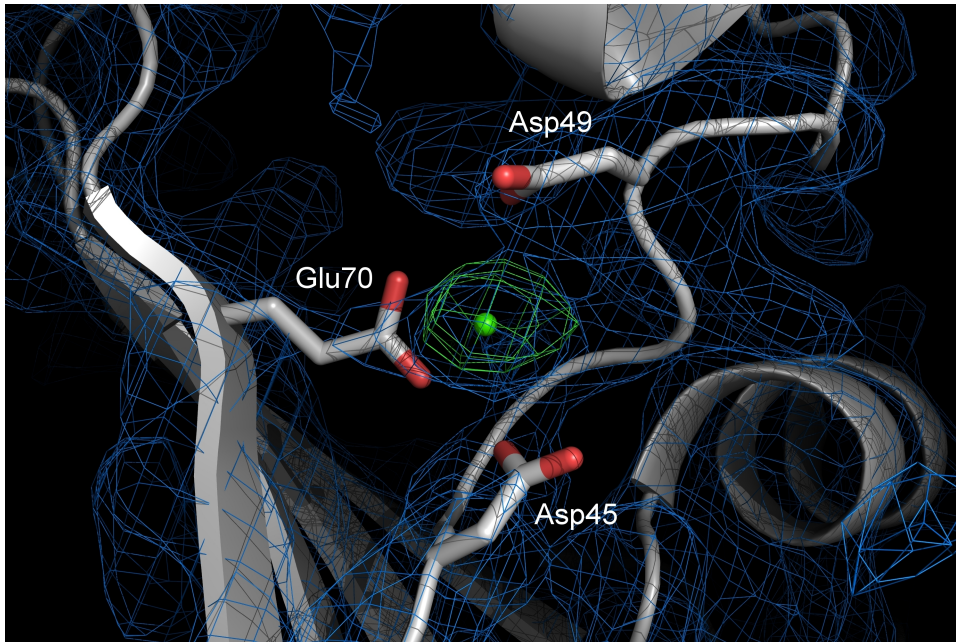


Fig. S1. Binding site of the divalent cation. 2FoFc map (blue) contoured at 2.0 σ , omit map (green) contoured at 6.0 σ .

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          ----S1-----          ----S2----          ----S3-----
TtoA .....AAKFSVEAGAGFYG.....GFGGQLAVVAEDLAPG.....LPLGVRLGVGFATSDALDDGYDLGGGT
NspA .....EGASGFYVQADAAHAKAS...SSLGSAKGFSPRISAGYRI.....NDLRFAVDYTRYKN.....
OmpA .....APKDNTWYTGAKLGWSQ....HEN....KLGAGAFGGYQVN.....PYVGFEMGYDWLGR.....
OmpW .....EAGEFFMRAGSATVRP....TE|GGFSVTNNTQLGLTFTYMATDN.....IGVELLAATPFRHKIG.TRAT..
OmpX .....ATSTVTGGYA.QSDA....QGQ...MNKMGGFNLKYRYEEDNSP....LGVIGSFYTYEKSRT.....
PagL .....ADVSAAVGAT.....GQS....GMTYRLGLSWDWDKSWWQTST..GRLTGYWDAGYTYWEGGDE.....
PagP TTFRENIAQTWQPEHYDLYIPAITWHARF|AER...PWGGGFGLSRWDE.....KGNWHGLYAMAFKDSW.....

          ---H1---          ----S4-----          -----S5-----          -----S6-----
TtoA TWGDVKEAGKFSEWGQNVTLSDVLYKP...SGLGLP...VEVAPYFGVRYNF.FSGGYTDPEDNLTIKAQTI.SS.NQLGLGLGV
NspA .....YKAPSTDFKLYSIGASAIYDF...D.TQSP...VKPYLGARLSLNR.ASVDLG.....GSDS.FSQTSLGLGLVT
OmpA .....MP|YAYKAQGVQLTAKLGYP....ITDD...LDIYTRLGGMVWR.ADTYSNV.....YGKN.HD.TGVSPVVFAG
OmpW .....GDIATVHHLPPTLMAQ.WY....FGDASSKFRPYVGAGINYTTFFDNGFNHDHGKEAGLSDLS.LKD....SWGAAGQV
OmpX .....ASSGDYKNQYYGITAGPAYRIN....DW...ASIYGVVGVGYGK.FQTTEYP.....TYKN.DT.SDYGFSYGA
PagL .....GAGKHSLSFAPVFVYEF....AGDSIKPFIEAGIGVAAFS.G.....TRVGDQN.LG.SSLNFEDRI
PagP .....NKWEPIAGYGWESTW....RPLADEN..FHLGLGFTAGVTA.RDNW.....NYIPLPVLPLLA

          -----          ----S7-----          --S9--          -S10--          --H2---          -----S8-----
TtoA RAAAYPLM.P...NLSLVGDLGVDYIF.QACFTRVEEDDSGNKSQSSVCPGDSGYEDVNKEVTQPEWVLKLRGAAAYRF... 207
NspA GVSAYVT.P...NVDLDAGYRYNYIGKVNT.....VKNVRSSELGELSAVVRVKF... 155
OmpA GVEYAIT.P...EIATRLEYQWTN|.....GMLSLGVSYRFG.. 137
OmpW GVDYL...INRD...WLVNMSVWYM...DIDTTANYKLGGAQQHDSVR.....LDPWVFMFSAGYRFH 182
OmpX GLQFNPMEN...VAL.DFSYEQSRIR.S.....VDVGTWI..AGVGYRF. 148
PagL GAGLKFA.N...GQSVGVRAIHYSNAGLKQP.....NDGIESYSLFYKIPI... 150
PagP SVGYG.....PVTFQMTYIP.....GTYNNGNVYFAWMRFQFLE... 147

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Fig. S2. Structural alignment of TtoA with all known eight stranded β -barrel proteins. β -strands are highlighted in gray, helices in dark gray. The numbering of the secondary structure elements of TtoA is shown at the top; S indicates β -strands and H α -helices. | marks sequence areas not resolved in the X-ray structure.

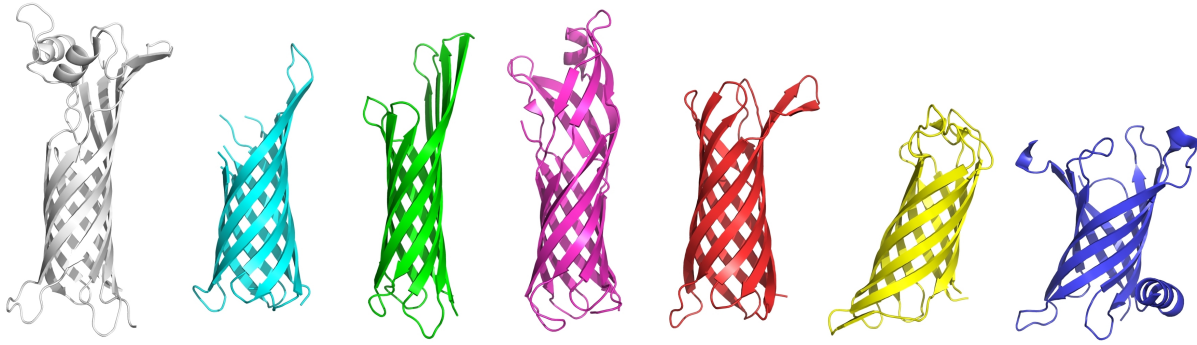


Fig. S3. Structure of TtoA (grey) compared to the structures of OmpA (cyan), OmpX (green), OmpW (pink), NspA (red), PagL (yellow), PagP (blue).