Supplementary material: Properties of an inward-facing state of LeuT – conformational stability and substrate release

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Table S1: Overview of residues used for each TM segment in helix tilt analysis												
TM	**1a**	**1b**	**2**	**3**	**4**	**5**	**6a**	**6b**	**7**	**8**	**9**	**10**
Residue	11-22	25-38	41-71	88-124	166-184	191-214	241-255	260-267	275-306	337-371	375-395	399-426

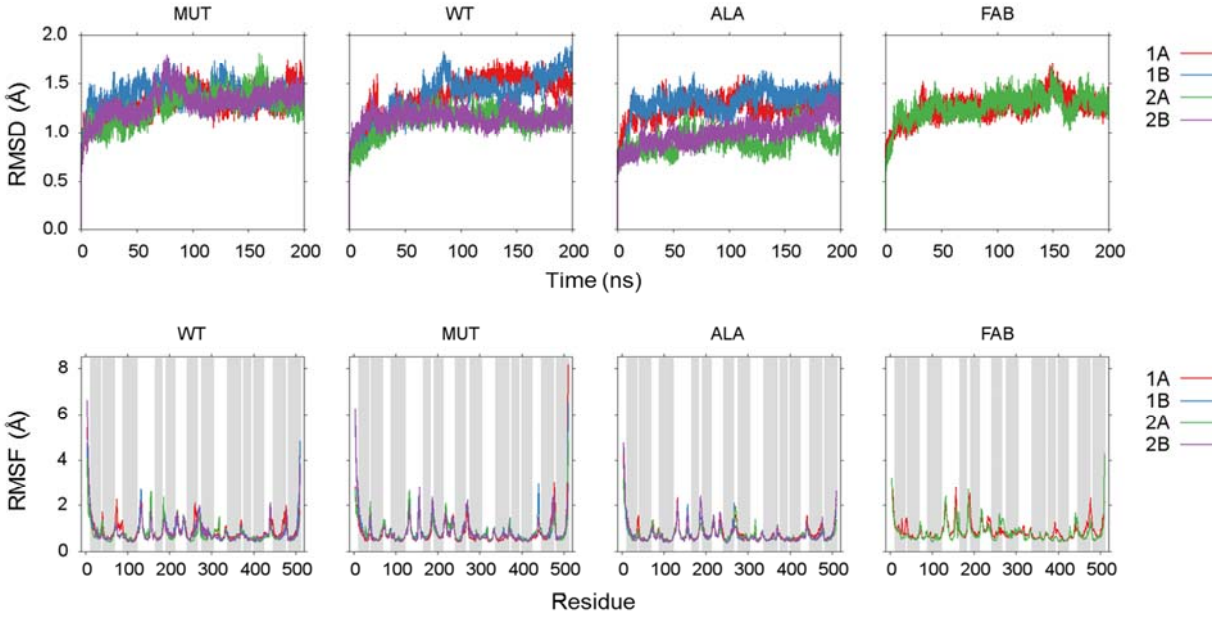

Figure S1: RMSD and RMSF for each setup. The RMSD is measured for the C_α atoms in the 12 TMs in LeuT with respect to the structure at 0 ns. The RMSF is calculated with respect to the average position of the C_α atoms in LeuT. The shaded grey areas in the RMFS plots correspond to transmembrane helical segments.

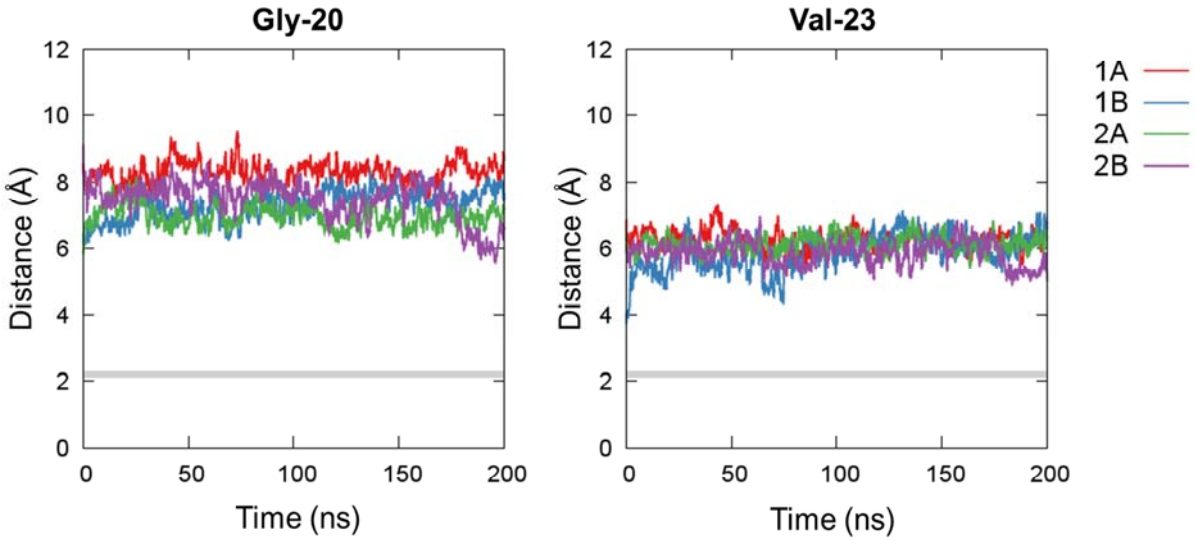

Figure S2: Distances from carbonyl oxygen atoms in Gly-20 and Val-23 to the center of Na2 site. The structures have been superimposed on three of the residues in the Na2 site (Ala-351, Thr-354, and Ser-355) in the Na^+ bound, outward-occluded crystal structure (PDB code 2A65), and the center of the Na2 site has been defined as position of the Na^+ ion in the Na2 site in the PDB structure. The grey line represents the oxygen to Na^+ distance in the Na^+ bound structure.

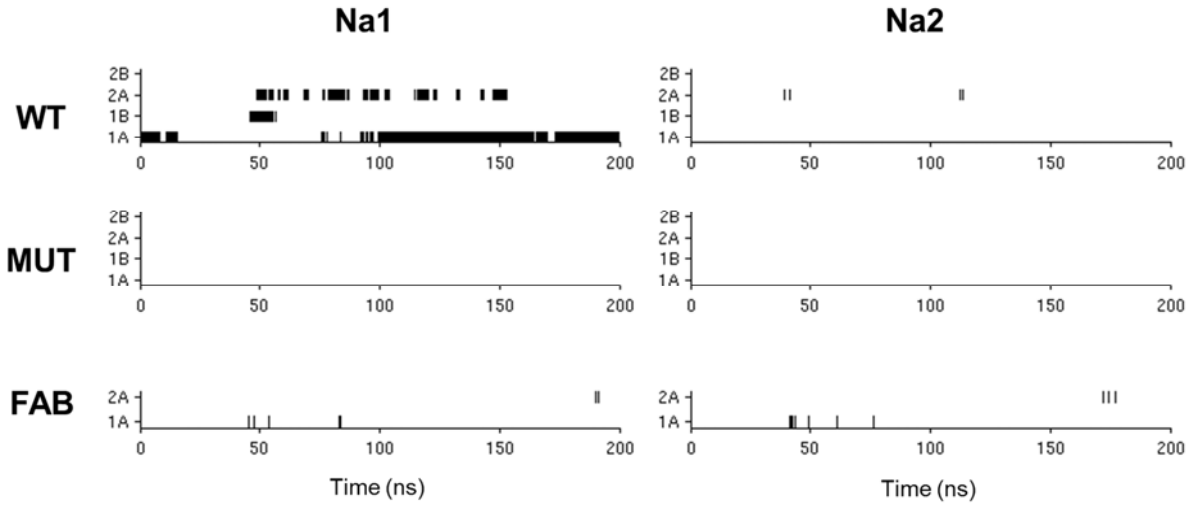

Figure S3: Occupancy of the Na1 and Na2 site. The occupancy was determined by identifying Na^+ ions within 4 Å of the center-of-mass of either Asn-27, Thr-254, and Asn-286 (Na1 site) or Val-23, Ala-351, and Ser-355 (Na2 site).