Conserved movement of TMS11 between occluded conformations of LacY and XylE of the Major Facilitator Superfamily suggests a similar hinge-like mechanism

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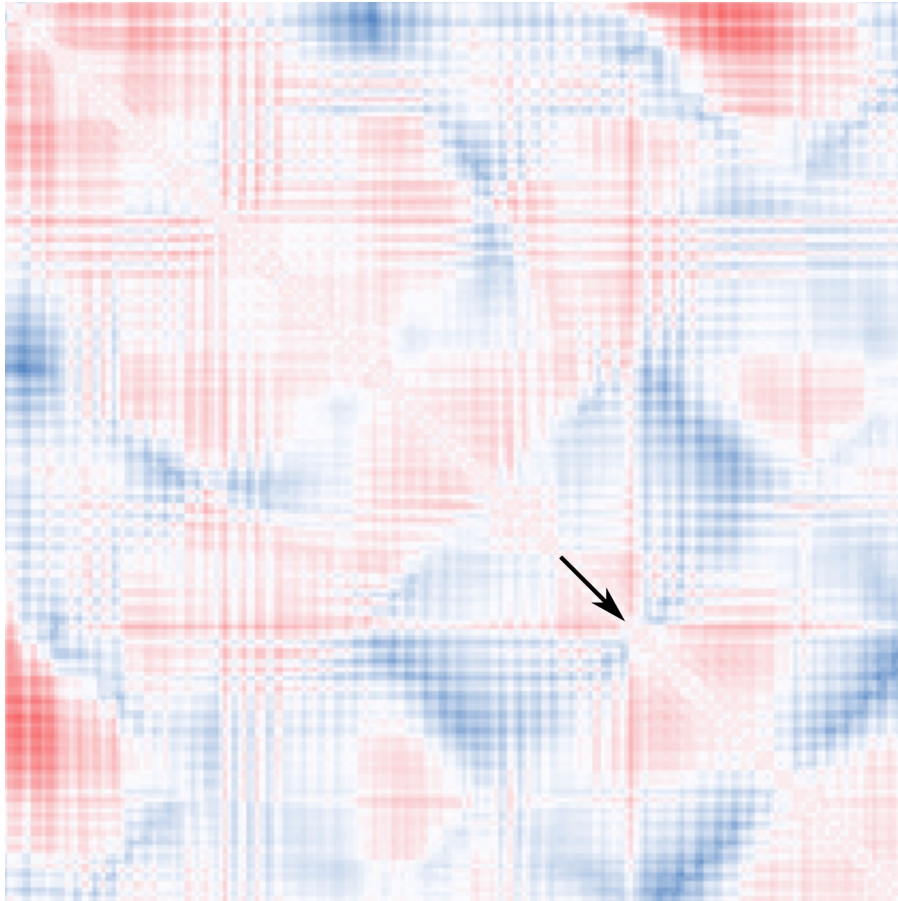
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Supplementary materials

Figure S1. *Δ-distance map of 4OAA-repeat swapped model (outward occluded minus outward open state of LacY).* The graph represents changes in distance between atom pairs during shifts in conformational state. According to conventions, the four quadrants of any intact Δ-distance map are numbered 1, 2, 3 and 4 anti-clockwise from the top right quadrant. This figure is limited to the C-terminal quadrant only (quadrant 4; the other quadrants have been removed) and the arrow points to the loop connecting TMSs 10 and 11.
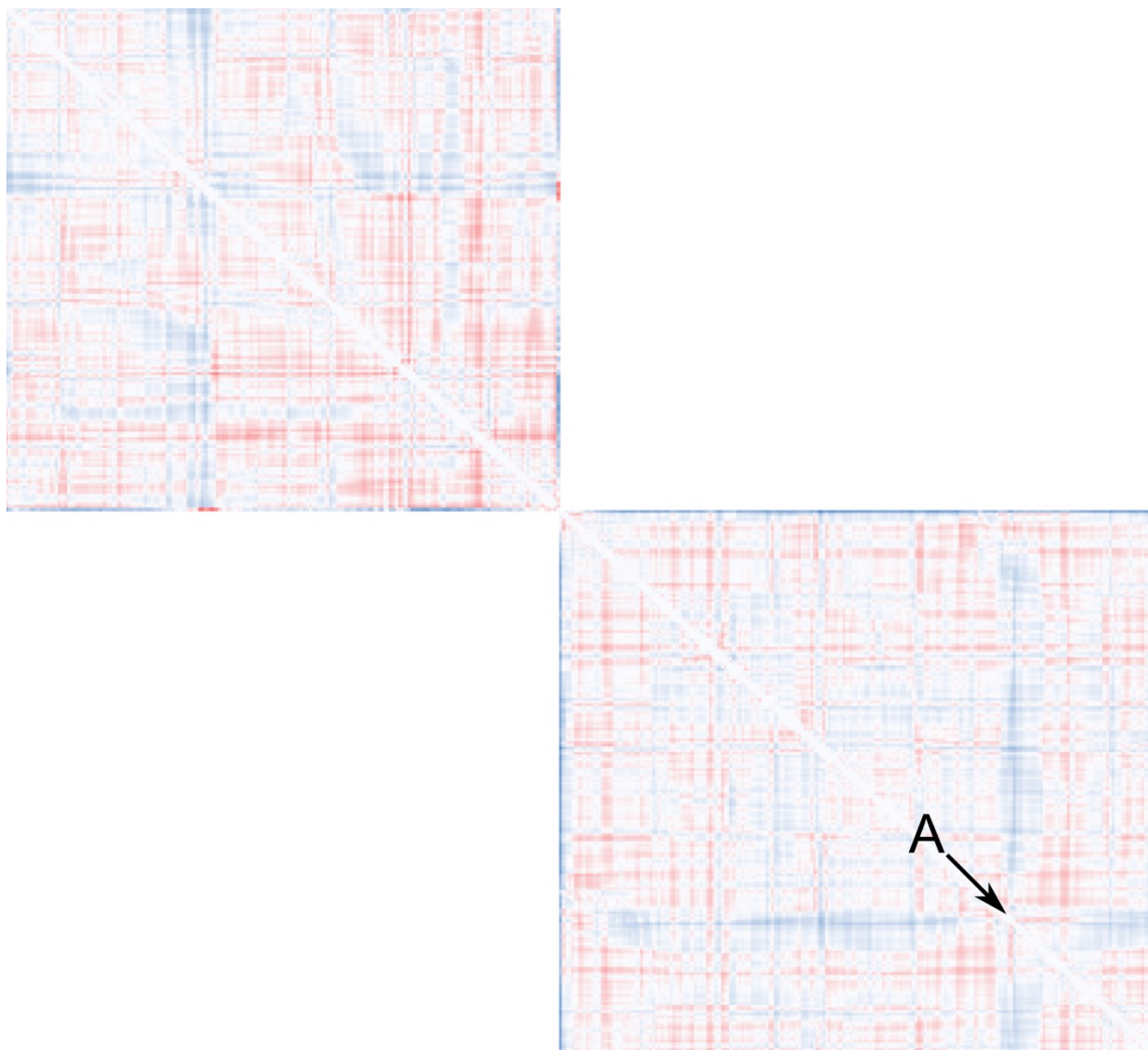
Figure S2. *Δ-distance map of 2V8N-2Y5Y (inward open state minus inward affinity inactivator-occluded states of LacY).* Here, quadrants 1 and 3 have been removed because they show a large conformational change that is due to the hinge-like movement between domain halves, not considered in this article. The white diagonal denotes areas where the Δ-distance is close to zero. **'A'** points to the N-terminal portion of TMS11.
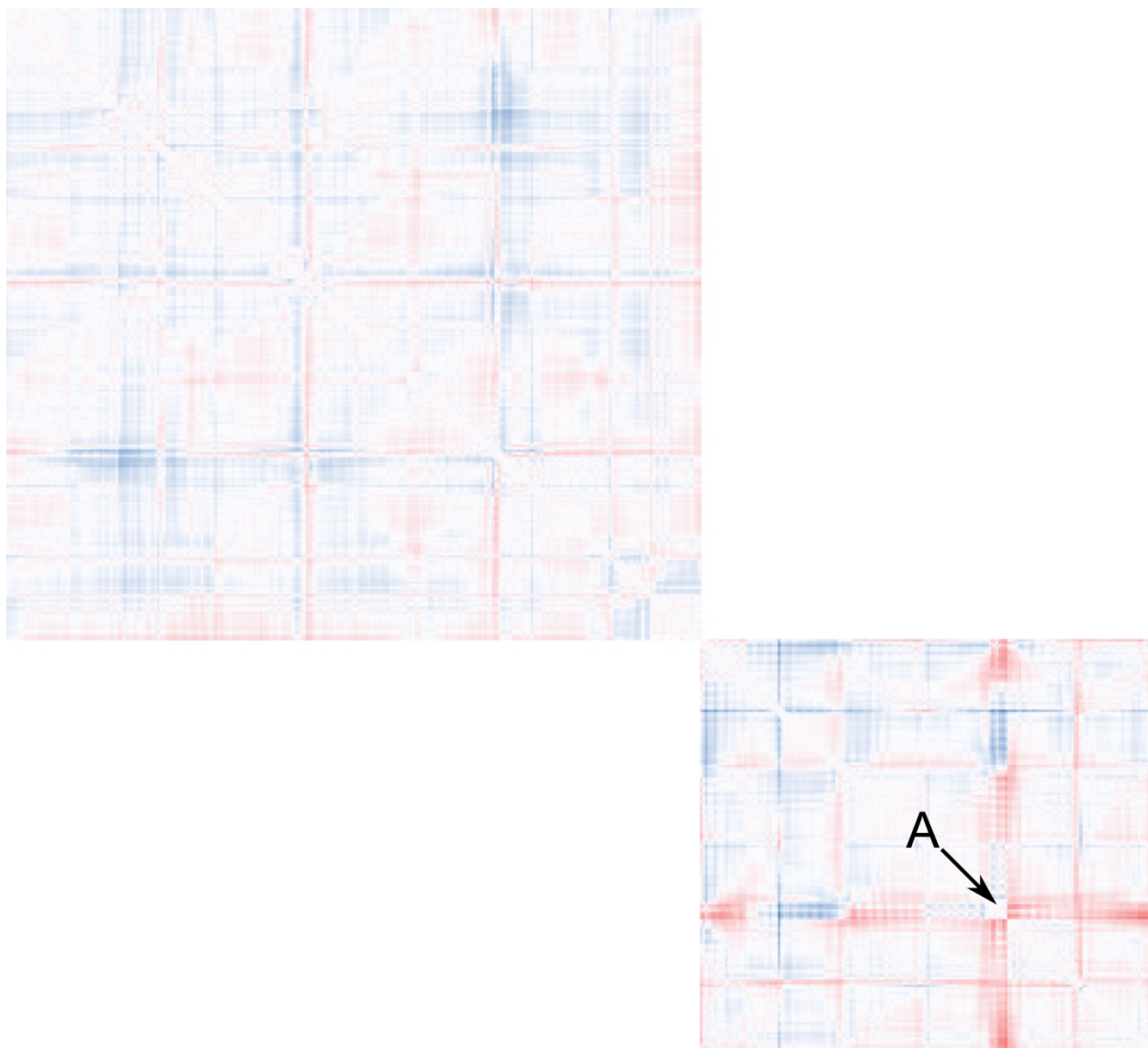
**Figure S3.** *Δ-distance map of 4JA4-4JA3 (inward open minus inward occluded states of XylE).* The blue segment of the "A" cross represents movement in relation to TMS 8. 'A' points to the N-terminal portion of TMS11.
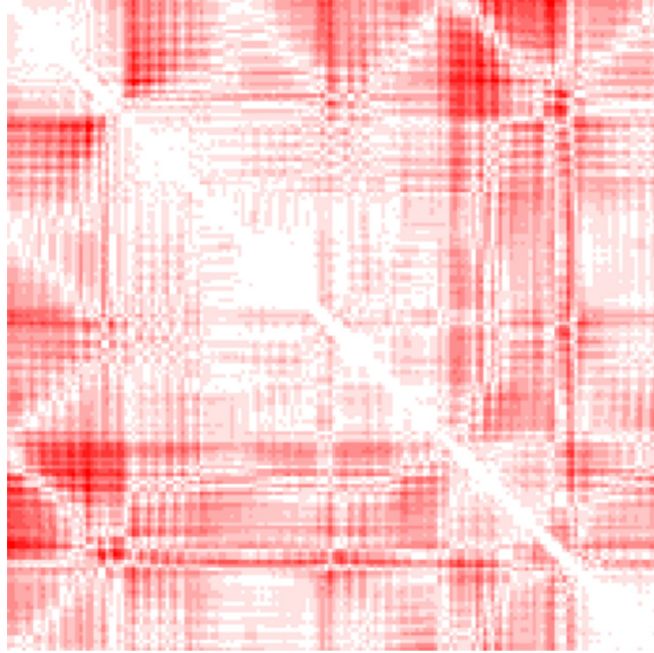
Figure S4A. *RR distance map comparing the standard deviation of distances between FucP in the outward open conformation and a repeat-swapped homology model of FucP in an inward open-like state.* The red color scale indicates the number of standard deviations of change. The cross-like area in quadrant 4 coincides with elevated standard deviation measurements.
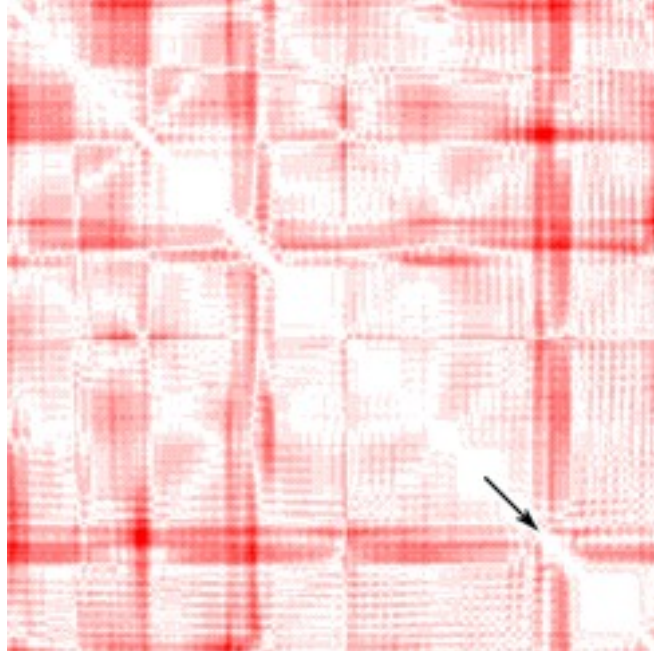
Figure S4B. *RR distance map comparing standard deviation of distances of NRT1 in the inward open conformation and a homology model of the outward occluded state of NRT1.* The black arrow points to a loop located between TMSs 11 and 12, which displays an elevated standard deviation of approximately 10-15 units.
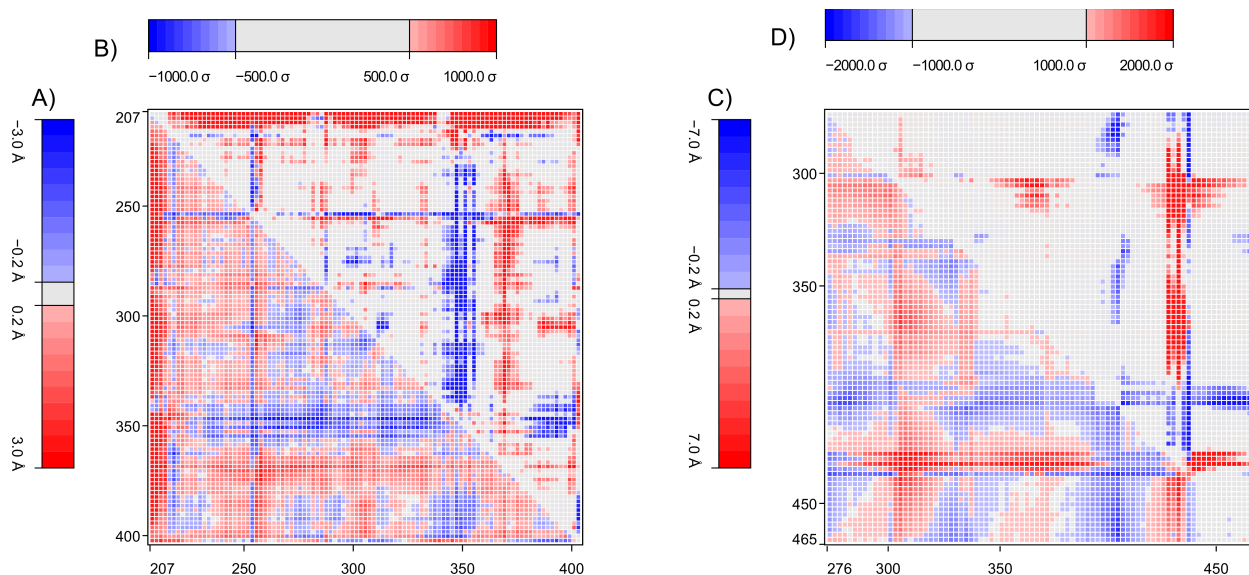
Figure S5. *Non-normalized (A and C) and error-scaled (B and D) difference distance matrices of 2Y5Y-4OAA (A and B; the inward affinity inactivator occluded state-the outward occluded state of LacY) and 4AJ3-4GBY (C and D; XylE in the inward occluded and outward occluded states) created using ESCET 0.7.*

For 2Y5Y, the parameters used were: cpl=97.7, d_{min}=3.38, n_{obs}= 35055, r_{free}=0.3027. For 4OAA, the parameters used were: cpl=95.3, d_{min}=3.50, n_{obs}=20954, r_{free}=0.293. For 4JA3, the parameters used were: cpl=82.3, d_{min}=3.80, n_{obs}= 17321, r_{free}=0.315. For 4GBY, the parameters used were: cpl=98.4, d_{min}=2.81, n_{obs}=19517, r_{free}=0.274. A) For the non-normalized matrix of 2Y5Y-4OAA, the scale went from -3 to 3 Angstroms. B) For the error-scaled matrix of 2Y5Y-4OAA, the scale went from -1000 to 1000 Angstroms, excluding the -500 to 500 range. C) For the non-normalized matrix of 2Y5Y-4OAA, the scale went from -7 to 7 Angstroms. D) For the error-scaled matrix of 2Y5Y-4OAA, the scale went from -2000 to 2000 Angstroms, excluding the -1000 to 1000 range. The TMS11-associated movement in the comparison between the occluded states of XylE is between 500 and 1000 standard deviations above the background noise, and for LacY, between 1000 and 2000 standard deviations above the background noise.