

Effect of the Southeast Asian Ovalocytosis Deletion on the Conformational Dynamics of Signal-Anchor Transmembrane Segment 1 of Red Cell Anion Exchanger 1 (AE1, Band 3, or SLC4A1) – Supplemental Information

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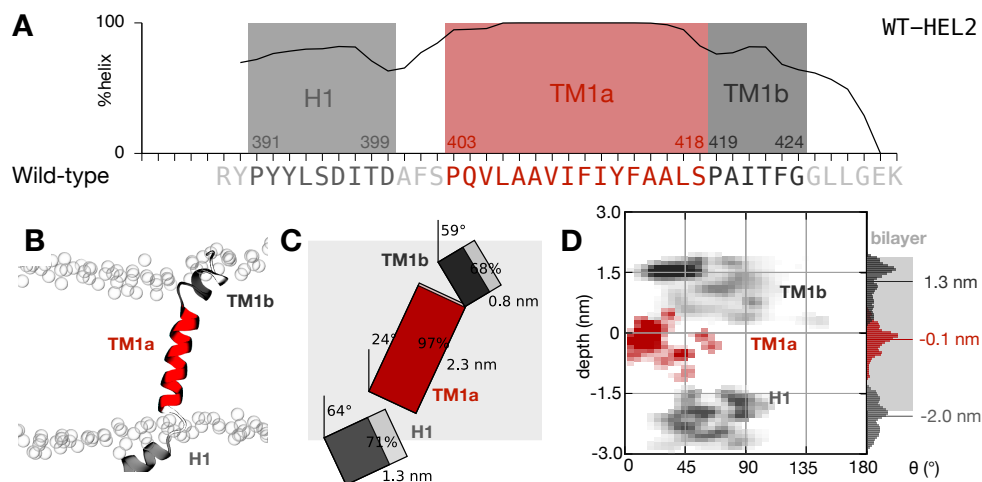


Figure S1: The same analysis as in Fig. 2 of the main body of the paper repeated for WT-HEL2, the shorter model helix that lacks the RDIRR sequence.

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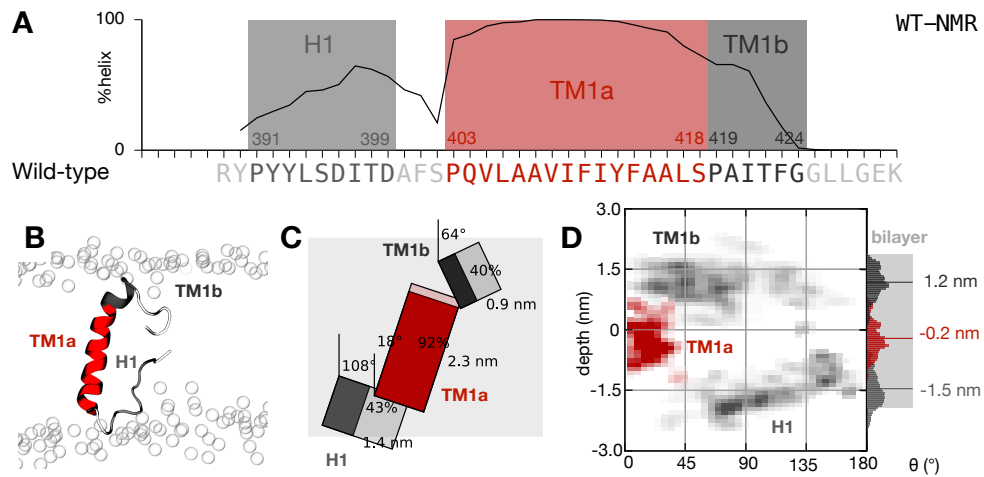


Figure S2: The same analysis as in Fig. 2 of the main body of the paper repeated for WT-NMR, the ensemble of 21 NMR structures of the wildtype Arg389-Lys430 sequence.

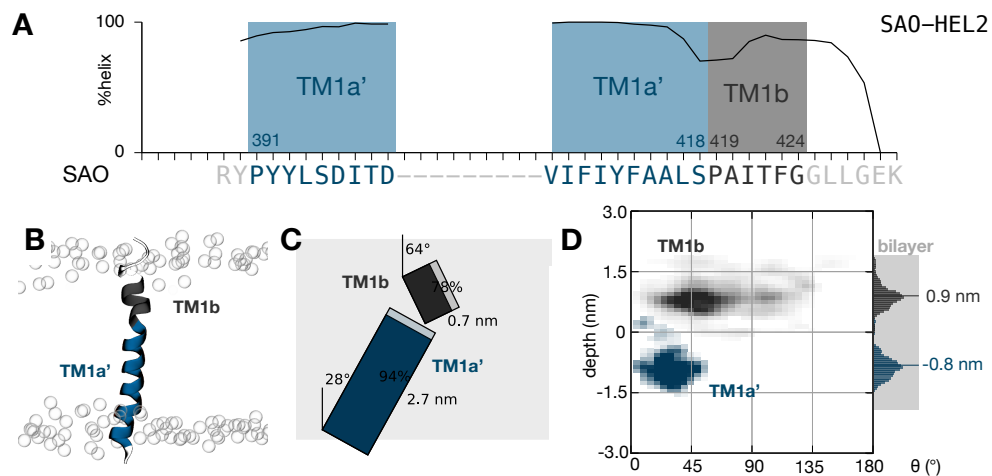


Figure S3: The same analysis as in Fig. 3 of the main body of the paper repeated for the shorter model helix that lacks the RDIRR sequence. Asp396 and Asp399 are protonated and are therefore neutral.

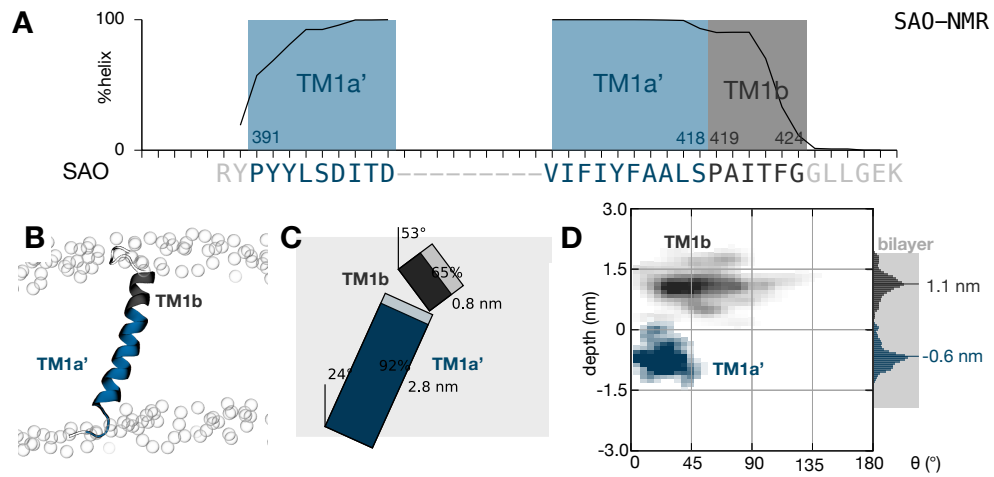


Figure S4: The same analysis as in Fig. 3 of the main body of the paper repeated for the ensemble of 21 NMR structures of the SAO deletion mutant of sequence Arg389-Lys430. Asp396 and Asp399 are protonated and are therefore neutral.

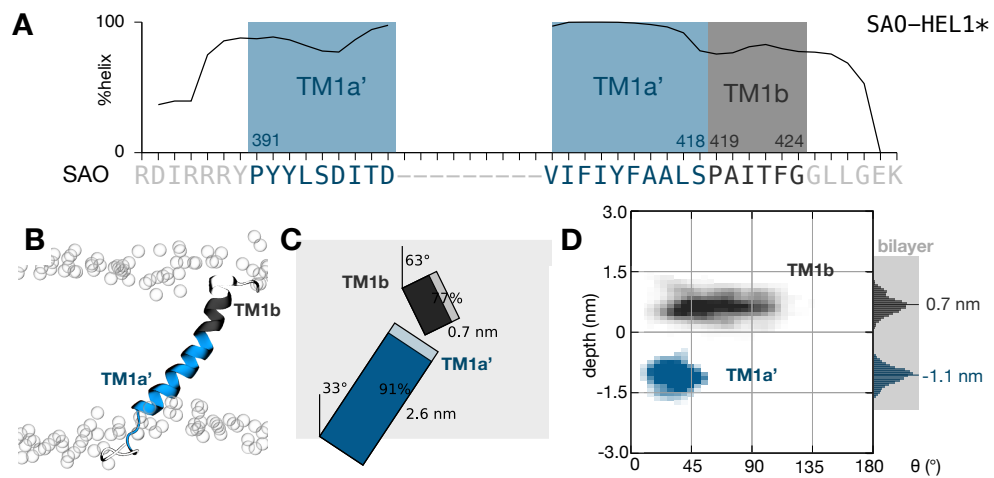


Figure S5: The same analysis as in Fig. 3 of the main body of the paper repeated for the shorter model helix that lacks the RDIRR sequence. Asp396 and Asp399 are deprotonated and therefore are charged.

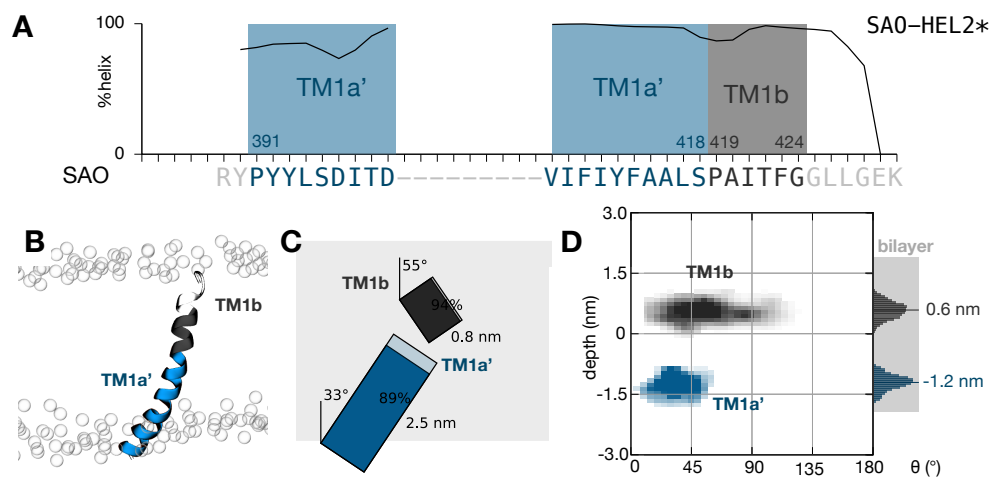


Figure S6: The same analysis as in Fig. 3 of the main body of the paper repeated for the same set of simulations, but with Asp396 and Asp399 deprotonated and therefore charged.

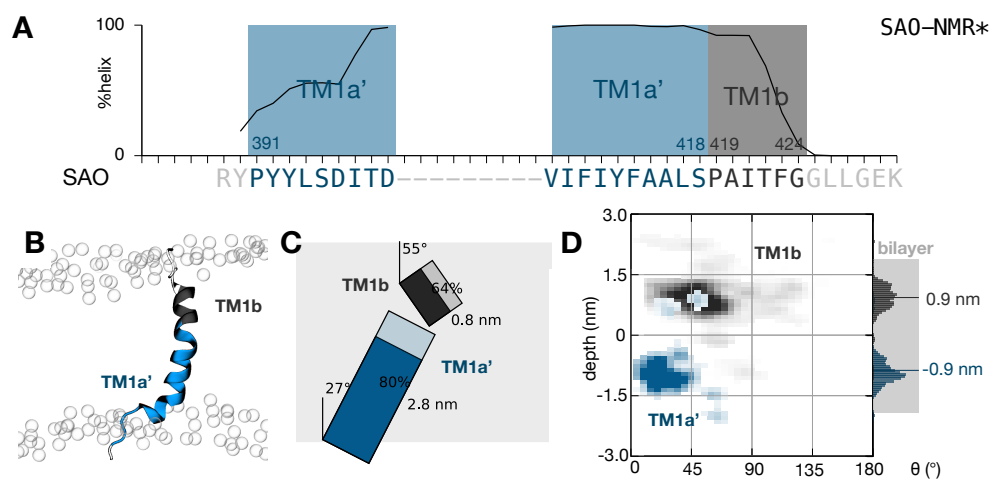


Figure S7: The same analysis as in Fig. 3 of the main body of the paper repeated for the ensemble of 21 NMR structures of the SAO deletion mutant of sequence Arg389-Lys430. Asp396 and Asp399 are deprotonated and are therefore charged.

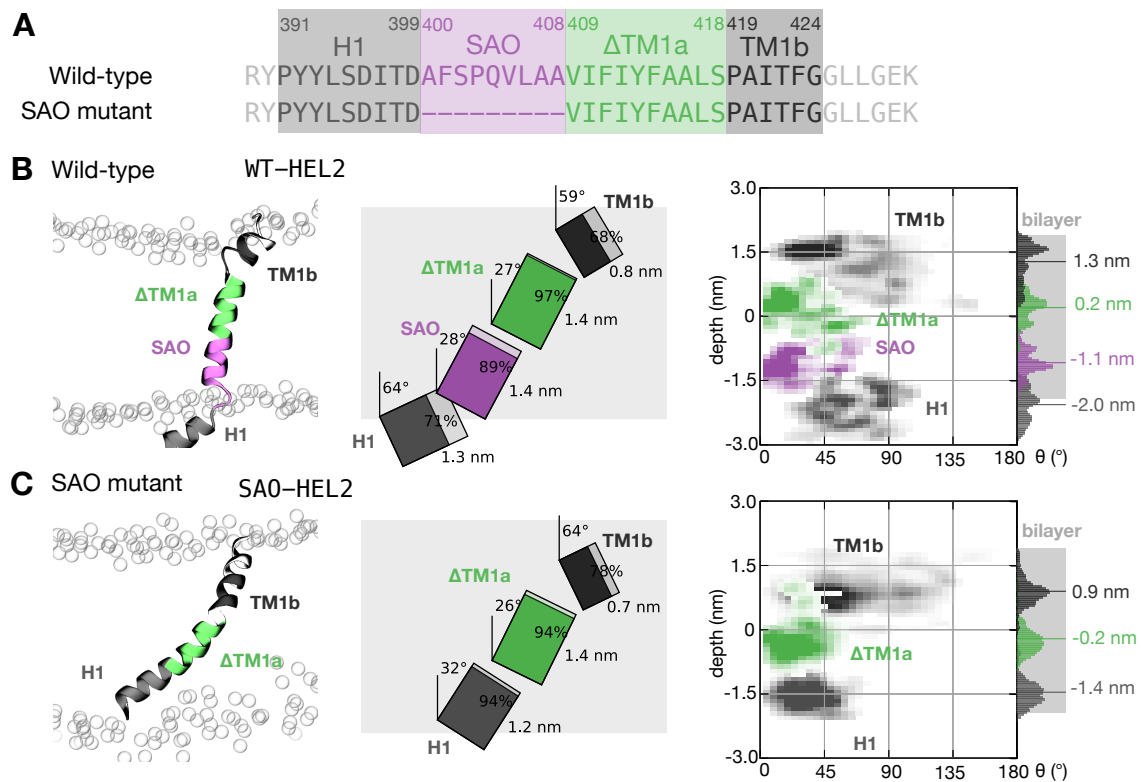


Figure S8: The same analysis as in Fig. 4 of the main body of the paper repeated for the shorter model helix that lacks the RDIRR sequence for both the (B) wildtype and (C) SAO deletion mutant. Asp396 and Asp399 are protonated and are therefore neutral.

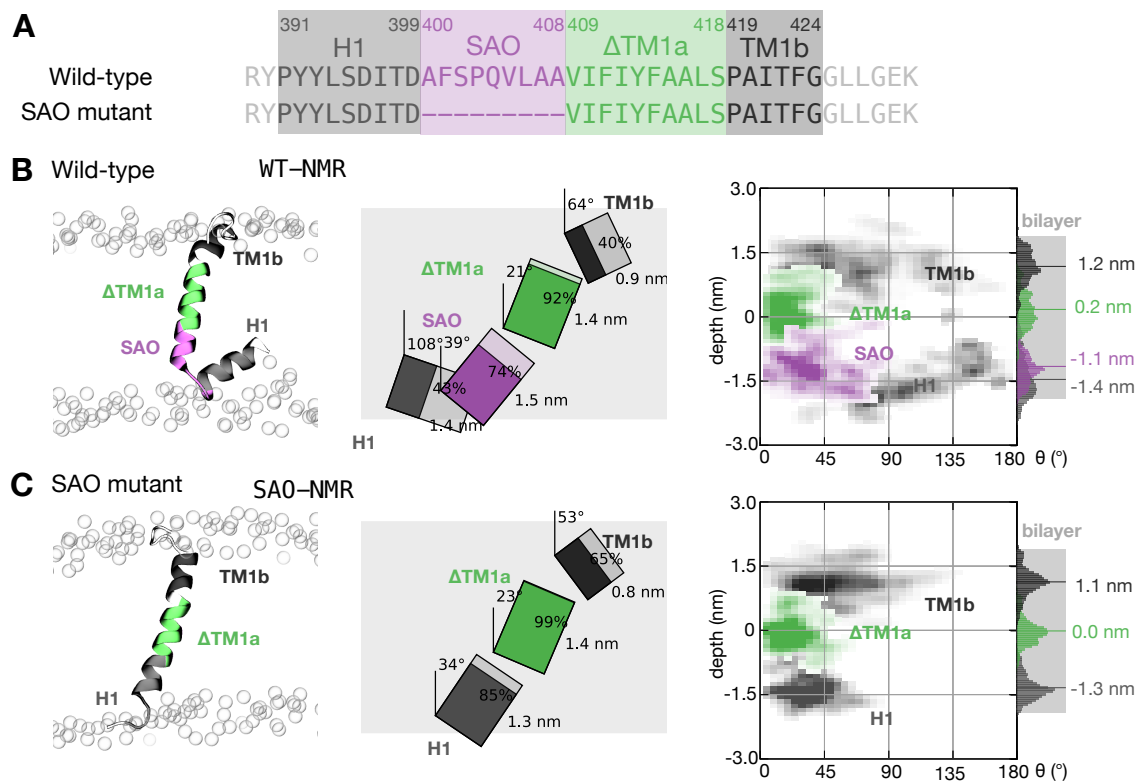


Figure S9: The same analysis as in Fig. 4 of the main body of the paper repeated for the ensembles of 21 NMR structures for both the (B) wildtype and (C) SAO deletion mutant. Asp396 and Asp399 are protonated and are therefore neutral.

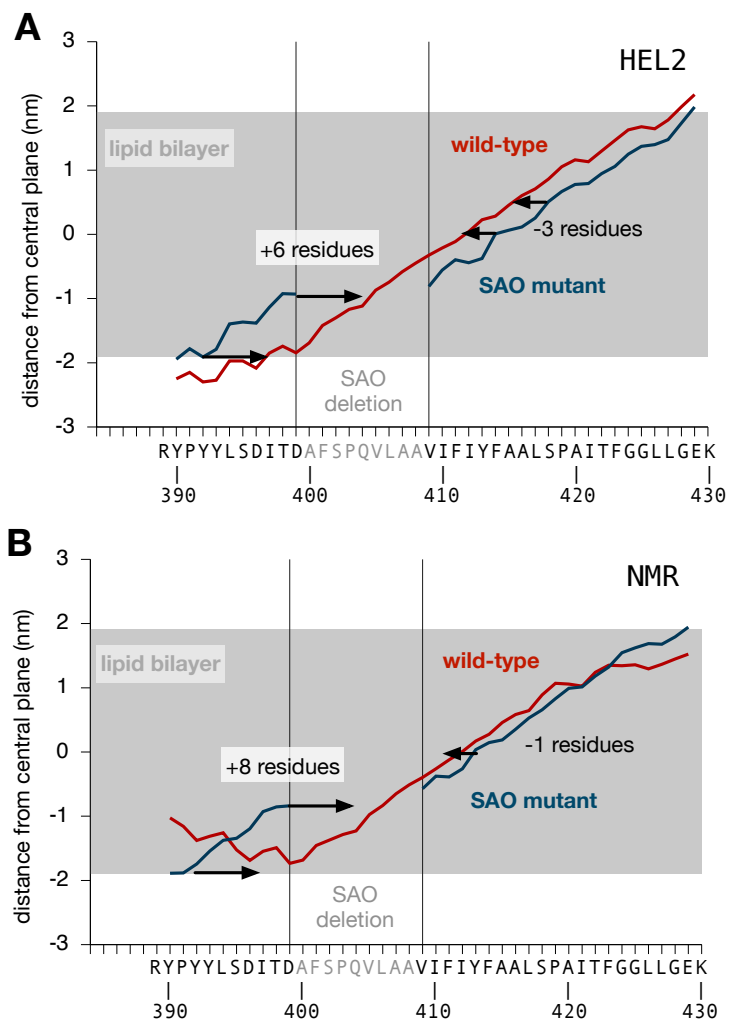


Figure S10: The same analysis as in Fig. 5A of the main body of the paper repeated for (A) the shorter model helix missing the N-terminal RDIRR motif and (B) the ensembles of 21 NMR structures. In the SAO deletion mutant Asp396 and Asp399 are protonated and are therefore neutral.

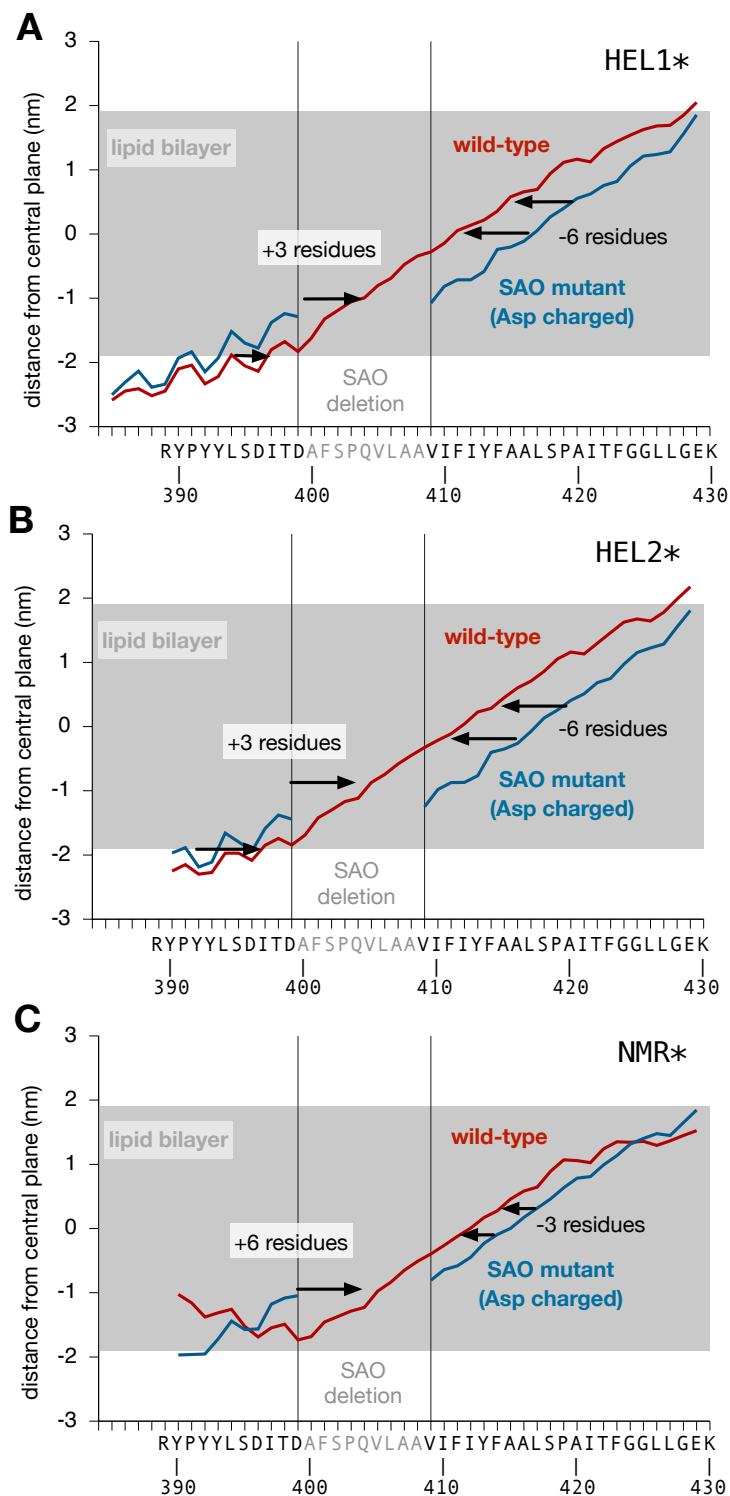


Figure S11: The same analysis as in Fig. 5A of the main body of the paper repeated for (A) the longer model helix that includes the RDIRR motif, (B) the shorter model helix missing the N-terminal RDIRR motif and (C) the ensembles of 21 NMR structures. In all three SAO deletion mutant Asp396 and Asp399 are deprotonated and are therefore charged.

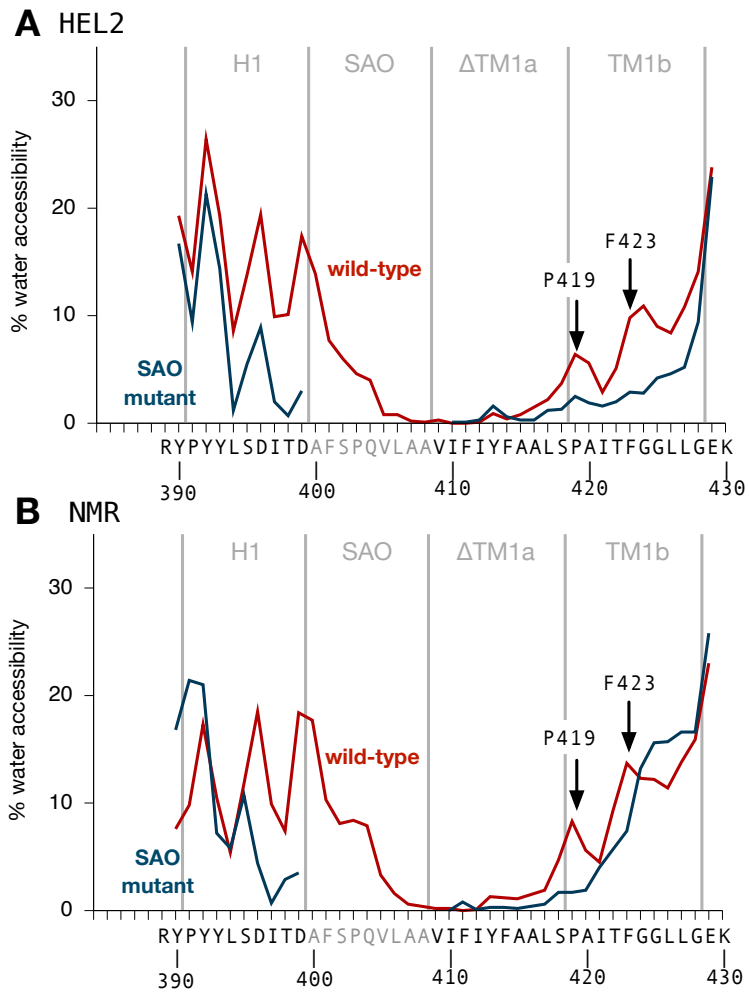


Figure S12: The same analysis as in Fig. 6 of the main body of the paper repeated for (A) the shorter model helix missing the N-terminal RDIRR motif and (B) the ensembles of 21 NMR structures. In the SAO deletion mutant Asp396 and Asp399 are protonated and are therefore neutral.

References

1. Chambers EJ, Bloomberg GB, Ring SM, Tanner MJ (1999) Structural studies on the effects of the deletion in the red cell anion exchanger (band 3, AE1) associated with South East Asian ovalocytosis. *J Mol Biol* 285:1289–307.
2. Arakawa T, Kobayashi-Yurugi T, Alguel Y, Iwanari H, Hatae H, Iwata M, Abe Y, Hino T, Ikeda-Suno C, Kuma H, Kang D, Murata T, Hamakubo T, Cameron AD, Kobayashi T, Hamasaki N, Iwata S (2015) Crystal structure of the anion exchanger domain of human erythrocyte band 3 *Science* 350:680–684.