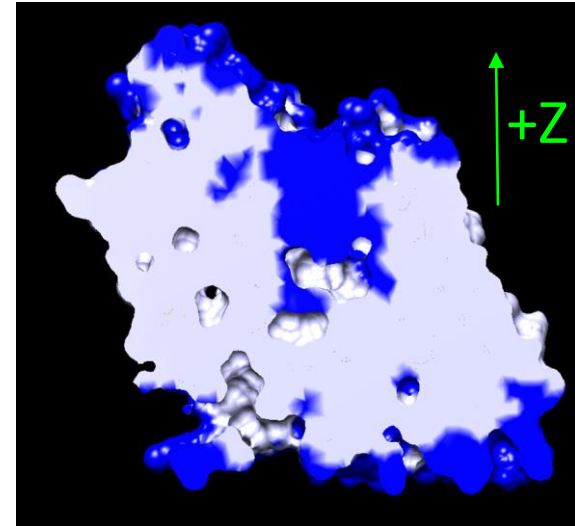


New Update Improves Cavities

Orientation	OLD APBSmem (e)	NEW APBSmem (e)
Original	-0.49	-0.60
Flipped X	-0.097	0.74
Flipped Y	-0.13	0.67
Flipped Z	-0.43	-0.66



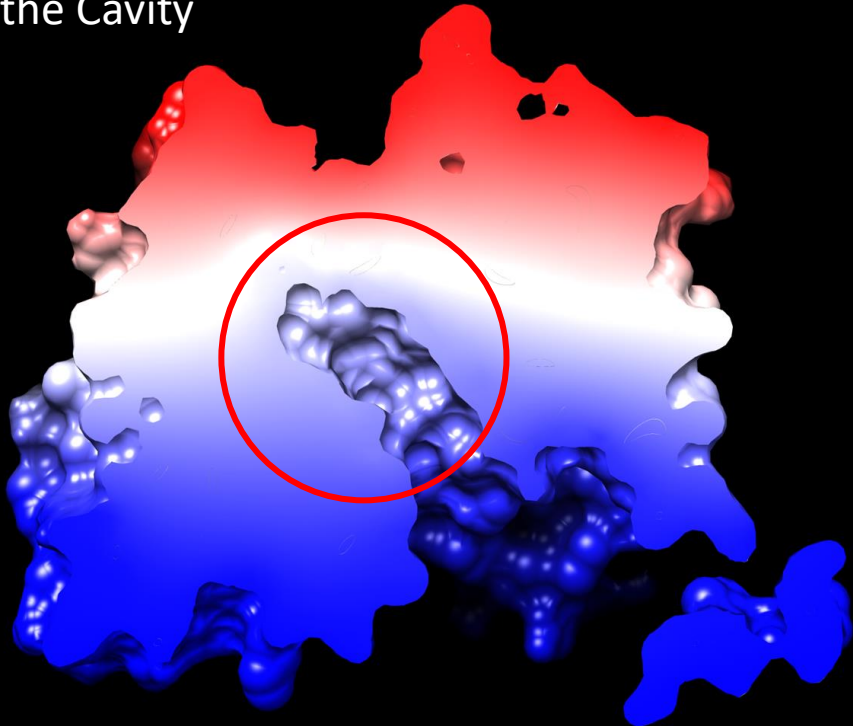
Dielectric Cross Section (Blue is 80)

These are good results because they show vSGLT has the same gating charge regardless of relative orientation in APBSmem

Updated APBSmem Improves Cavities

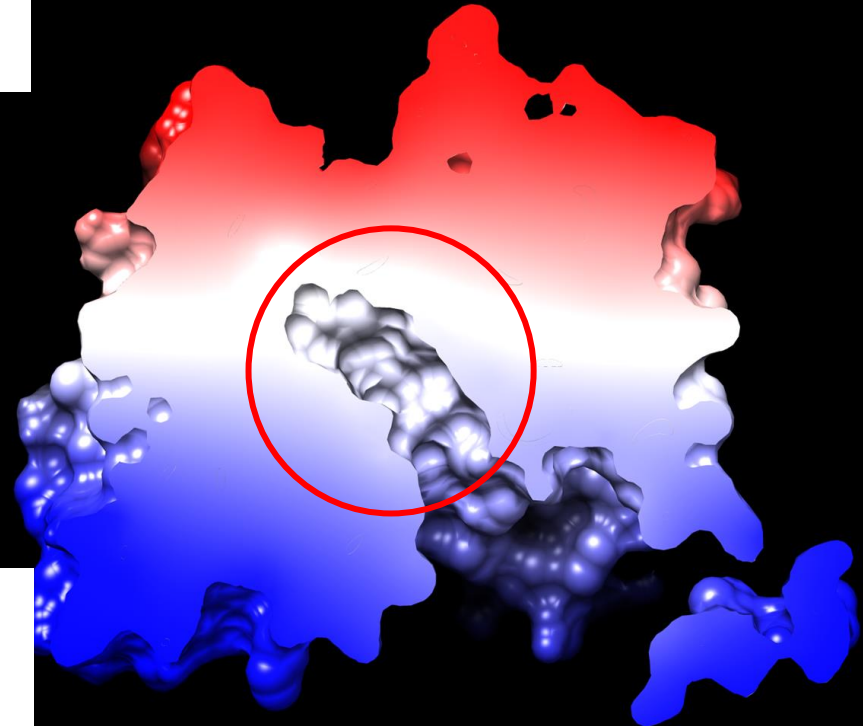
NEW APBSmem

More Charge Density
in the Cavity



OLD APBSmem

0
Potential

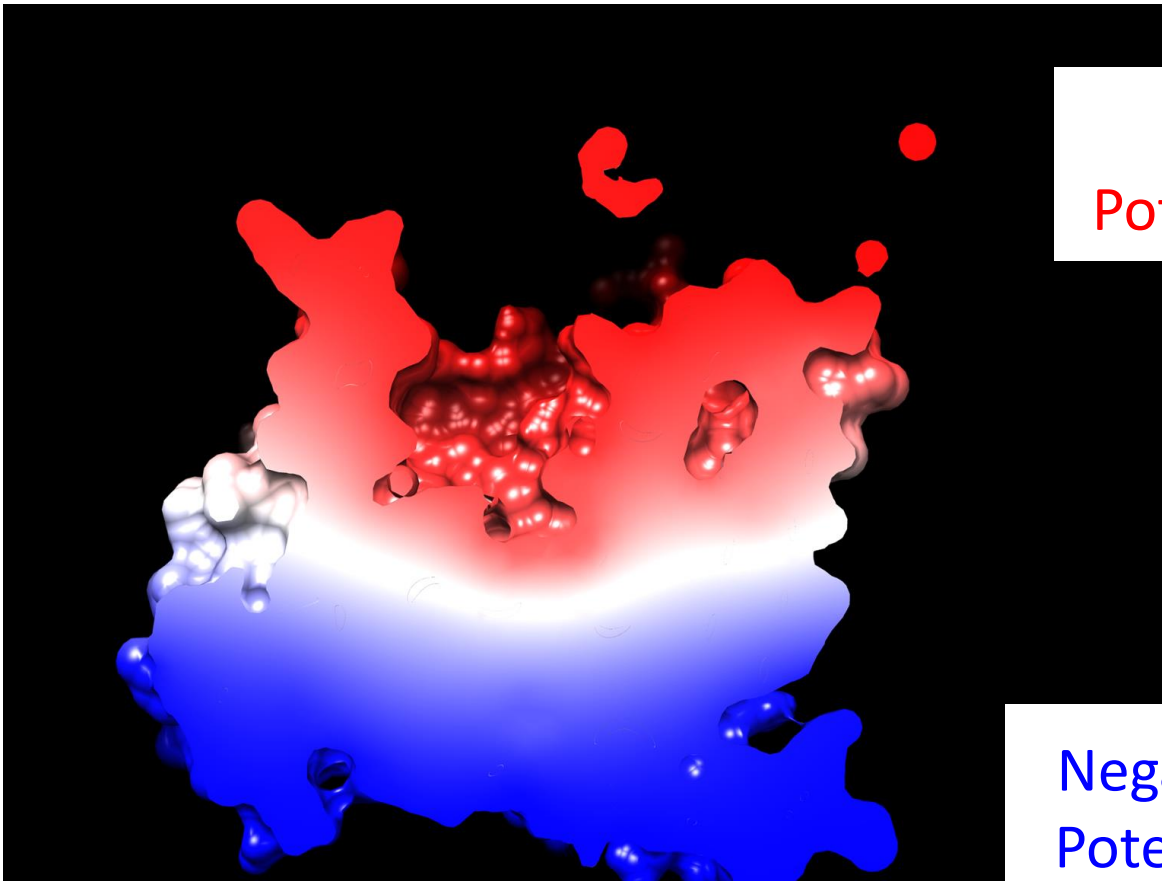


Negative
Potential

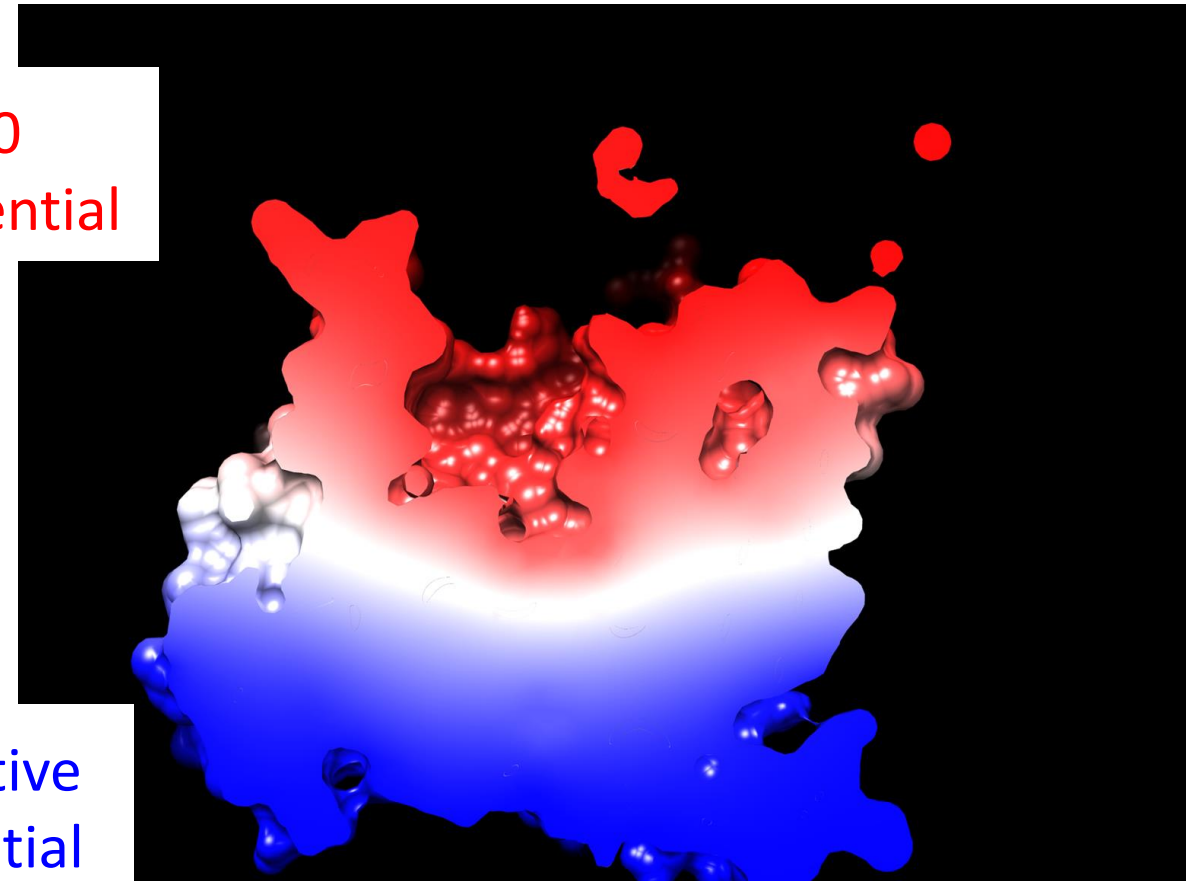
Updated APBSmem Improves Cavities

Positive Z Potential Not Affected- already working as intended

NEW APBSmem



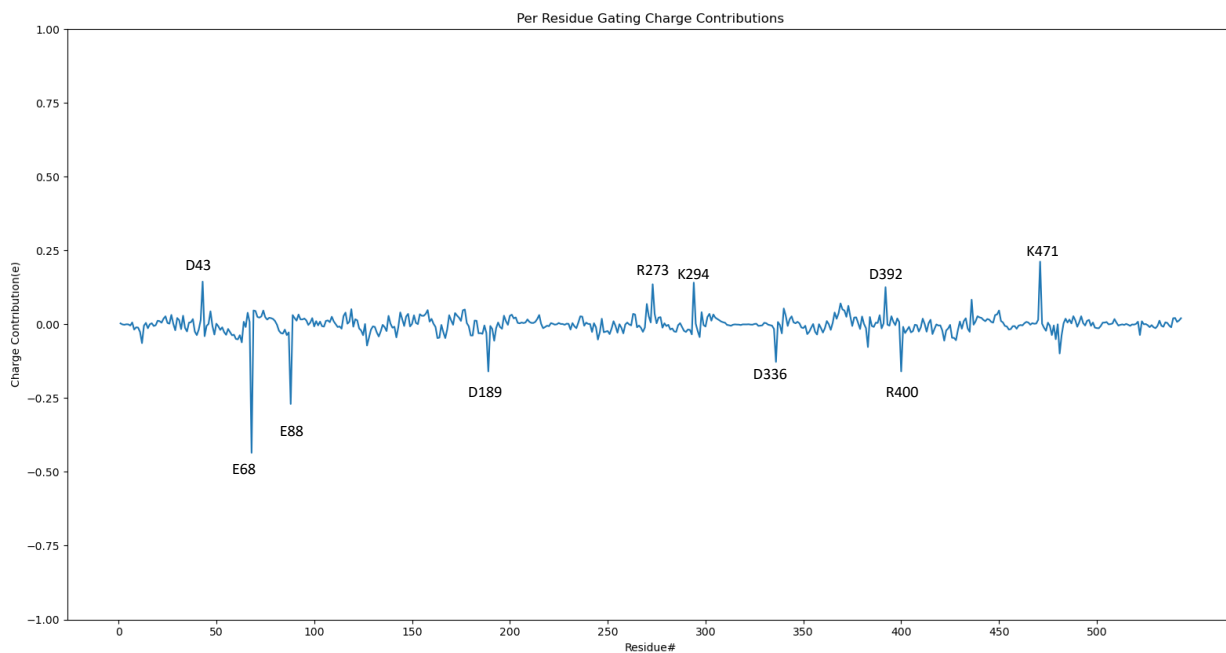
OLD APBSmem



0
Potential

Negative
Potential

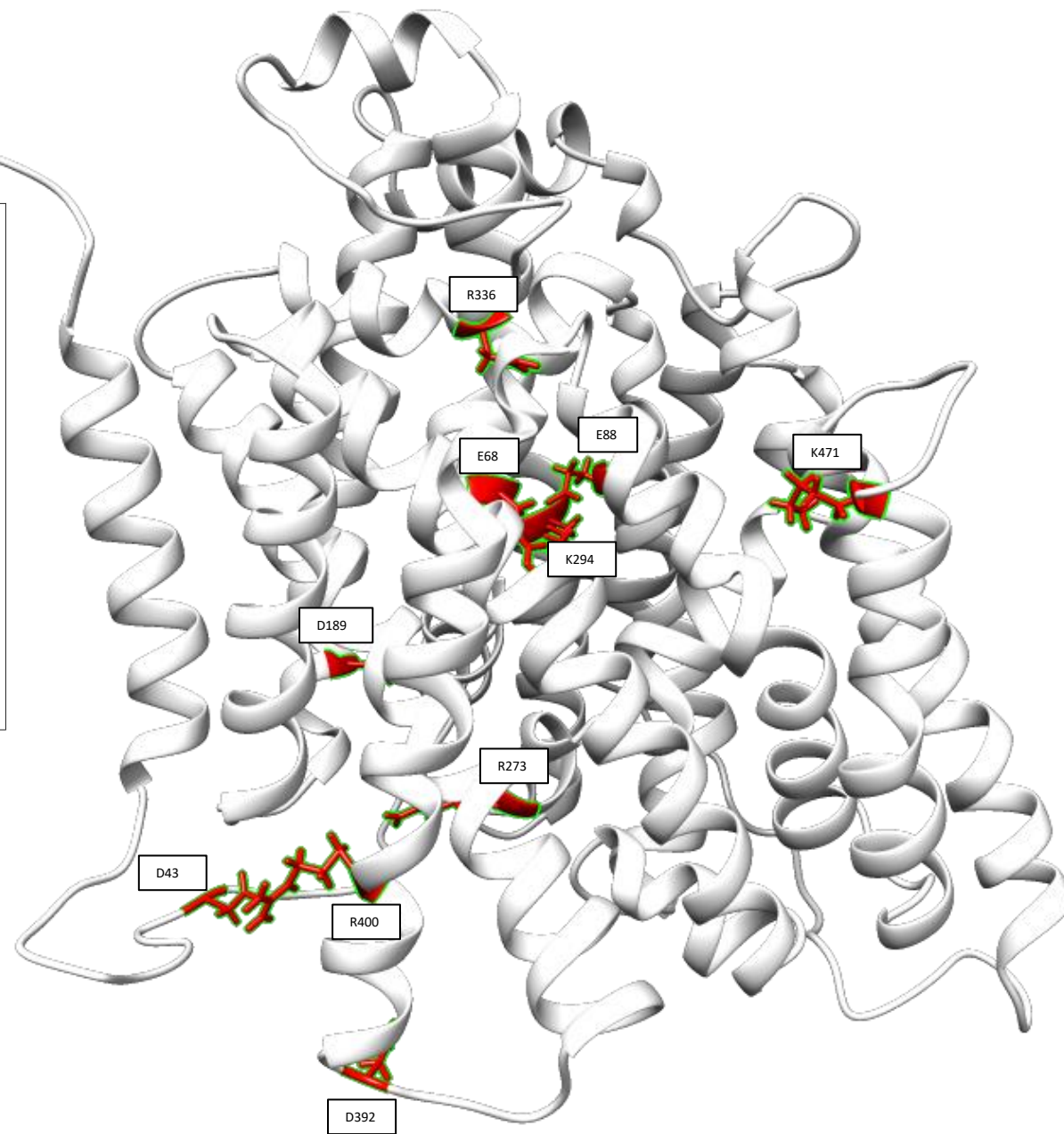
vSGLT Gating Charge



Net Charge +flooding = 0.6e

Residues seemingly not involved in catalytic cycle:

D43, D189, D336, D392, R400, K471



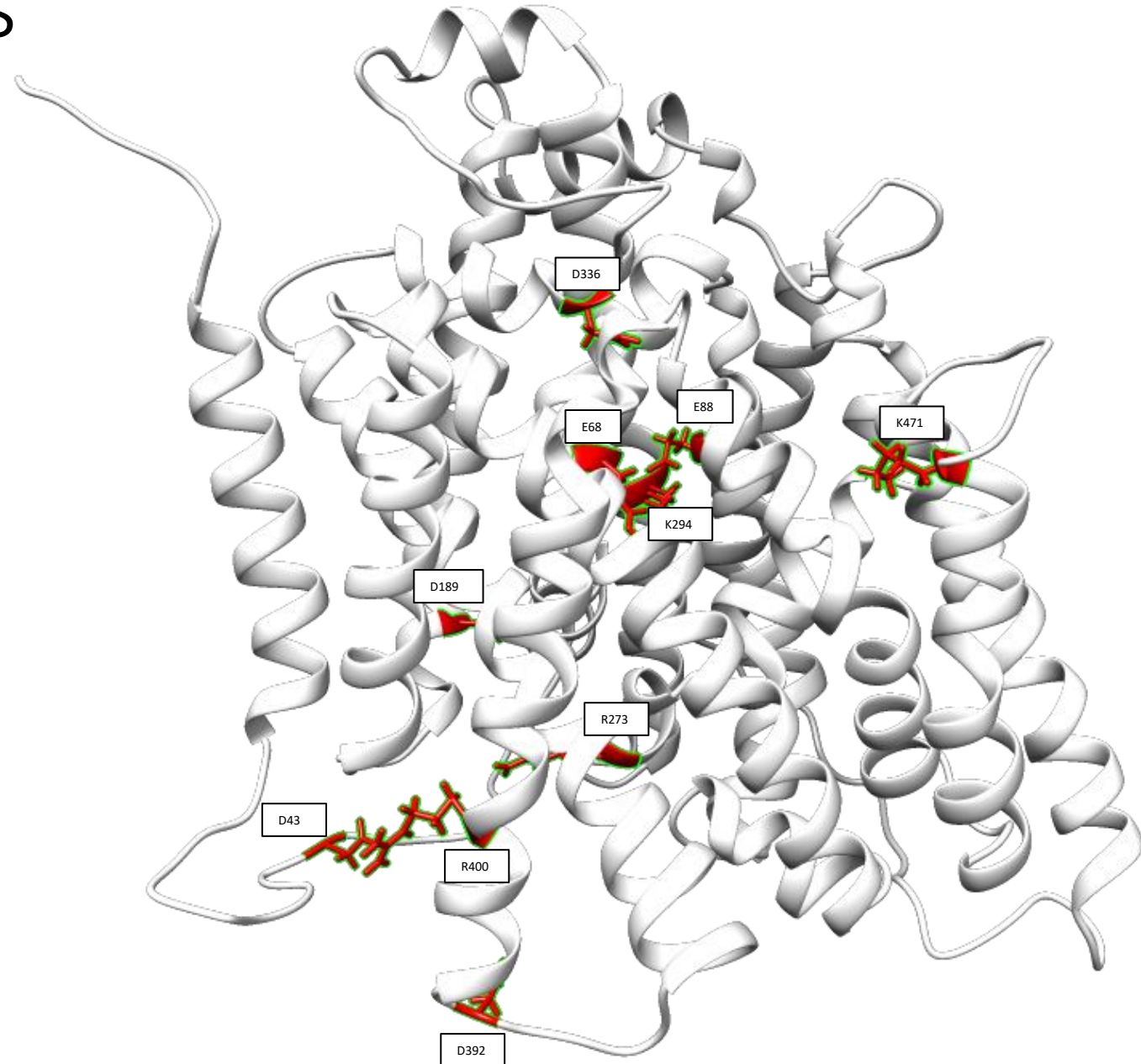
Mutation Predictions

Residues seemingly not involved in catalytic cycle:

D43, D189, D336, D392, R400, K471

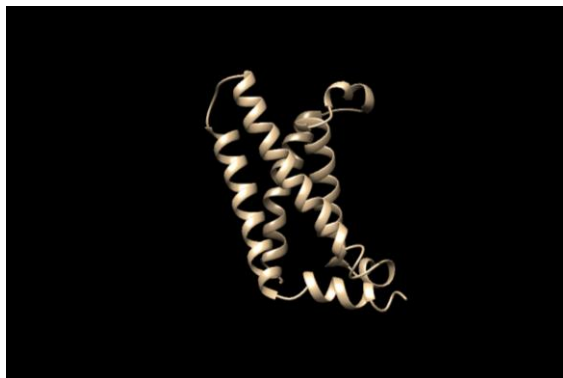
Normal |Charge|: 0.6e

Residue	Zero Charge in PQR / Flood	MODELLER ALA Mutation w/Flood
D43	0.0787/0.604	0.818
D189	0.00385/0.296	0.528
D336	0.0358/0.436	0.659
D392	0.0817/0.609	0.812
R400	0.0571/0.569	0.779
K471	0.16/0.83	0.976



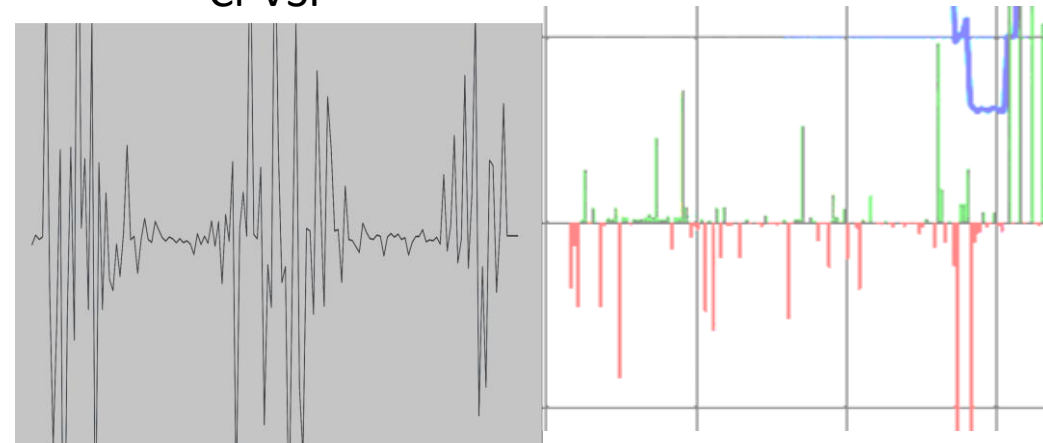
Reproducing Machtens Et al. Data

Ci-VSP Voltage Sensing Domain:

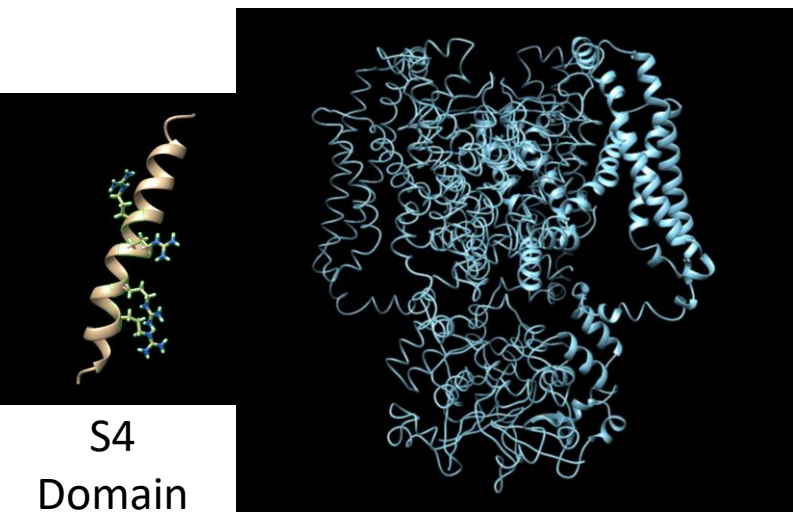


Machtens Gating charge: $\sim 0.95e$
APBSmem: $0.887e$

Overlaid Per-residue charges Ci-VSP



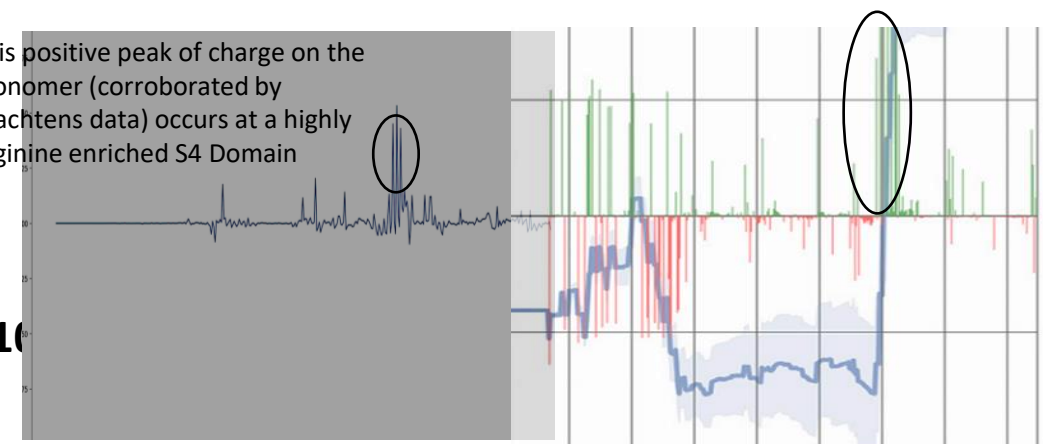
Kv1.2 Potassium Channel:



Machtens Gating charge: $\sim 10.10e$
APBSmem: $13e$
Note: Literature reports a range of 10

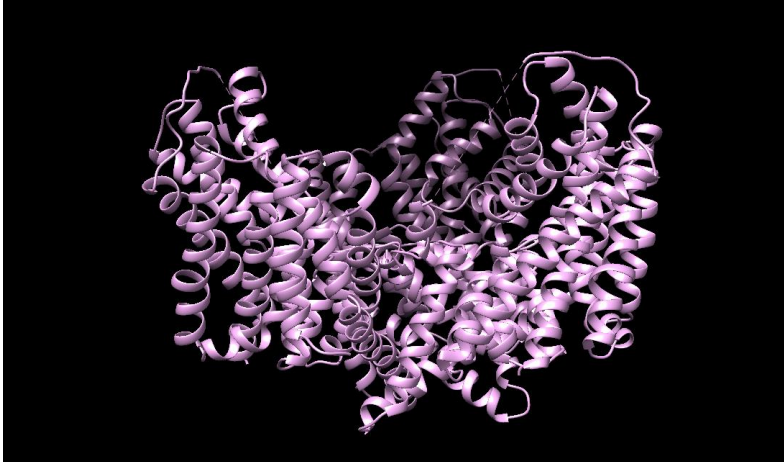
Overlaid Per-residue charges (monomer) Kv1.2

This positive peak of charge on the monomer (corroborated by Machtens data) occurs at a highly arginine enriched S4 Domain



Glt[ph]

Have not been able to reproduce exactly what Machtens got with their structures. Machtens did not do a per-residue study



Machtens /trimer	APBSmem different monomers
~0.55e	0.157e
	0.128e
	0.058e