

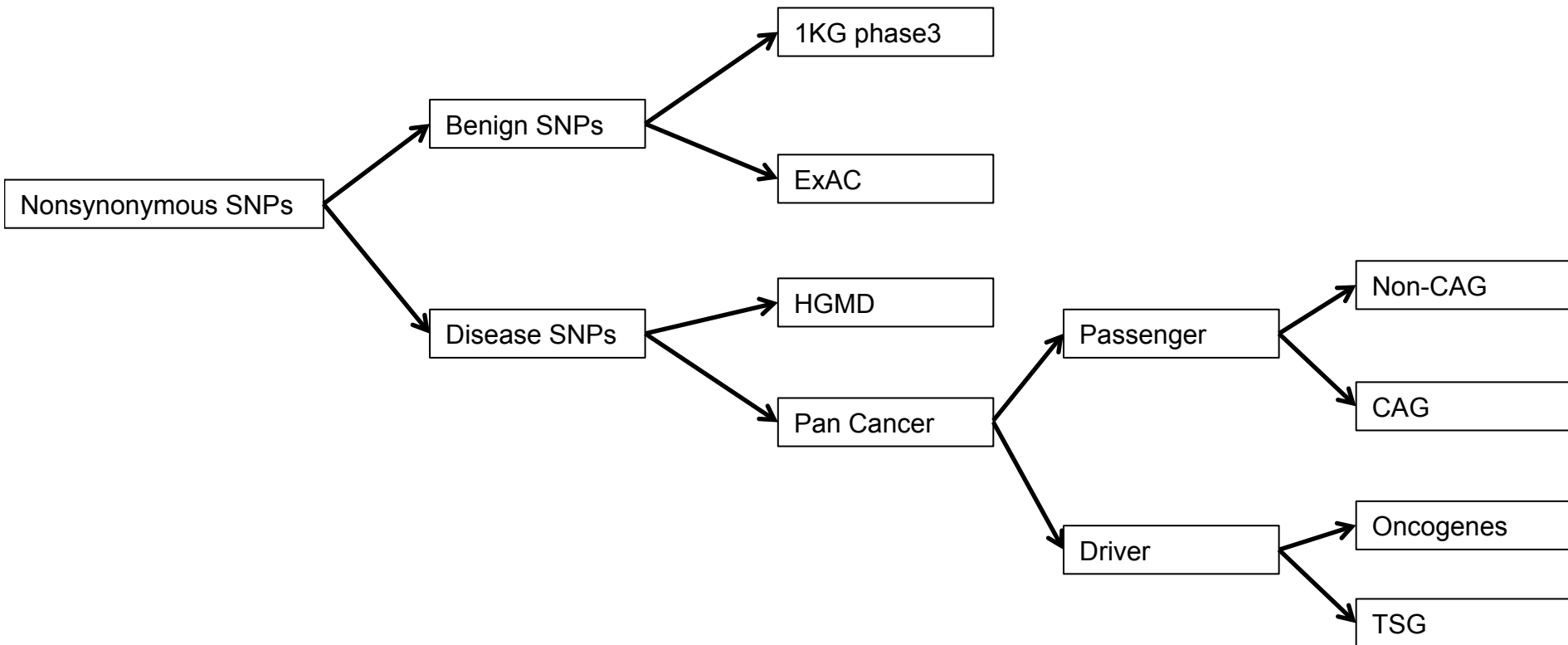
Frustration Analysis

Objective of the work

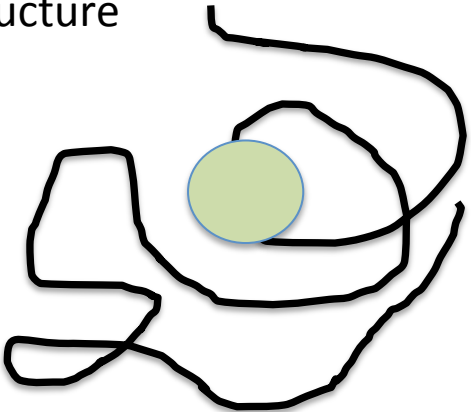
Investigate the impact of non-synonymous single nucleotide polymorphism on the localized frustration profile of protein structures and its interactions.

Comparison of the localized frustration profile of SNPs mapping to protein structure from the 1000 Genome, EXAC, HGMD and Pancancer data.

SNV datasets for frustration analysis



Native structure

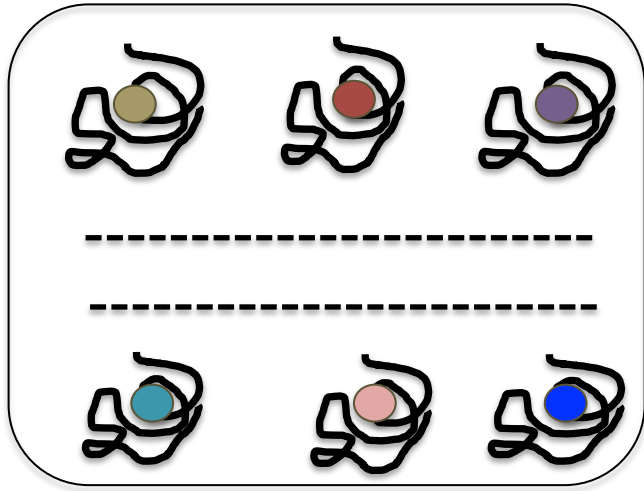


$$F_i = \frac{E_i^{T,N} - \langle E_i^{T,U} \rangle}{\sqrt{1/N \sum_{k=1}^n (E_{i'}^{T,U} - \langle E_{i'}^{T,U} \rangle)^2}}$$

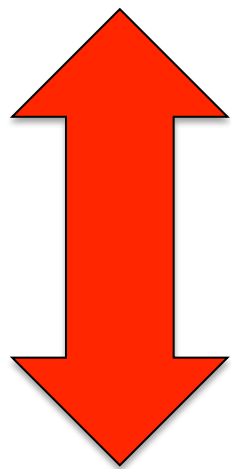
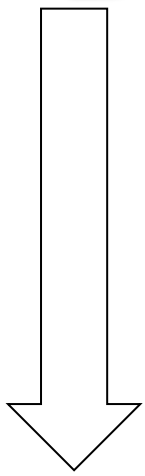
$F_i \geq 0.78$ (minimal frustrated)
 $F_i \leq -1.0$ (maximal frustrated)



Native Residue Frustration Index (NRFI)

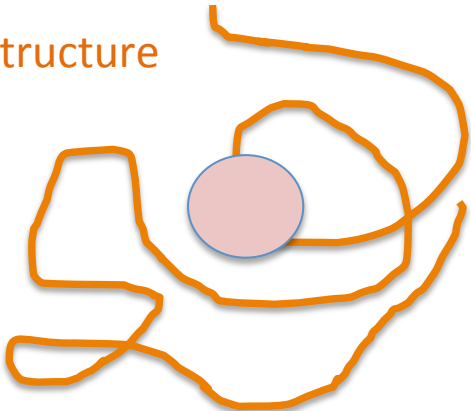


HOMOLOGY MODELLING

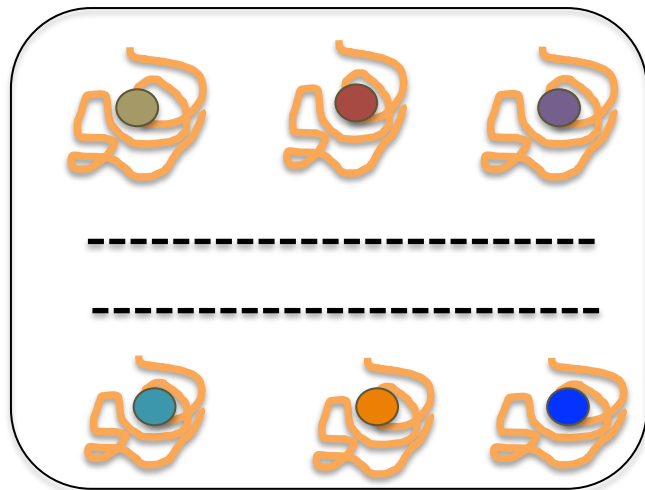


$$\Delta \text{Residue frustration} = \text{MRFI} - \text{NRFI}$$

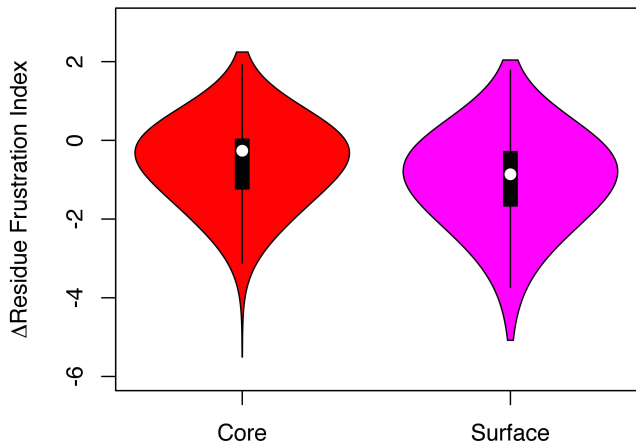
Mutated structure



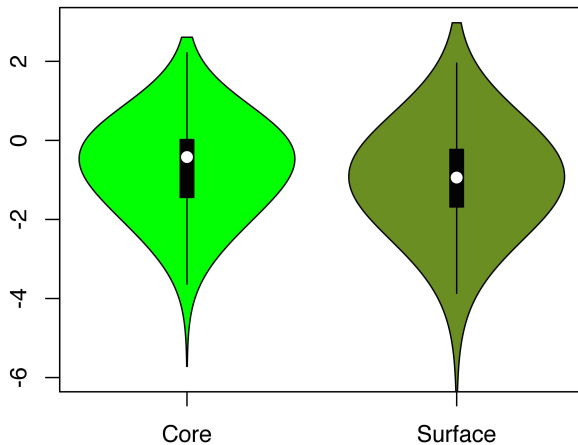
Mutated Residue Frustration Index (MRFI)



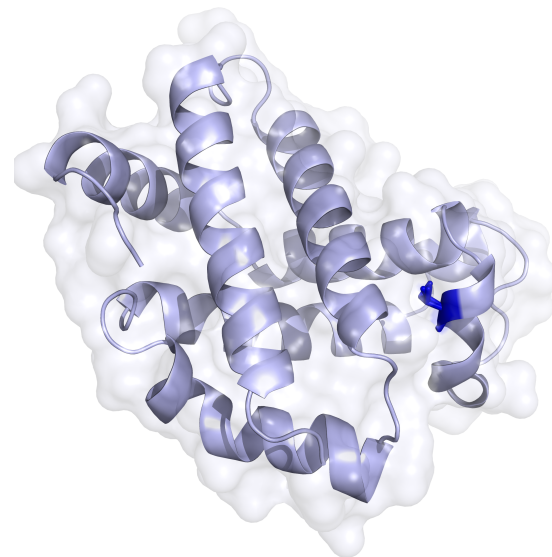
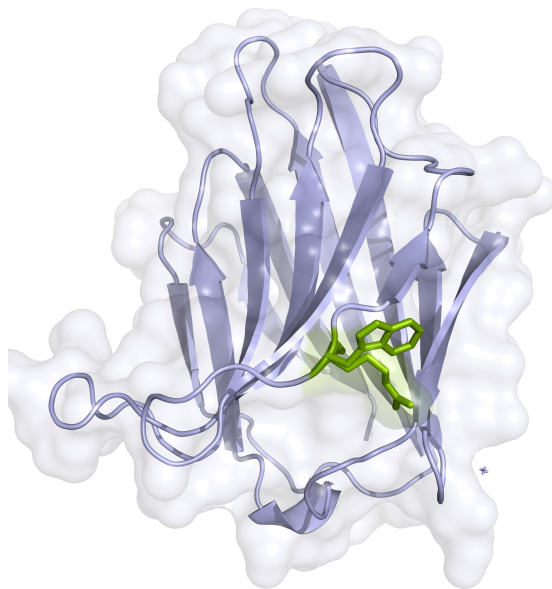
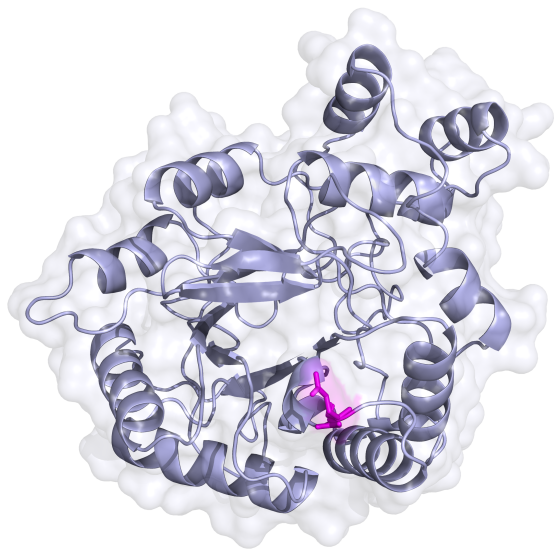
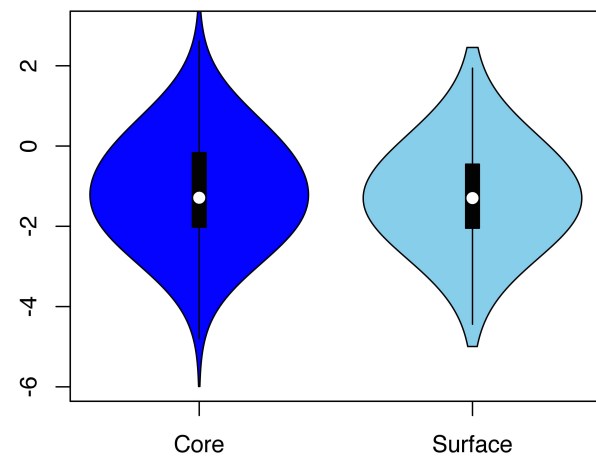
1KG min frustrated

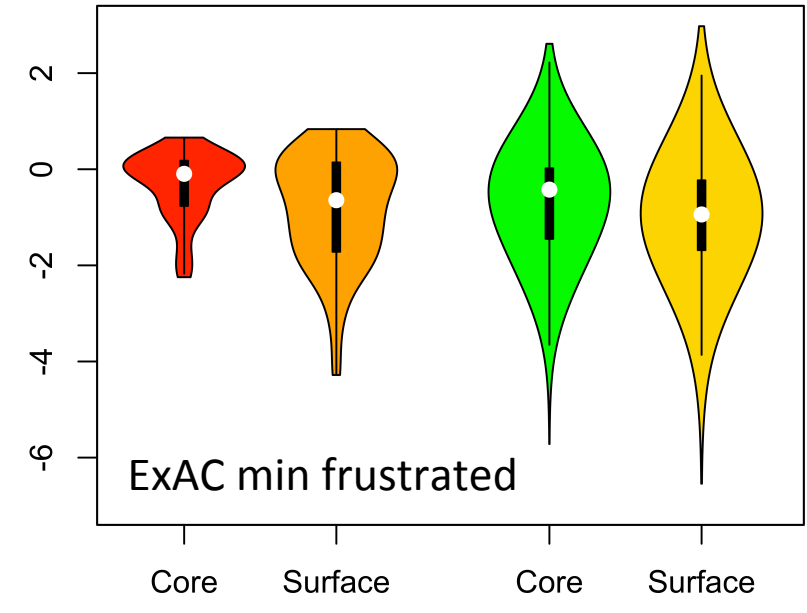
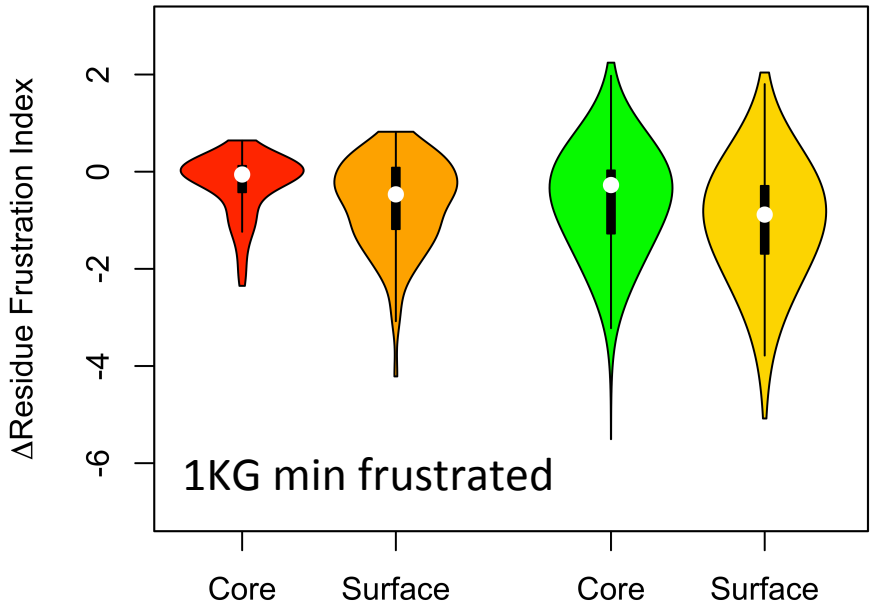
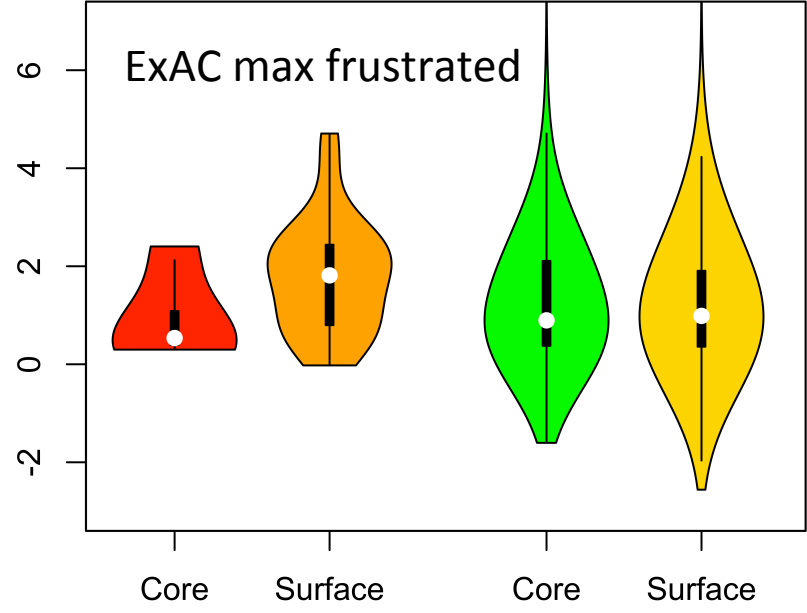
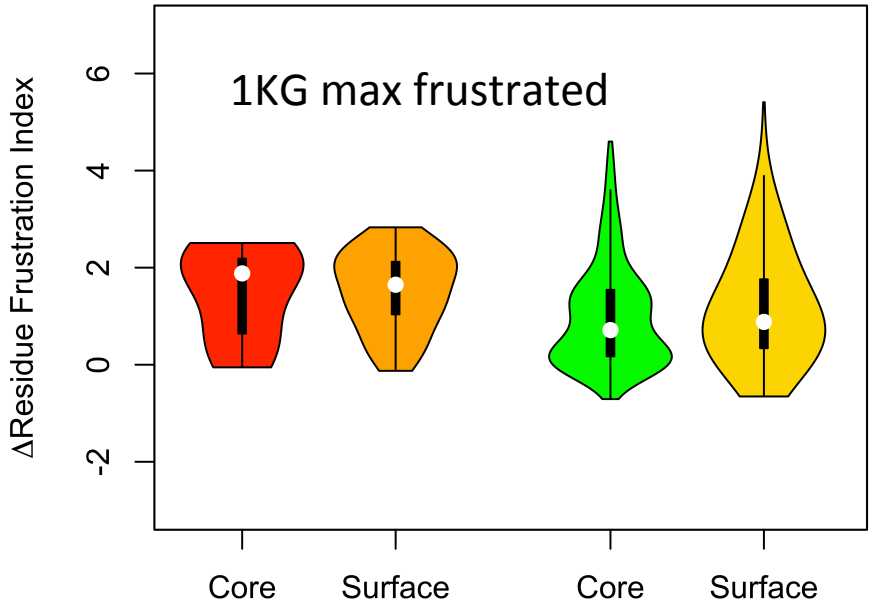


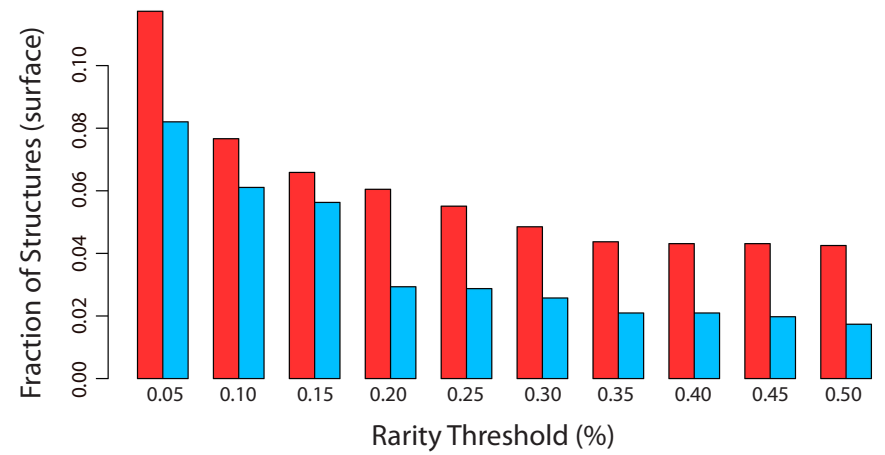
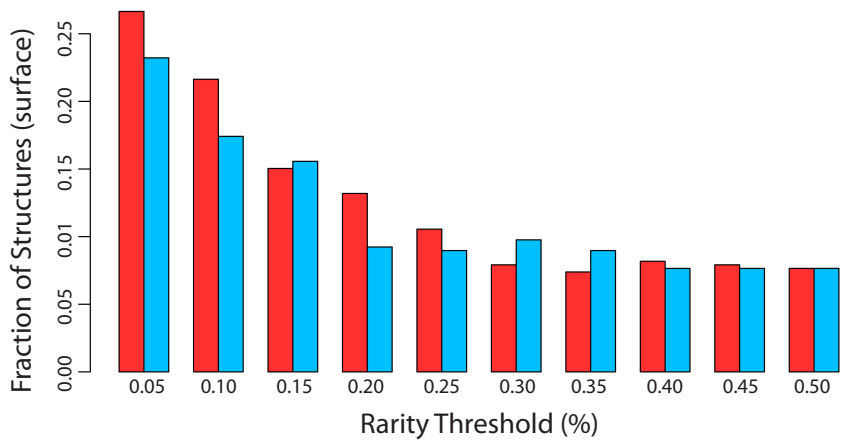
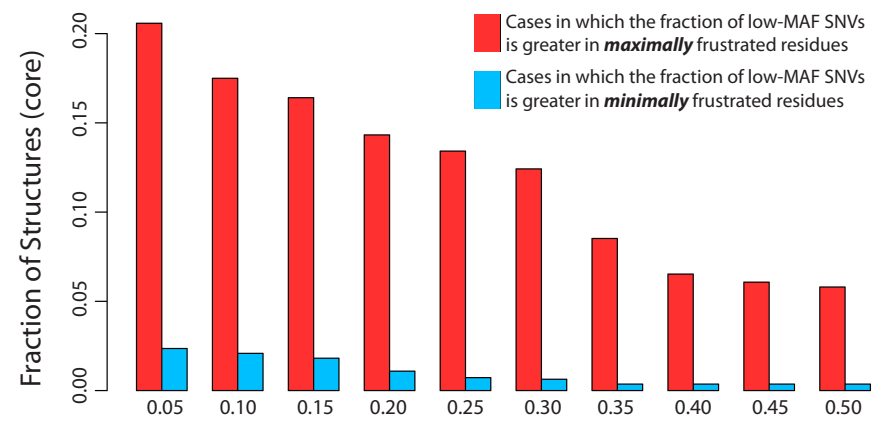
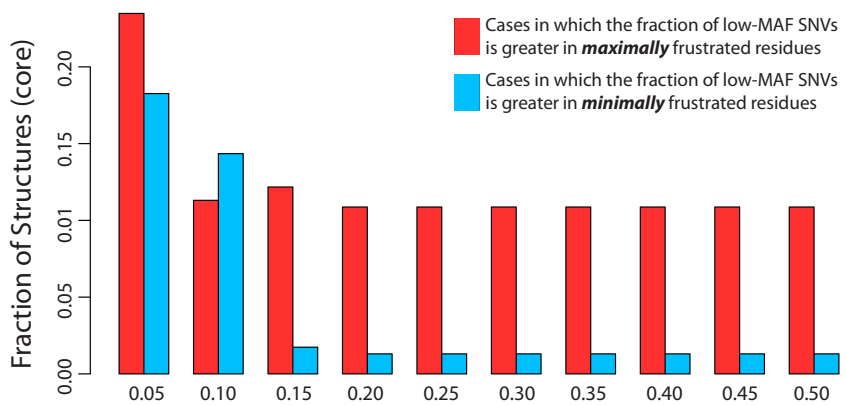
EXAC min frustrated



HGMD min frustrated

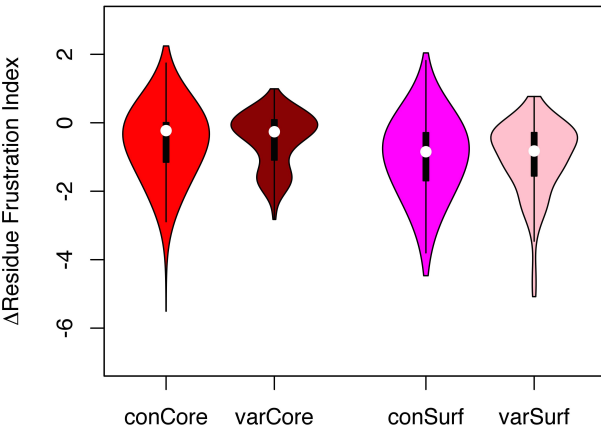




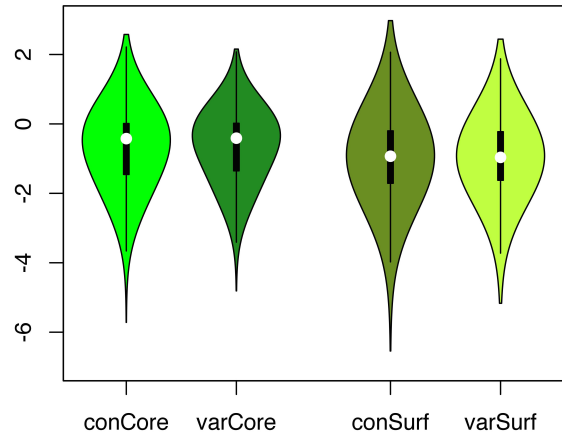


GERP score based analysis

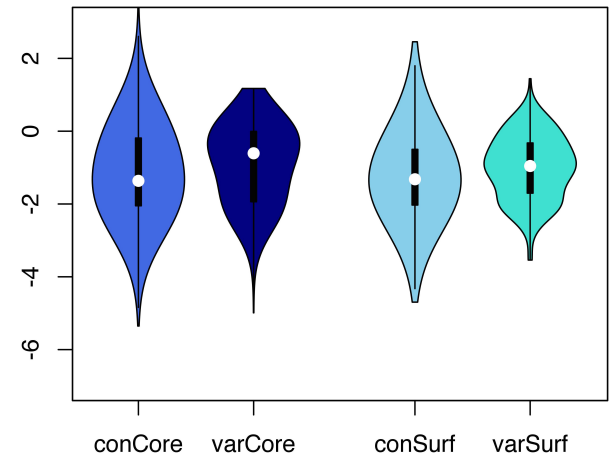
1KG min frustrated



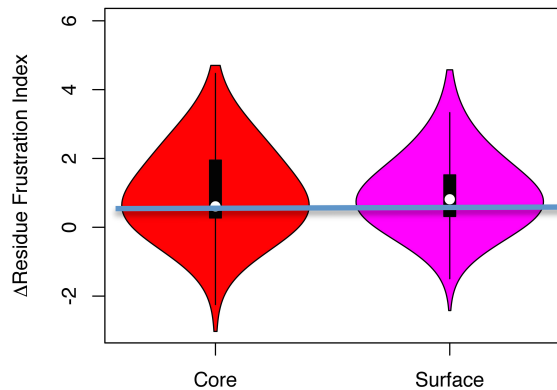
ExAC min frustrated



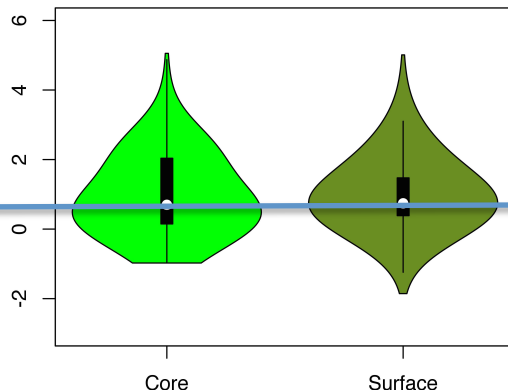
HGMD min frustrated



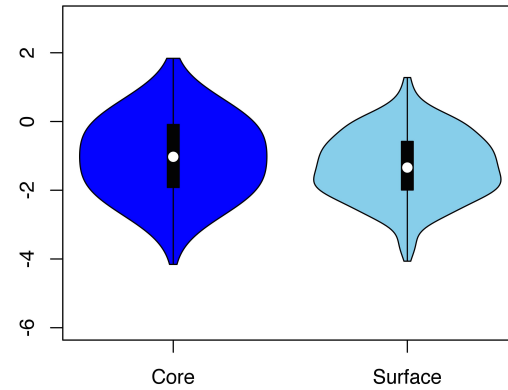
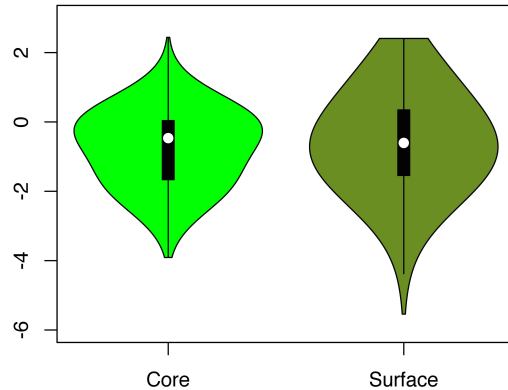
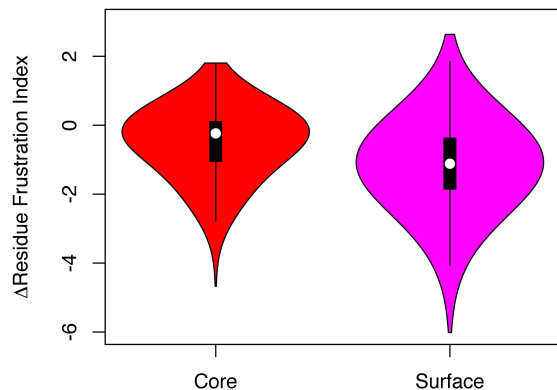
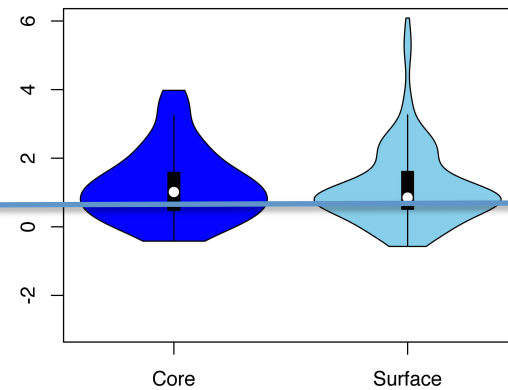
nonCAG max frustrated



CAG max frustrated



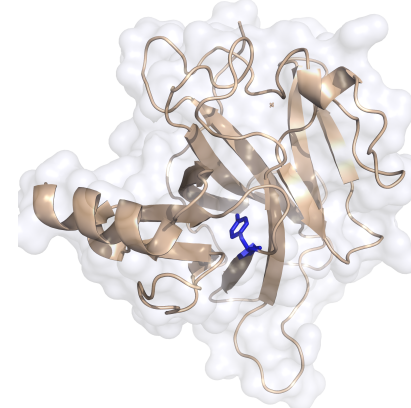
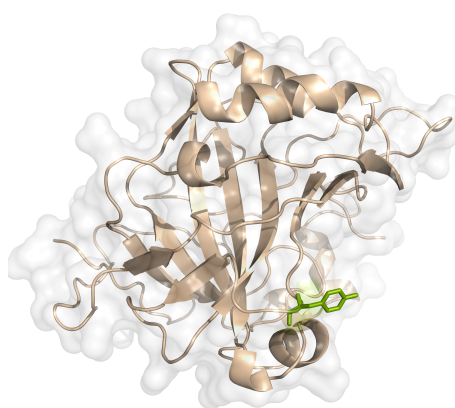
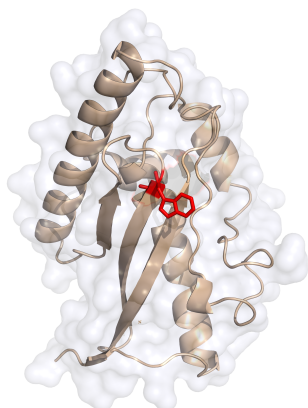
driver max frustrated

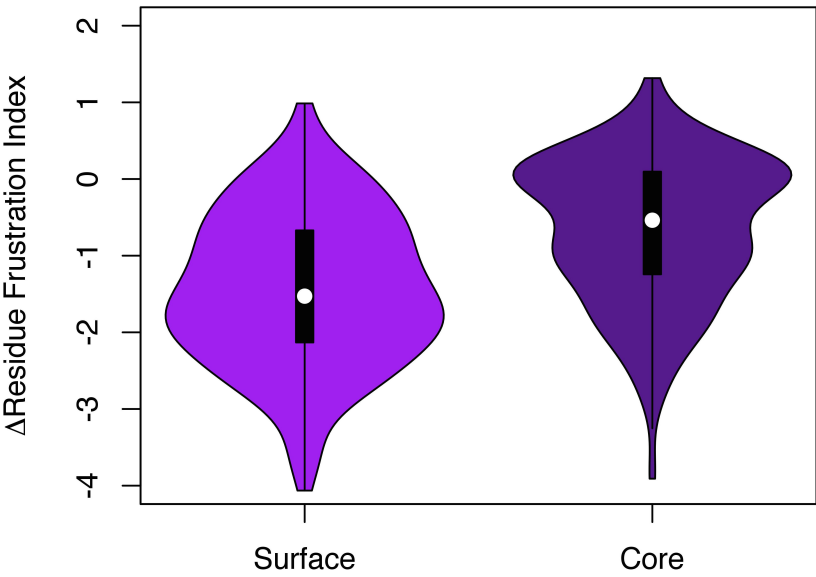


nonCAG min frustrated

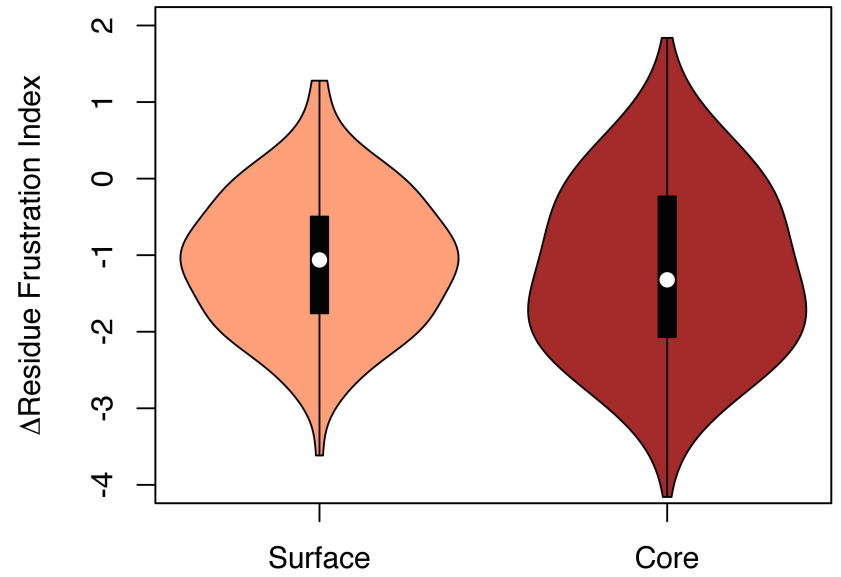
CAG min frustrated

driver min frustrated





Oncogene min frustrated



TSG min frustrated