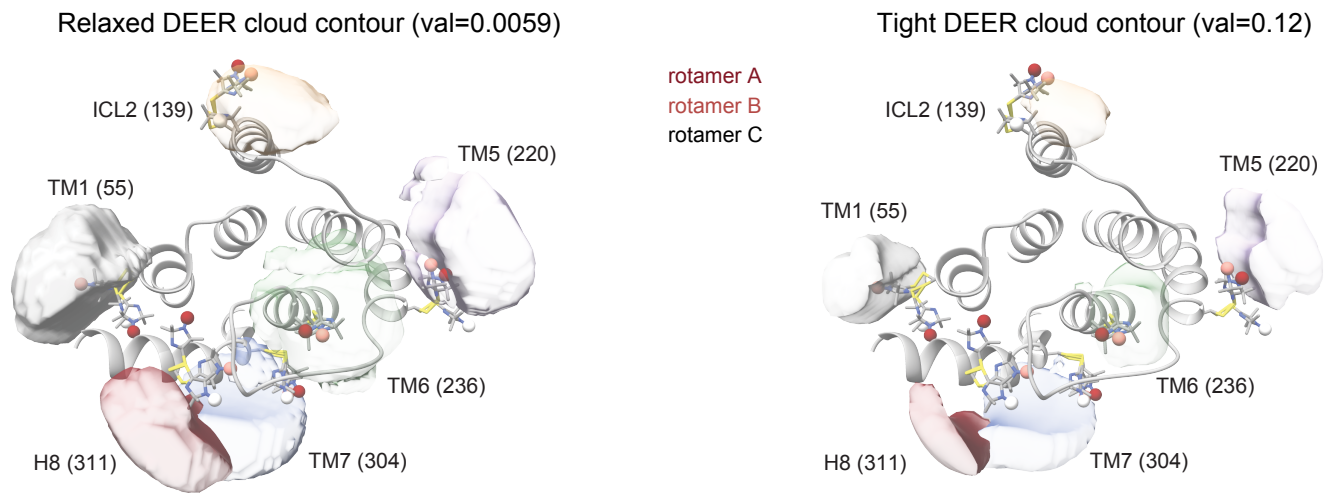


**D** High probability V1 rotamers attached to crystal structure exhibit minimal overlap with DEER clouds at several sites



**E** Fraction of MD simulation frames containing a high probability V1 rotamer in DEER cloud

