

Supplementary Material

Self-assembly and the conformational change in the oligomeric structure of the ectodomain of TBEV E protein studied by XRD, SAXS and molecular dynamics.

Supplementary Figures

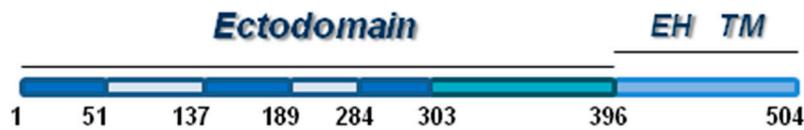


Figure S1. Scheme of protein E organization. Domain I (regions 1-51, 137-189, 285-302), domain II (regions 52-136, 190-284) and domain III (regions 303-396) of an ectodomain colored dark blue, light grey and teal respectively. Stem (EH) and transmembrane (TM) helices (region 397-504) colored blue. Residue numbering is shown as linear peptide.

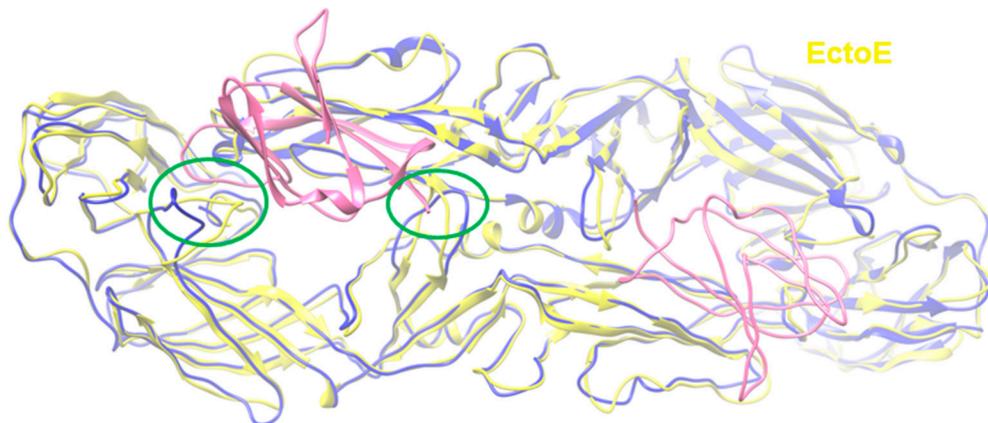


Figure S2. Superposition of ectoE (yellow) and 7QRE (protein E colored blue, pr protein colored pink) structures. Difference in α -trace of ectoE and E protein of Neudorfl strain due to protein pr binding (7QRE) is highlighted by green ovals.

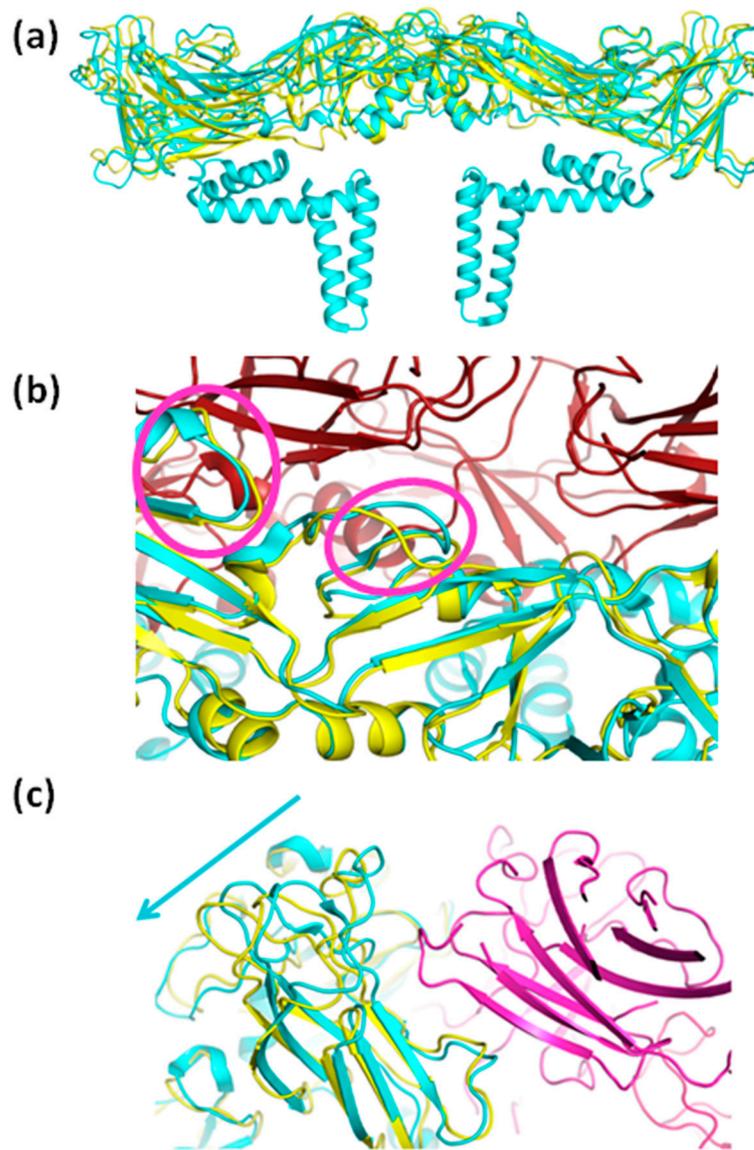


Figure S3. Influence of crystal packing on ectoE dimer conformation. (a) Superposition of ectoE (colored yellow) dimer from crystal structure (from CCT tetramer) and dimer from asymmetric part of cryo-EM structure of Kauutsalo-14 strain (colored cyan). (b) Zoom of region 79-90 (highlighted by pink oval) and 229-237 (highlighted by pink oval) of ectoE (colored yellow) superimposed with protein E in asymmetric part of structure of Kauutsalo-14 strain (colored cyan). Other dimer of CCT is colored brown. (c) Superposition of ectoE dimer of ECT (colored yellow) with dimer from asymmetric part of cryo-EM structure of Kauutsalo-14 strain (colored cyan). Other dimer of ECT colored magenta. Concerted movement of regions 300-312, 346-356 and 360-372 of domain III of ectoE due to neighbor subunit position in ECT is shown by blue arrow.