Electrostatics in Biomacromolecules

- Electrostatics important in (at least)

- binding for

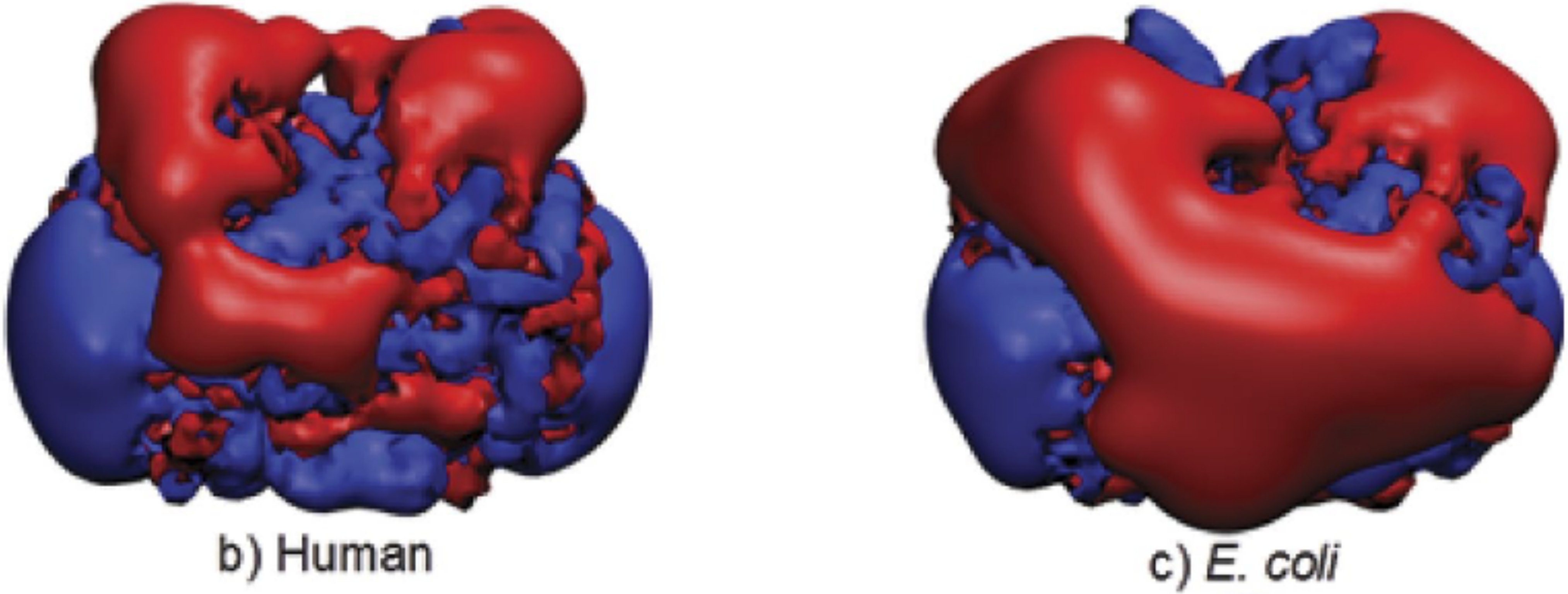
- steering, facilitating approach of species

- complexation, as complementarity means lower potential energy

- enzyme catalysis, as electric potential stabilizes transition state

- Thus, electrostatic potential usually conserved near functional sites

Thymidylate Synthase



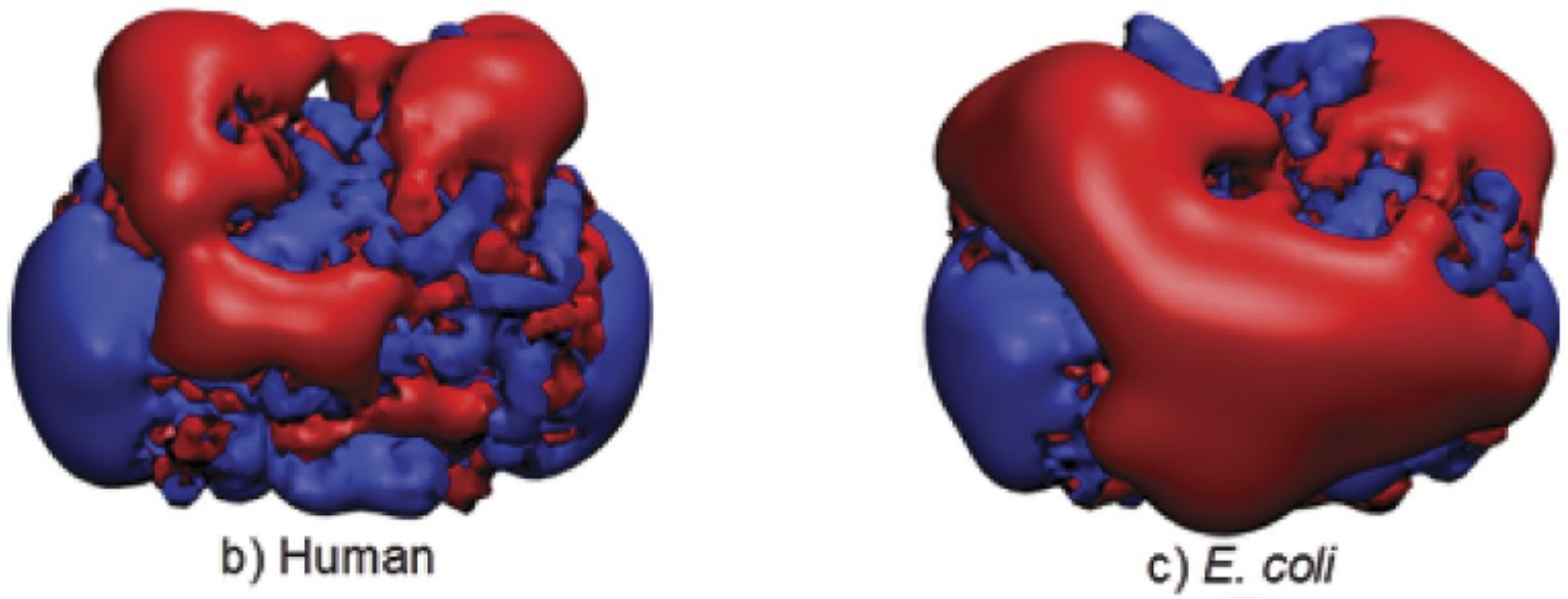
blue isocontours +1 kT/e,
red isocontours -1 kT/e
From Fig 1 of Garg *et al*. (2015).

2

Electrostatics in Biomacromolecules

- Electrostatics important in (at least)
  - binding for
    - steering, facilitating approach of species
    - complexation, as complementarity means lower potential energy
  - enzyme catalysis, as electric potential stabilizes transition state
- Thus, electrostatic potential usually conserved near functional sites

Thymidylate Synthase



blue isocontours +1 kT/e,
red isocontours -1 kT/e
From Fig 1 of Garg *et al*. (2015).

Modeling Electrostatics

- In biological macromolecules, the electrostatic potential is usually calculated based on the Poisson-Boltzmann equation
  - The Poisson equation describes the potential field due to a given charge distribution. Atoms in the biomolecule are assumed to have a fixed charge.
  - The Poisson-Boltzmann equation assumes that (infinitely small) ions surround a biomolecule in accordance with the Boltzmann distribution
- The PB equation is a partial differential equation that is solved numerically
- The equation is often linearized to be more numerically stable
- Chun Liu in Applied Math has worked on versions
  - that are time-dependent
  - account for the finite size of ions