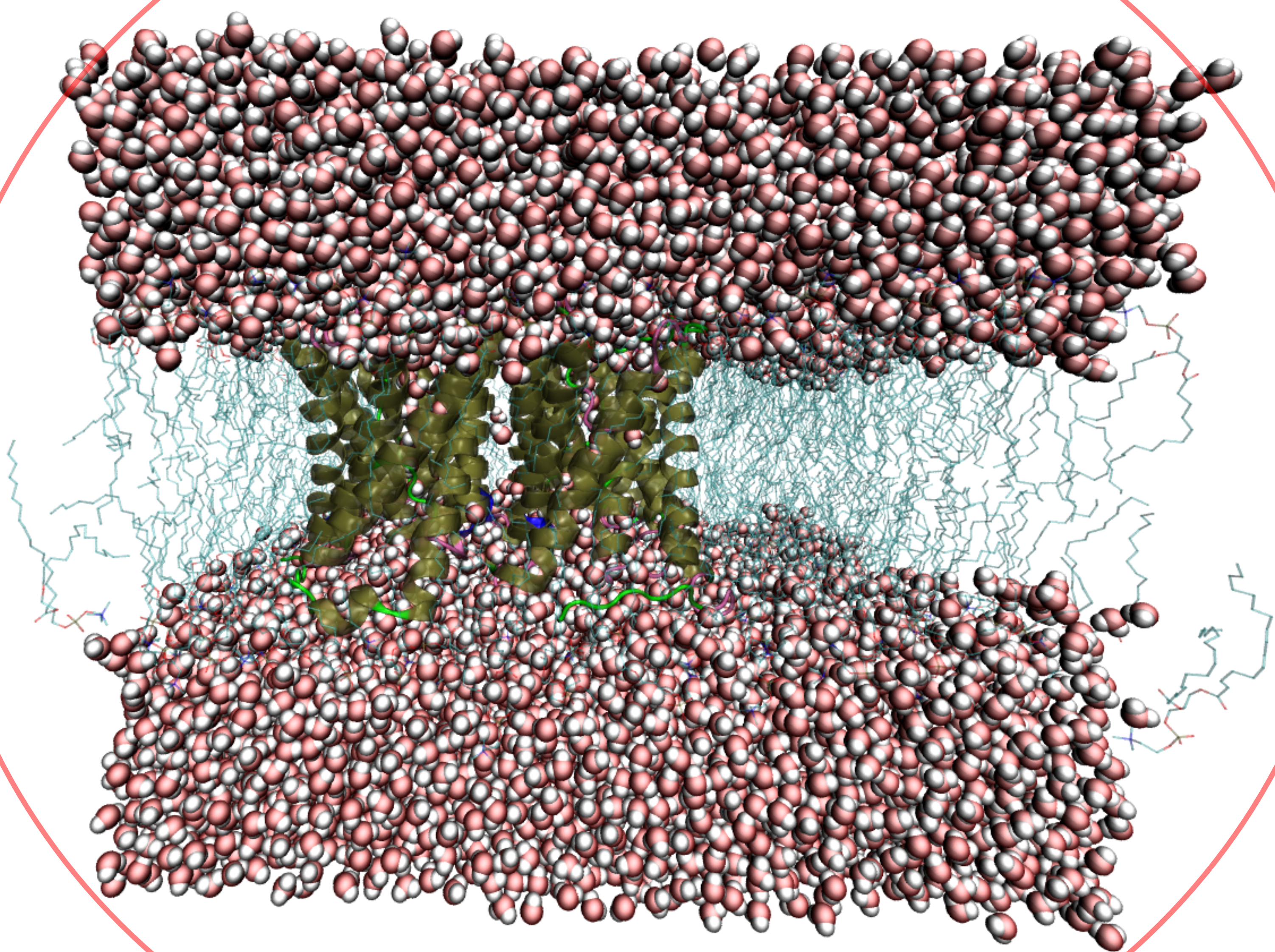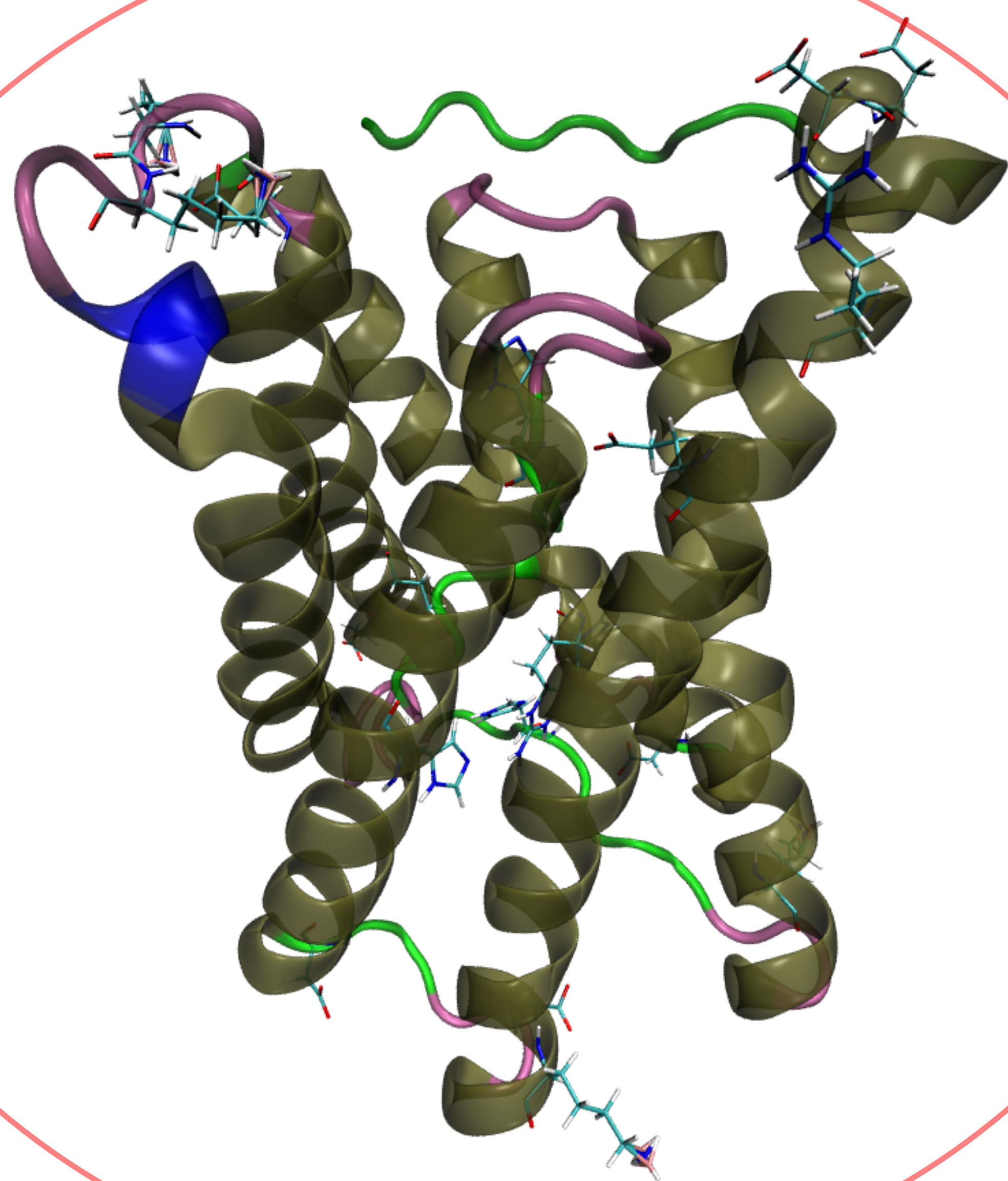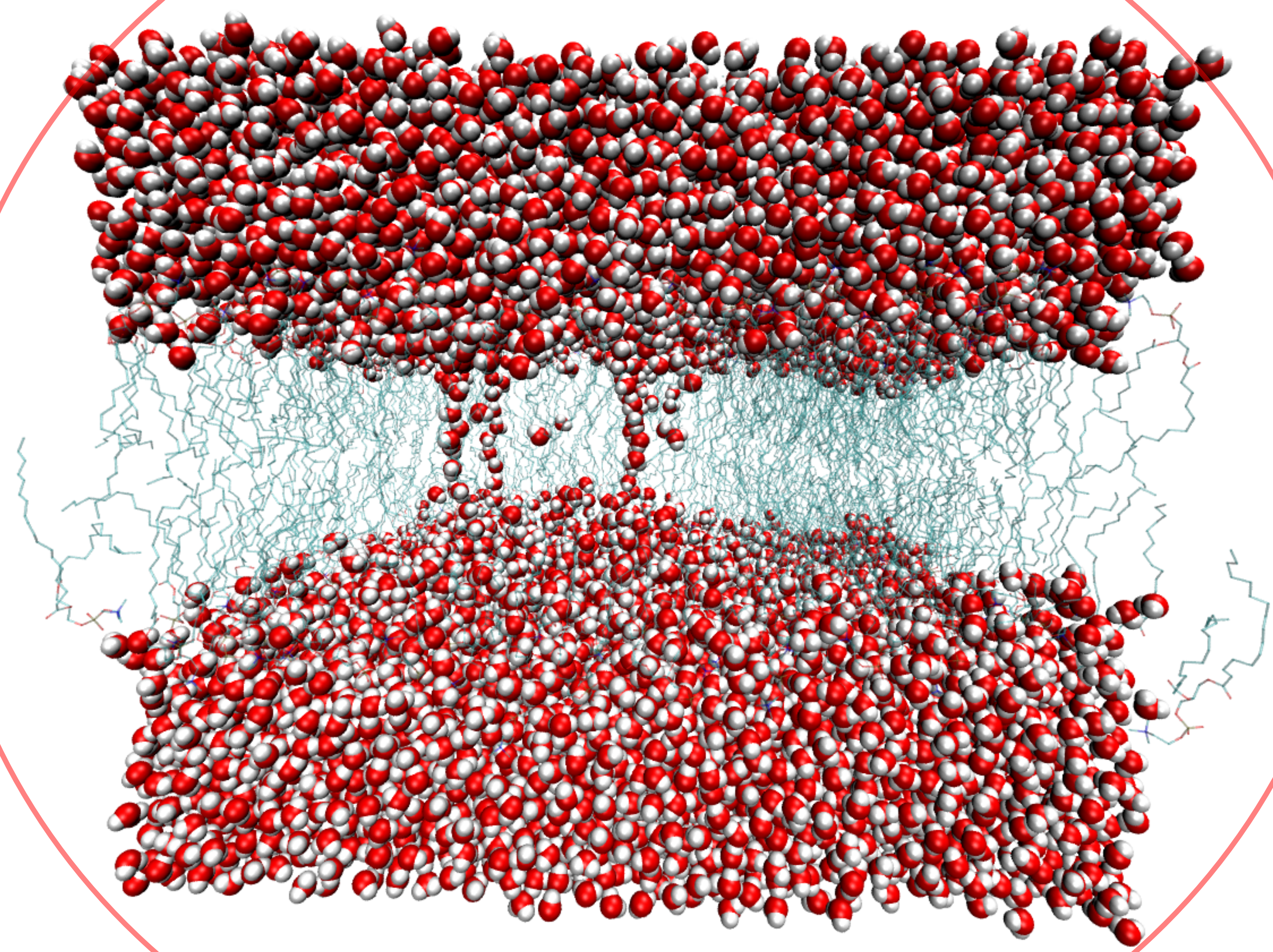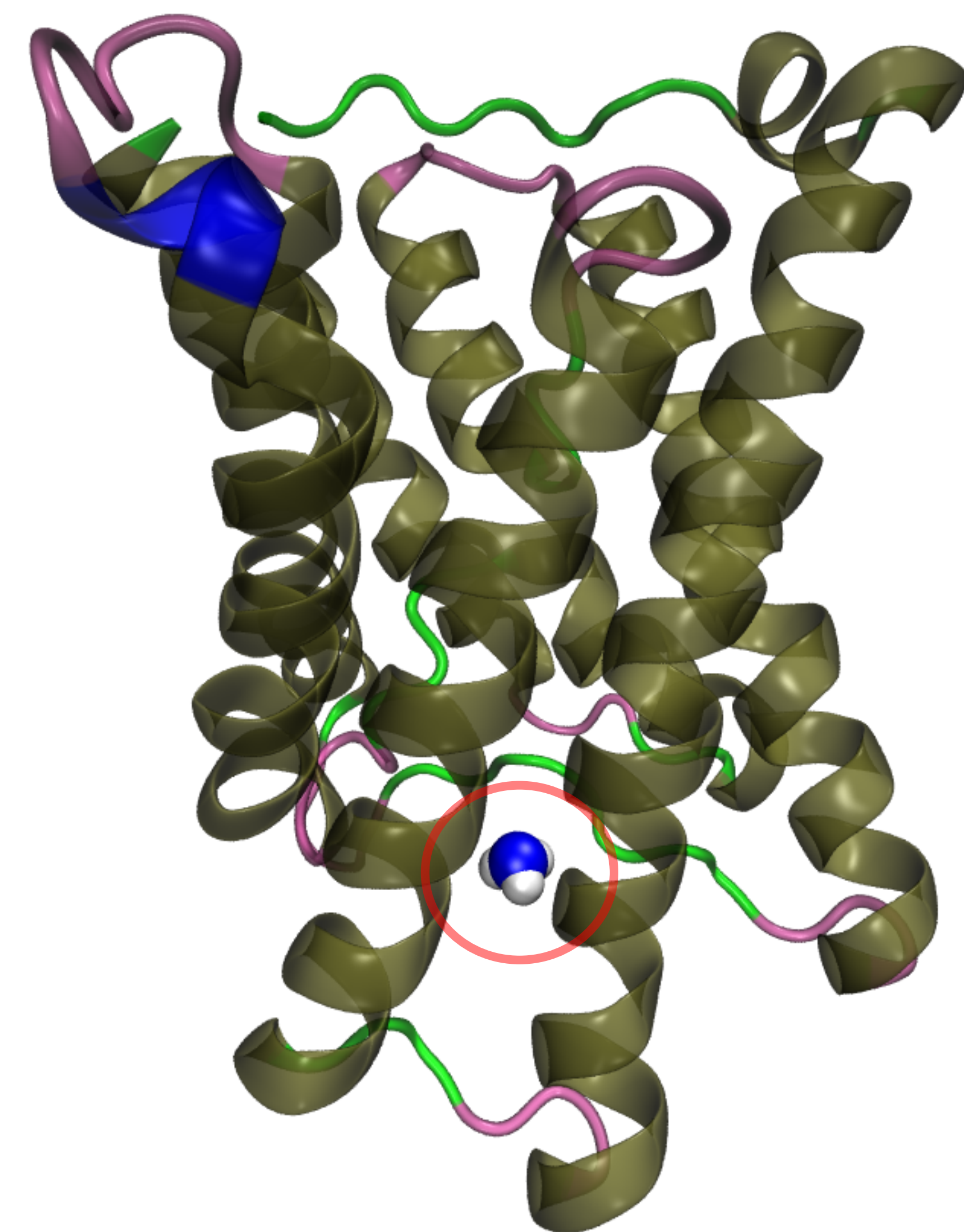Complete system for coordinate output

Partial system for e.g. temperature coupling

Partial system for interaction analysis

Single molecule for e.g. Umbrella sampling