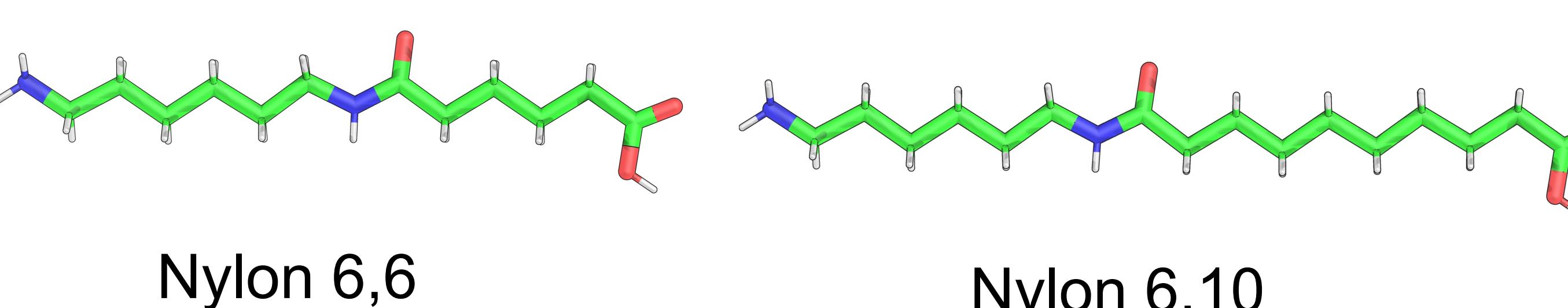
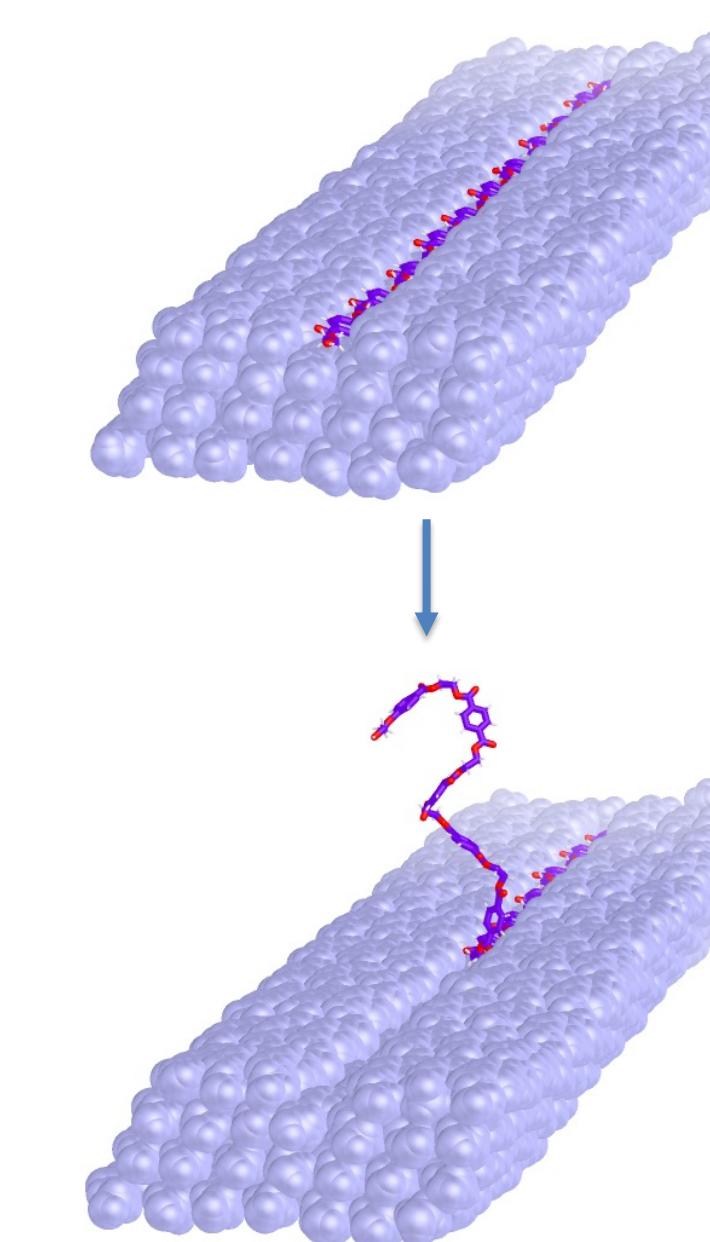


From Simulation to Solution: Decoding Nylons for a Sustainable Future

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Background

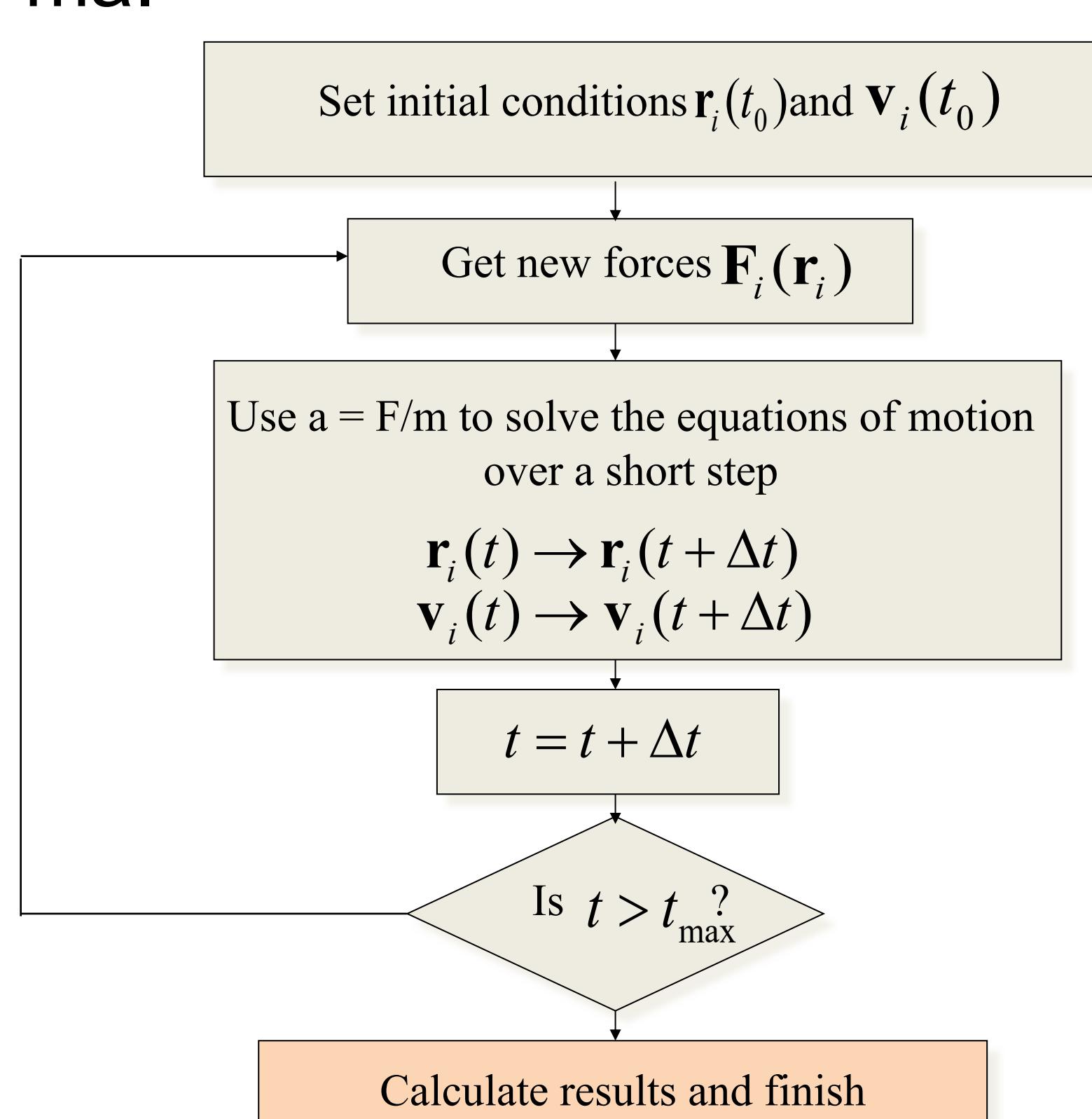
- Plastics are indispensable in modern life but pose environmental challenges
- Strategies to address plastic waste: enzymatic decrystallization
- Decrystallization energy calculation in cellulose, chitin and polyester
- Nylons:** versatile synthetic polymers
- Semi-crystalline in nature
- Uses: textiles, automotive components, medical devices, and more.



Methods

Molecular Dynamics (MD) Simulation

- Computer-based simulation method used to observe and study how atoms and molecules move and interact with each other over time.
- Based on Newton's second law or the equation of motion, $F=ma$.



Software

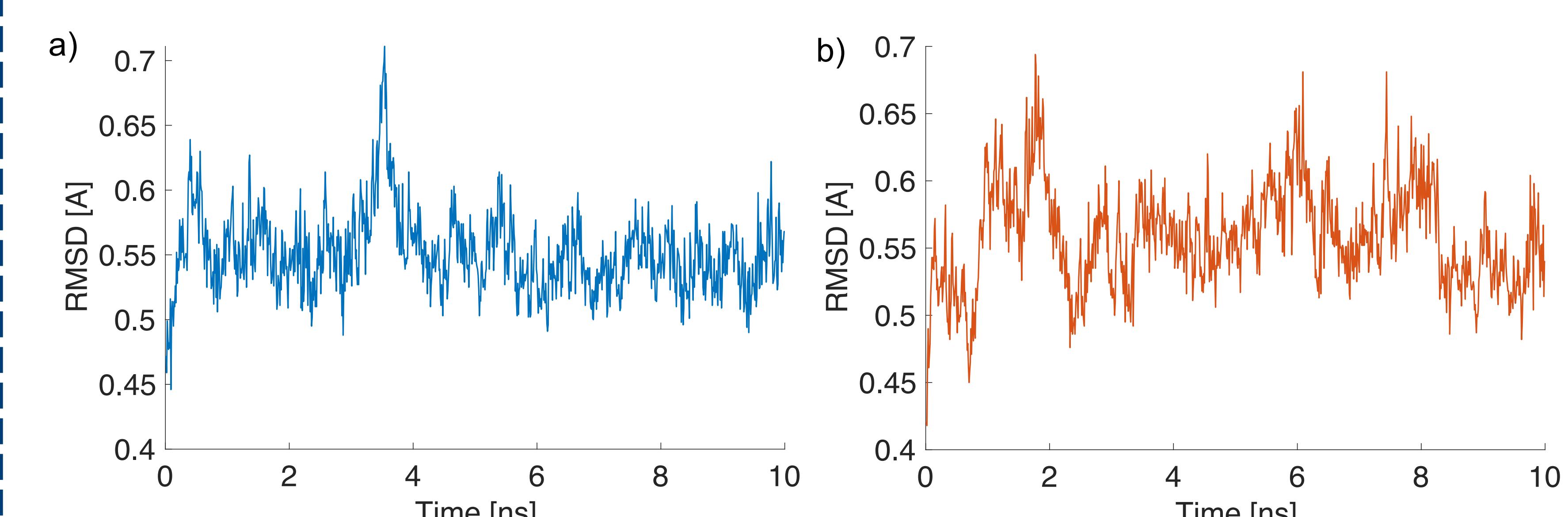
- Simulation Software:** **N**anoscale **M**olecular **D**ynamics (NAMD), CHARMM (Chemistry at **H**ARvard **M**olecular **M**echanics)
- Force field:** CHARMM36 forcefield
- Visualization Software:** Visual Molecular Dynamics (VMD), Pymol

System Building & Analysis

- Crystal structures of nylon 6,6 and nylon 6,10 were constructed using CHARMM. The initial coordinates and crystallographic information were obtained from the Cambridge Structural Database (CSD).

Fig 1: Snapshot of Nylon 6,6 chain

RMSD



System Building & Analysis

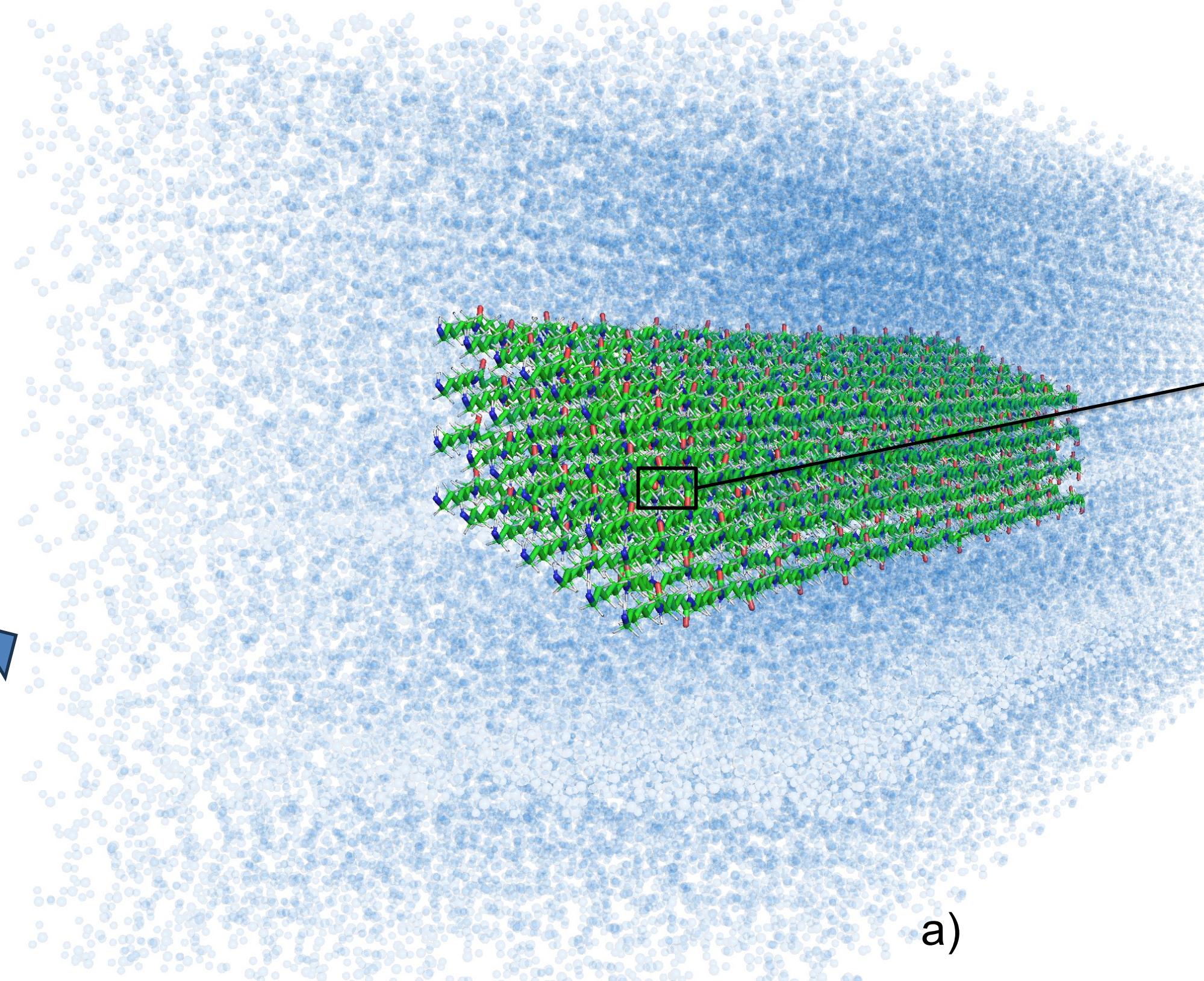
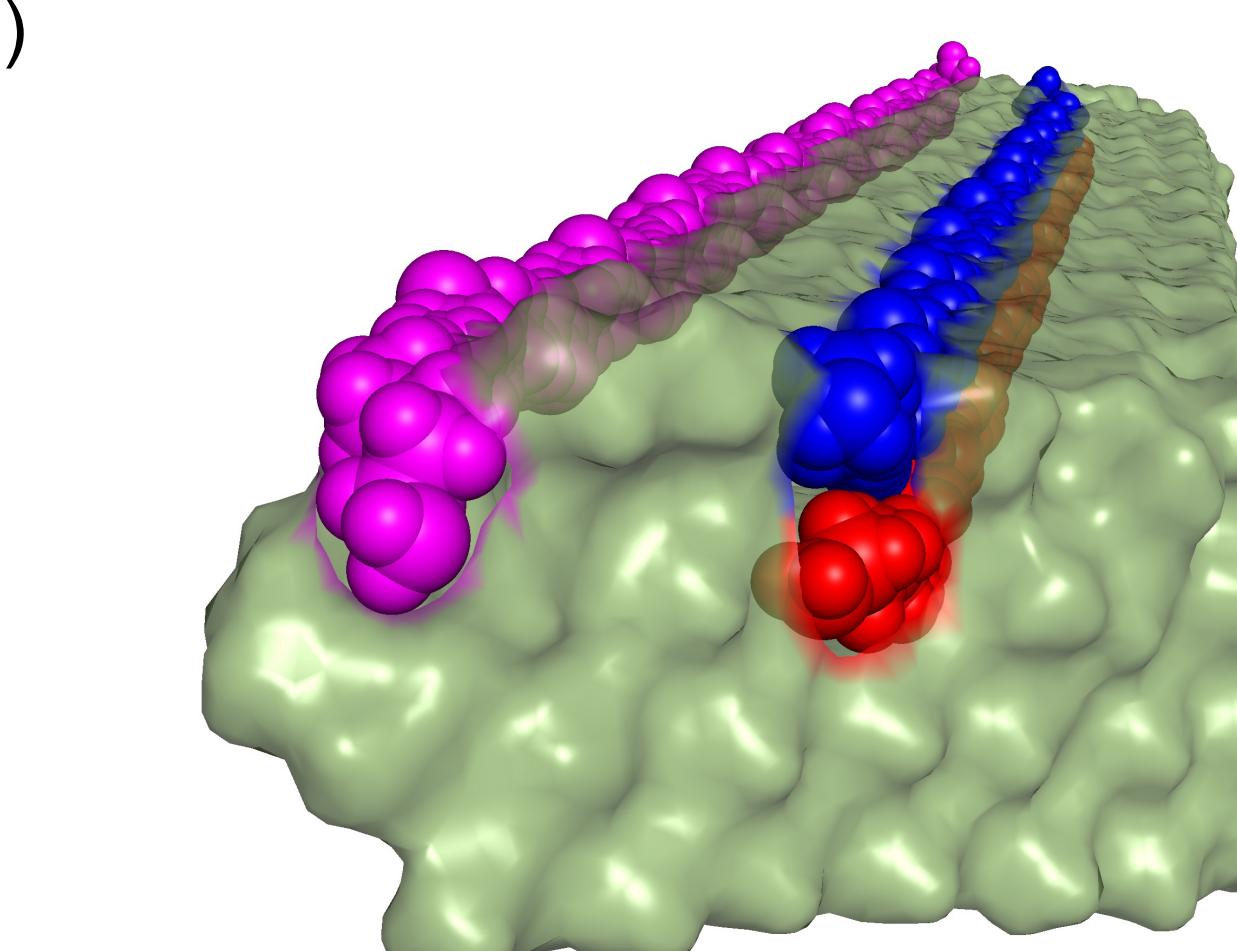


Fig 2: Snapshot of Nylon 6,6 crystal solvated in water

a)



RMSF

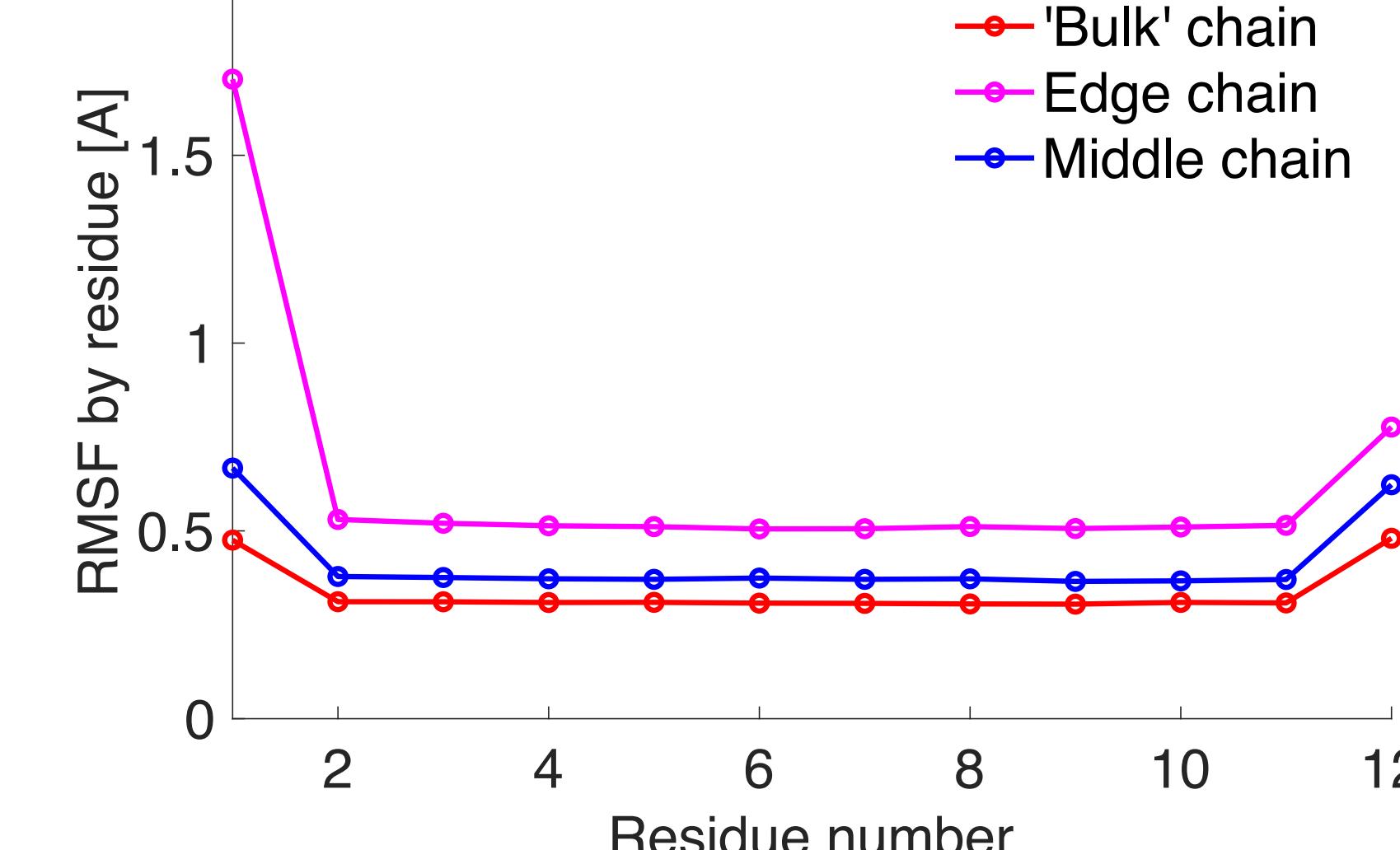
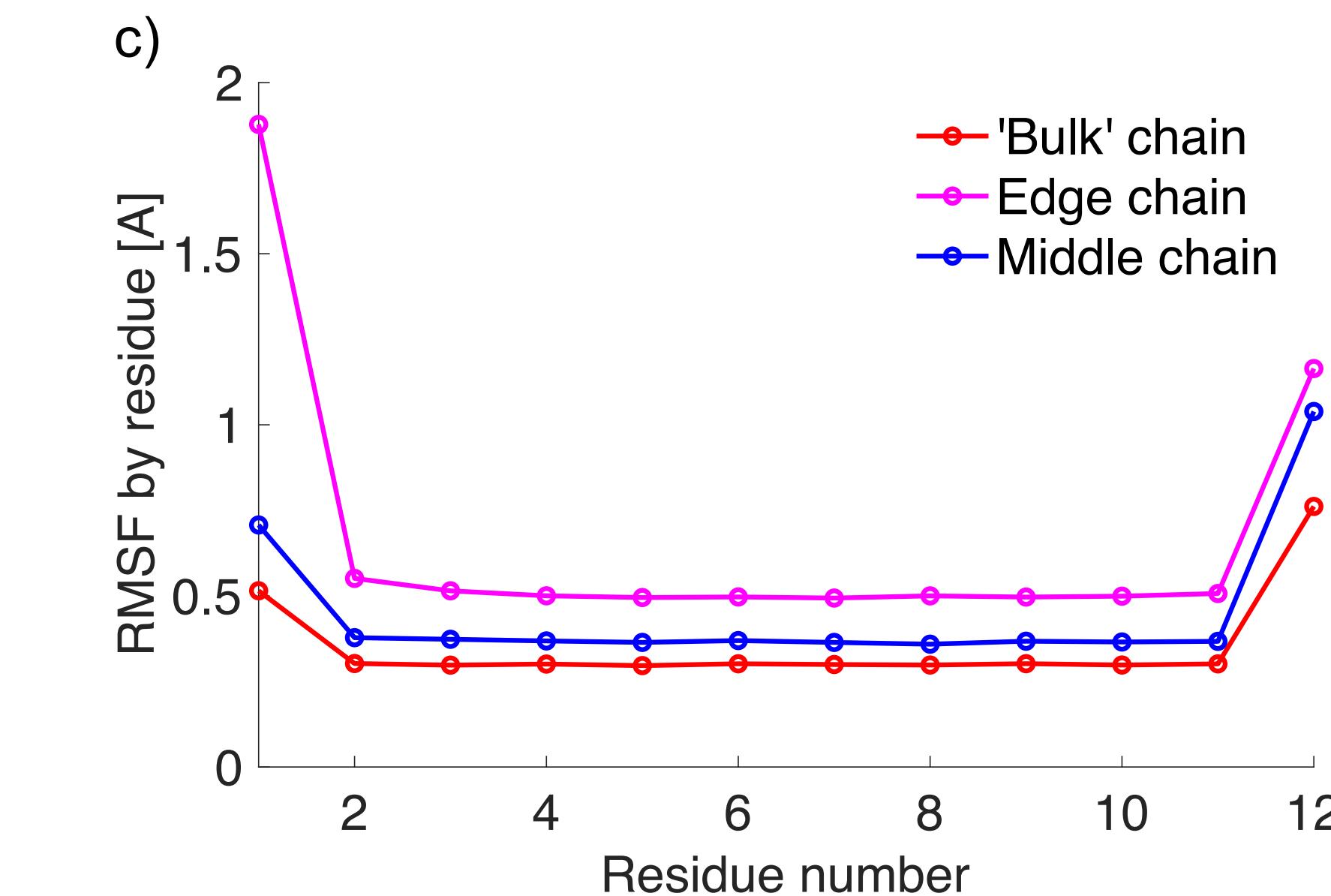
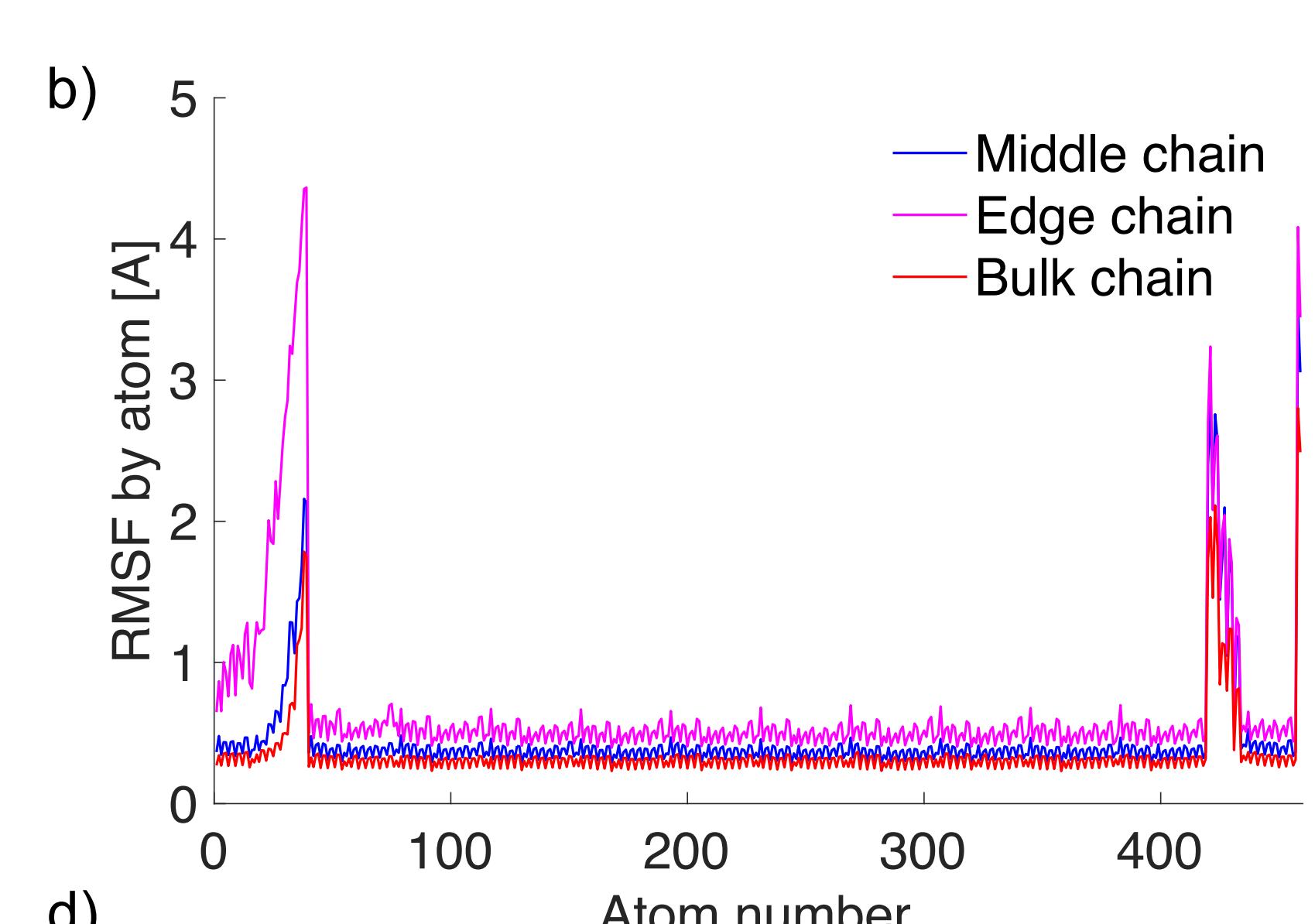
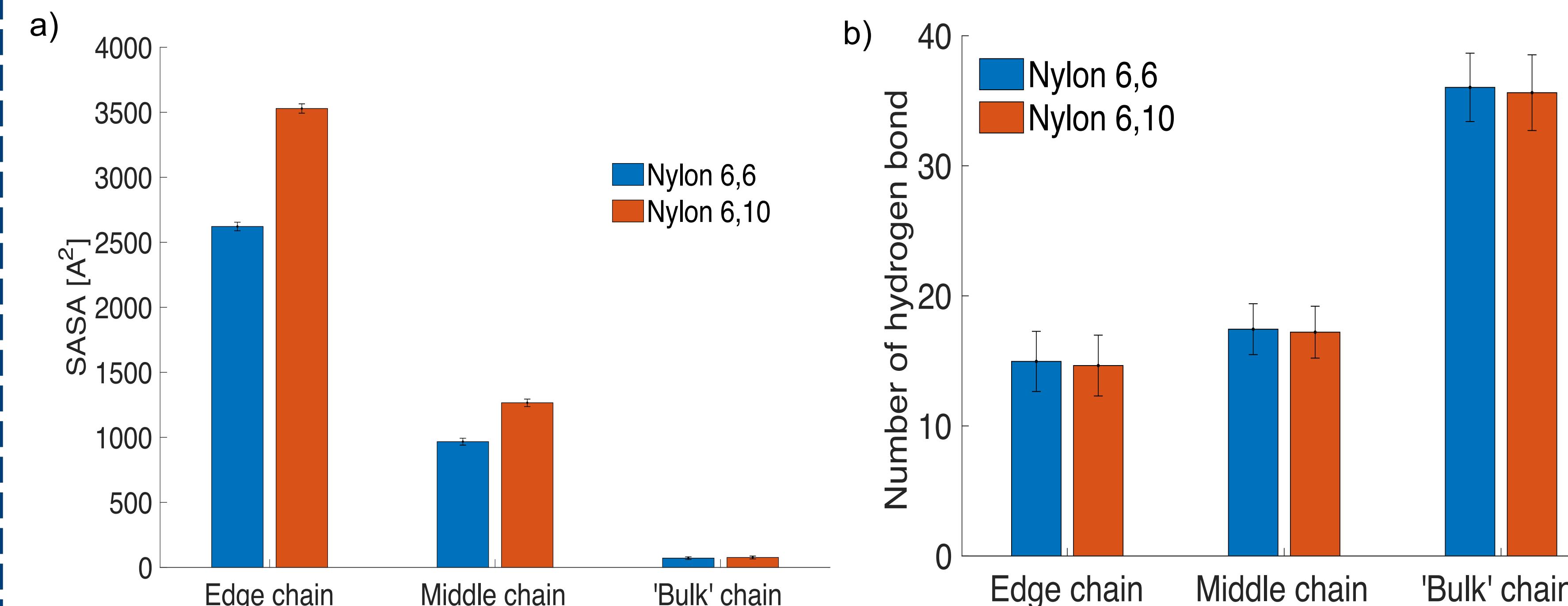


Fig 5: a) Snapshot of surface diagram of Nylon 6,6 crystal highlighting chains of interest: "Bulk" chain(red), edge chain(magenta) and middle chain(blue). b) Root mean square fluctuations by atom in Nylon6,6 crystal. Root mean square fluctuations by residue in c) Nylon6,6 crystal and d) Nylon 6,10 crystal.

- Rapid equilibration and minimal deviation from the initial crystal structure are observed in RMSD graphs for both crystals.

SASA & Hydrogen Bond Analysis



- Edge chains are more exposed to water, and form fewer hydrogen bonds, while bulk chains are less exposed to water, and form more hydrogen bonds.

Conclusions & Future Work

- Two types of nylon crystals were modeled.
- During the MD simulations, polymer crystals maintained their structure, only end caps showed high fluctuations.
- Bulk chain and middle chain formed more hydrogen bonds with the surrounding chains than edge chains.
- Expand the work to different types of nylons and calculate the free energy of decrystallization for these systems.

References

- Beckham et al. - The Journal of Physical Chemistry B – 2011
 Beckham and Crowley - The Journal of Physical Chemistry B – 2011
 Payne et al. - The Journal of Physical Chemistry Letters - 2011

