Characterizing Variation of PSII Water Channels Between Cyanobacteria and Higher Plants

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Abstract

- Water channels bring substrate water into the Oxygen Evolving Complex (OEC) and remove product protons to the lumen.
- Photosystem II (PSII) water channels have been well studied in cyanobacteria with 3 channels characterized.
- MCCE was used to trace hydrogen bond networks in *Pisum sativa* PSII and compare it with earlier studies of *T. vulcanus* PSII.
- **Conclusions**: Near the OEC the water chains are remarkably conserved in Pea but the end of the 3 previously characterized channels seems not to be the same found in *T. vulcanus.*
- Calculations are preliminary as they do not have all waters included. This leads to breaks in the chains.

Background

- Water is a primary reactant for oxygenic photosynthesis.
- Water passes through channels, from the lumen to the oxygen evolving complex to be split, using light energy, into oxygen, protons, and electrons, storing the energy for downstream reactions.
- PSII is susceptible to water limitation, as water is both a solvent and substrate
- Water limitation is a growing concern in agriculture, which has led to reduction and loss of crop yields.
- Water limitation has been largely studied in the physiology of plants, but little has been done at the protein level of PSII
- The end goal is to characterize water dynamics through PSII in higher plants.

Methods

- Multi-Conformational Continuum Electrostatics (MCCE)
- Compare cyanobacteria and higher plant PSII water channels
  - *Thermostichus vulcanus* (PDB_ID: 4UB6) (*T. vulcanus*)
  - *Pisum sativum* (PDB_ID:5XNL) (Pea)

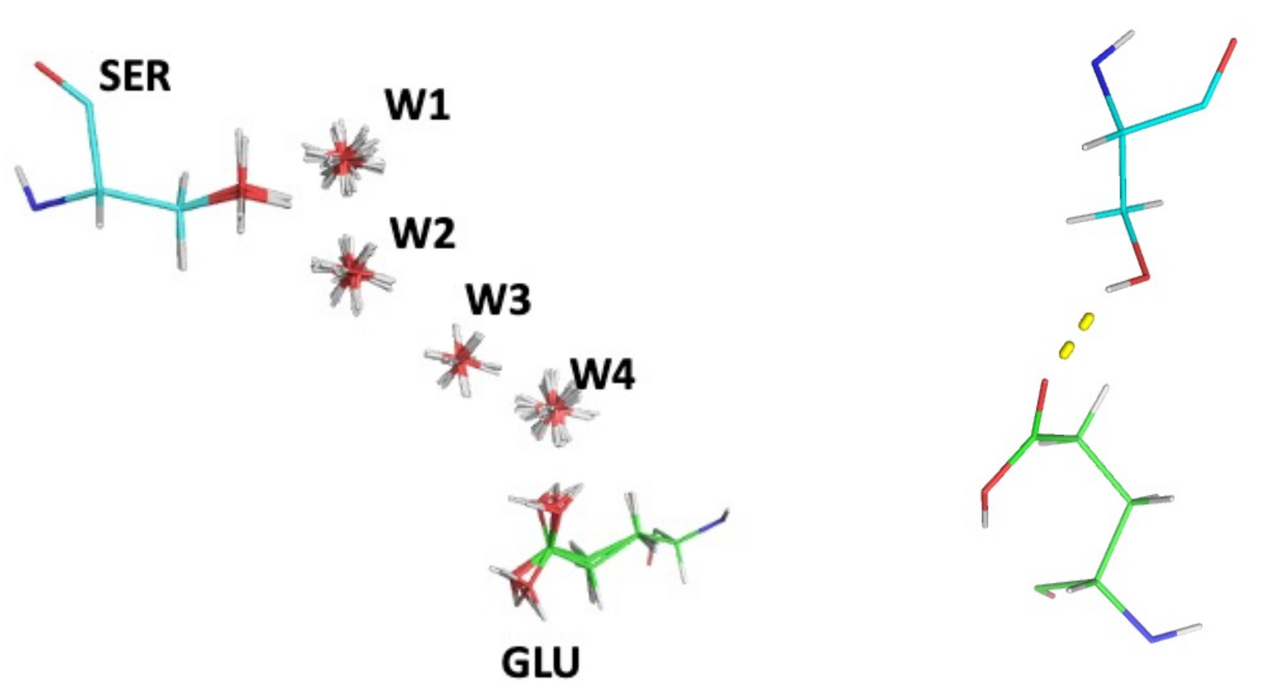

Figure 1.: MCCE samples multiple protonation and conformation states of side chains and waters. It finds the probability of conformations being selected that can make hydrogen bonds. The hydrogen bonds are organized into networks leading from the OEC

Acknowledgments

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Comparison of hydrogen bonded chains in T. vulcanus and Pea PSII

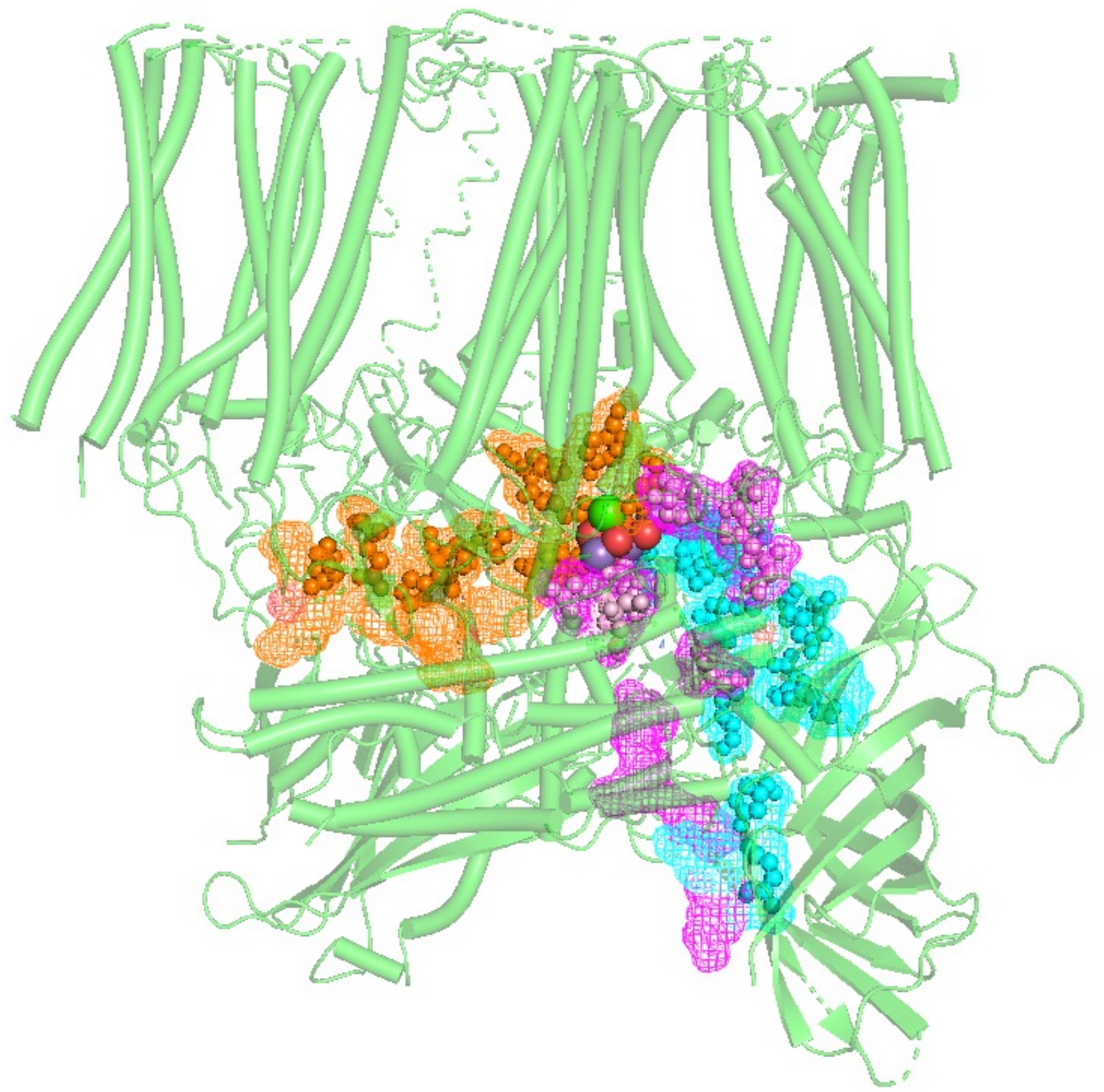

Figure 2: Structure of PS II *P. sativum* (PSB_ID: 5XNL). Water channels identified in Kaur et al. 2021 are identified in colored mesh, with OEC indicated by large spheres. Network residues in 5XNL are indicated by small spheres. Large (orange), narrow (magenta), and broad (cyan) channels.

List of residues 4UB6 → 5XNL		
Large	Broad	Narrow
SERP39 →THRC397	ASPM102 → ASPO110	SERA85 → THRA85
LYSP47 → LYSP170	ASPM99 →ASPO107	GLUO93**
LYSO104 → GLYO164	GLUM97 → GLUO105	ASPO96**
LYSP103 → PROQ32	GLUD313*	
	GLUD311*	
	ASPD222 →ASPD225	
	HISM228 → ASP227	
	ASPD309*	
	ASPD224 → ASPD227	
	LYSM188 → LYSO191	

Table Comparison of residues in channels in 4UB6 and 5XNL. Residues are an output of MCCE hydrogen bond network analysis. Single asterisks indicate shift in sequence position by one, double asterisks indicate no residue in analogous position in 5XNL. Arrows connect residues in 4UB6 (identified by Kaur) with 5XNL. .

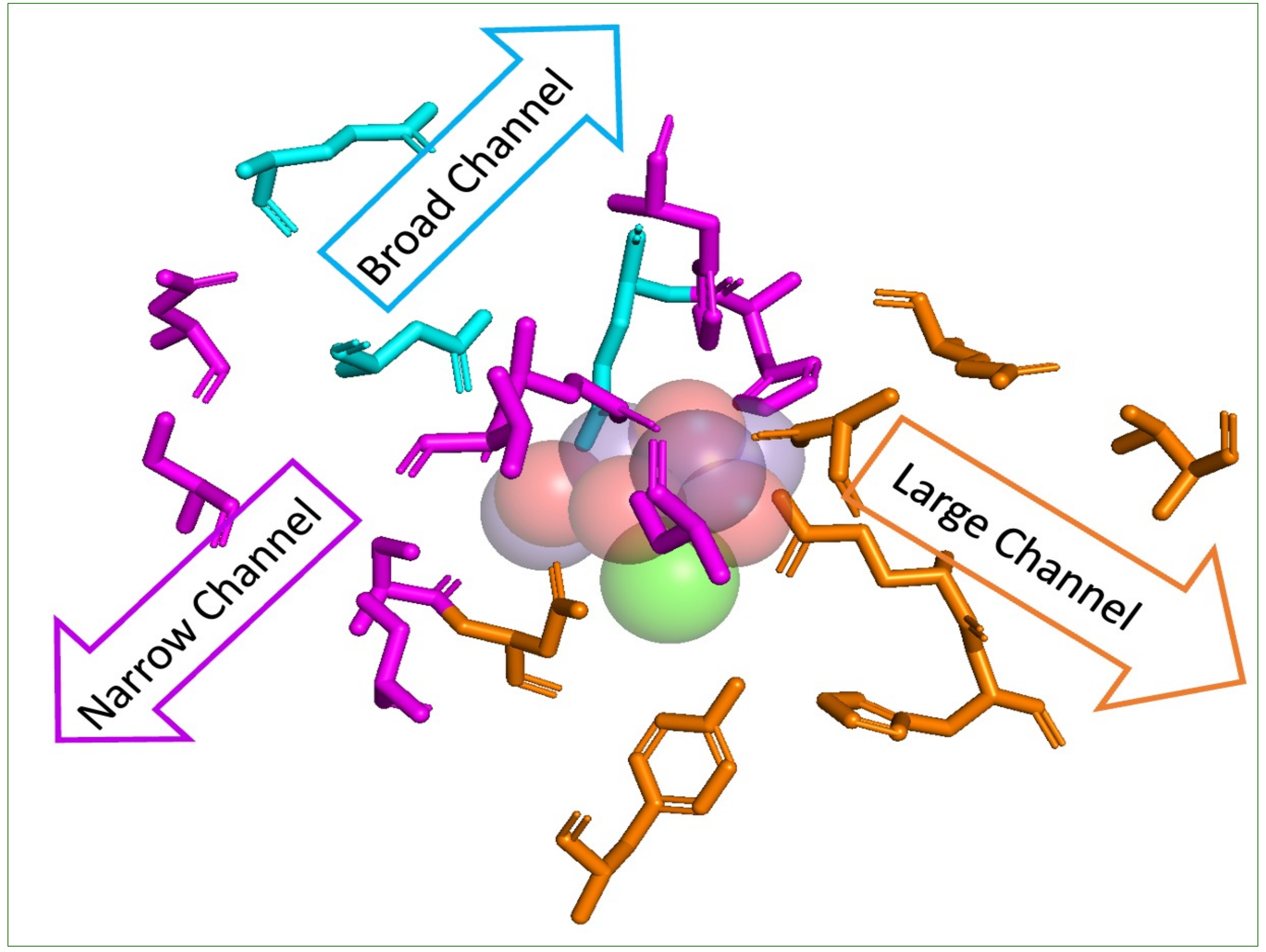

Figure 3: Residues surrounding OEC within a 10 Å radius. Residues present indicate overlap between 5XNL and 4UB6 structures. Channels are identified by large (orange), small (magenta), and broad (cyan). Residues within 10 Å of the OEC in the 3 *T. vulcanus* water channels are fully conserved in Pea.

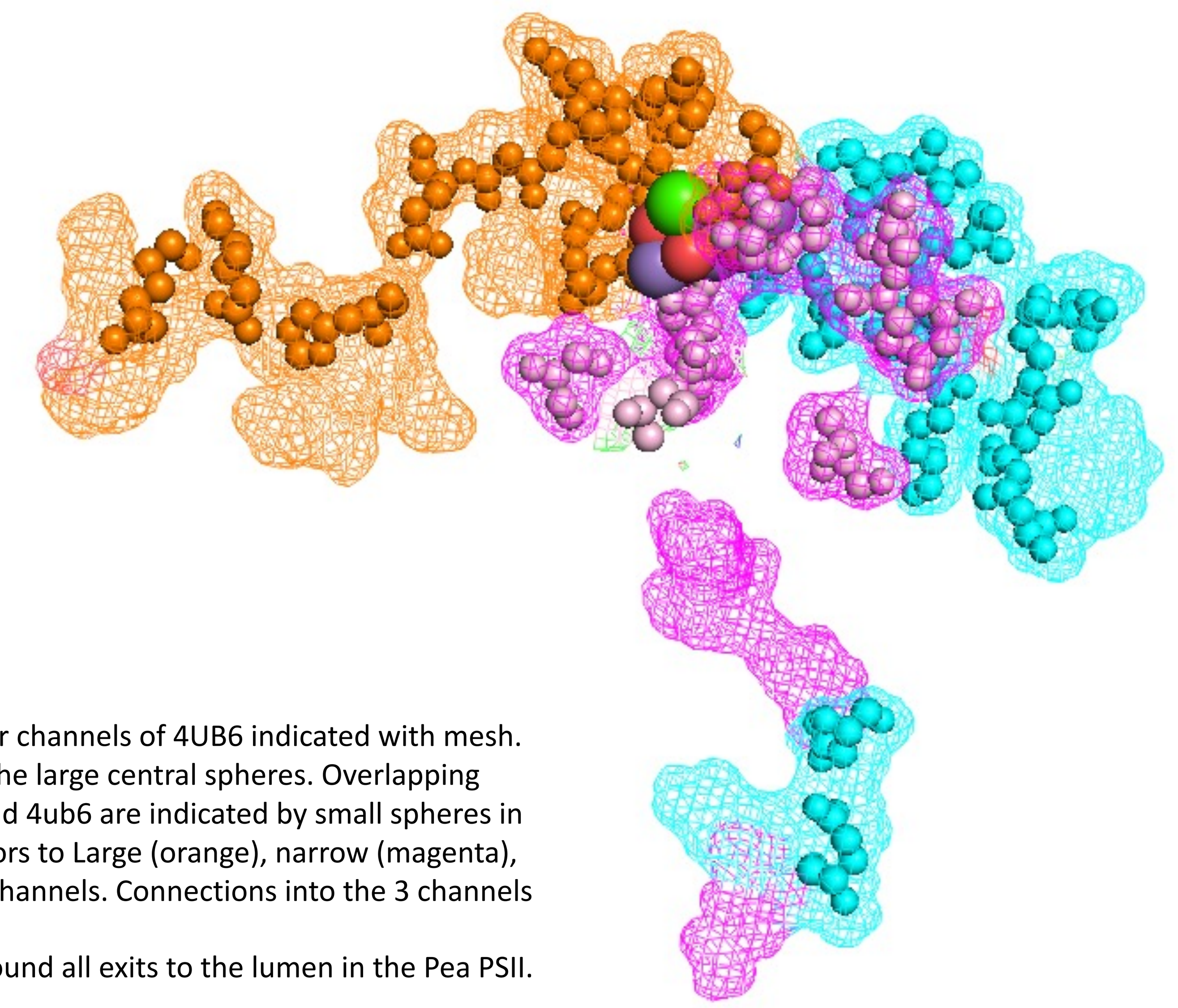

Figure 4: PSII water channels of 4UB6 indicated with mesh. OEC indicated by the large central spheres. Overlapping residues of 5xnl and 4ub6 are indicated by small spheres in corresponding colors to Large (orange), narrow (magenta), and broad (cyan) channels. Connections into the 3 channels are conserved.
We have not yet found all exits to the lumen in the Pea PSII.

Conclusion

- Overlap of residues that extend beyond the OEC core when comparing higher plants and cyanobacteria.
- High conservation of residues for all 3 channels.

Future Work

- Add water to calculations to fully connect the residues in the pea PSII networks
- Add more side chain conformations to find more connections.
- Use a reduced chemical potential for water in hydrated calculations to simulate drying and see if connections are broken.

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