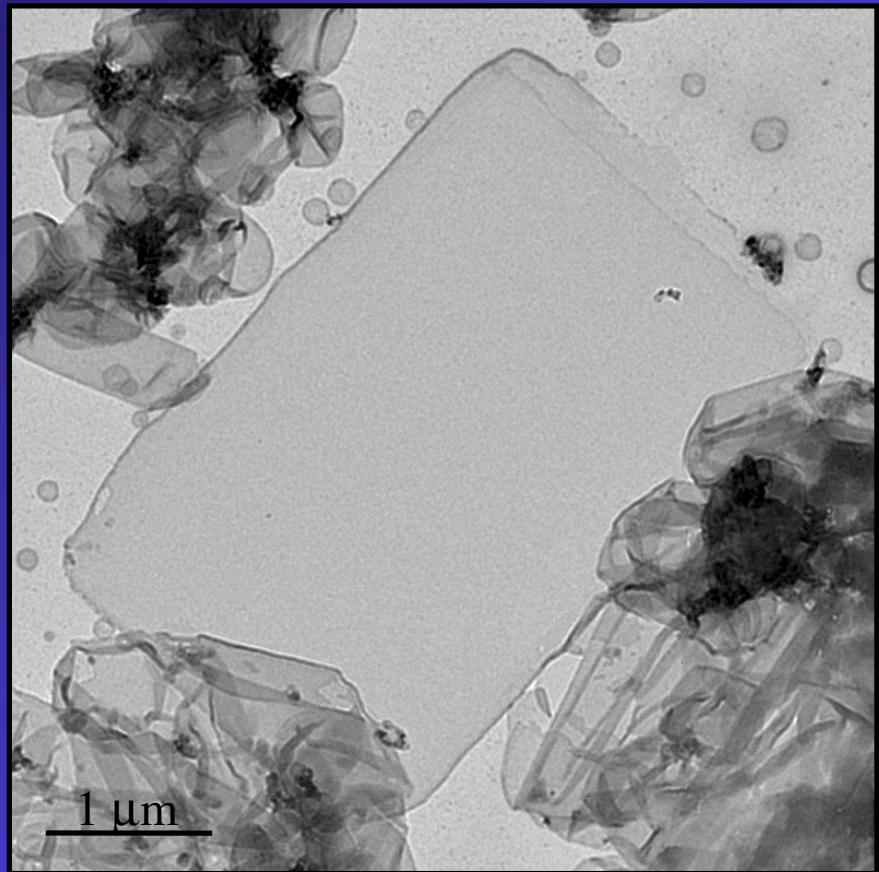
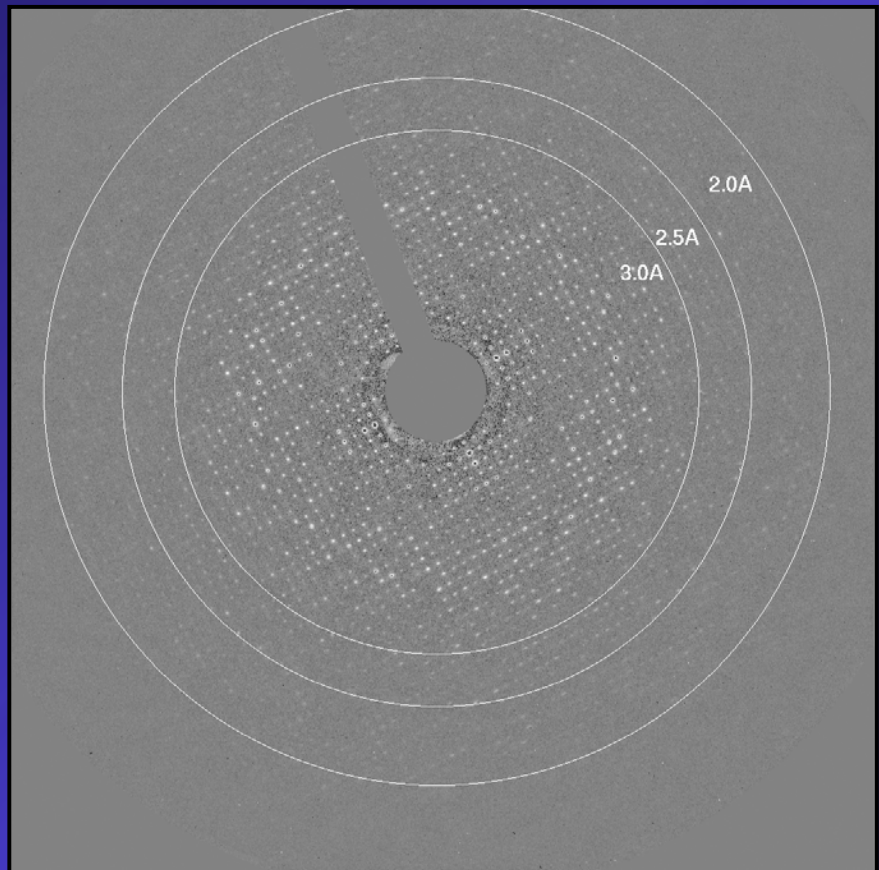




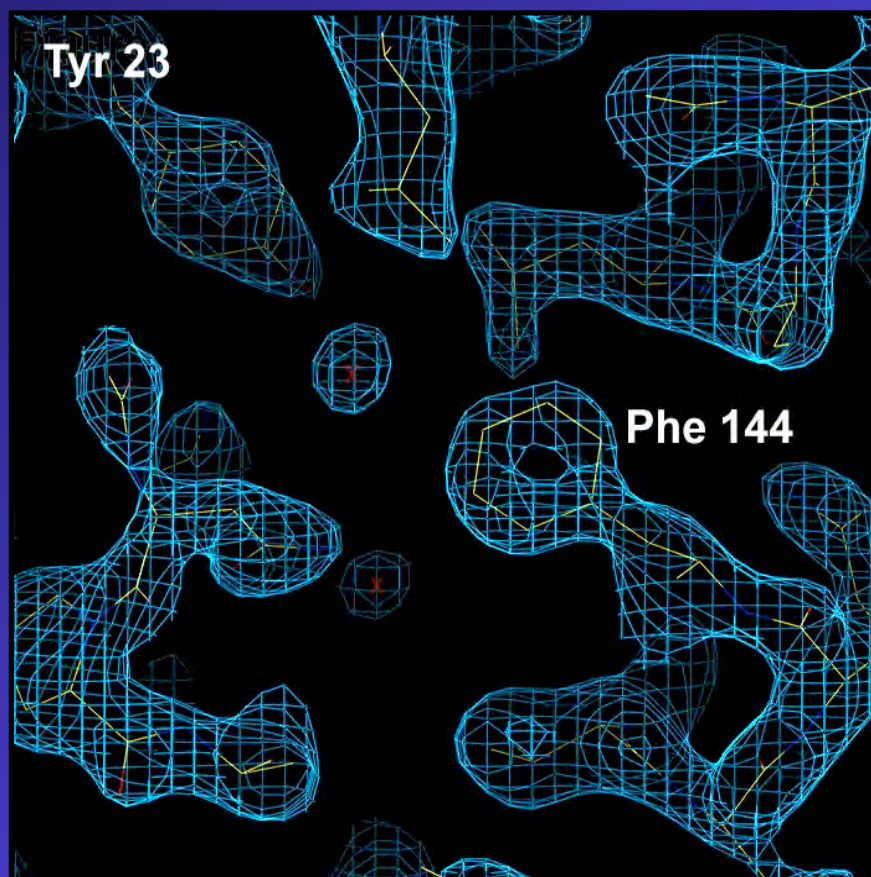
**Double-layered  
2D crystals  
of AQPO**



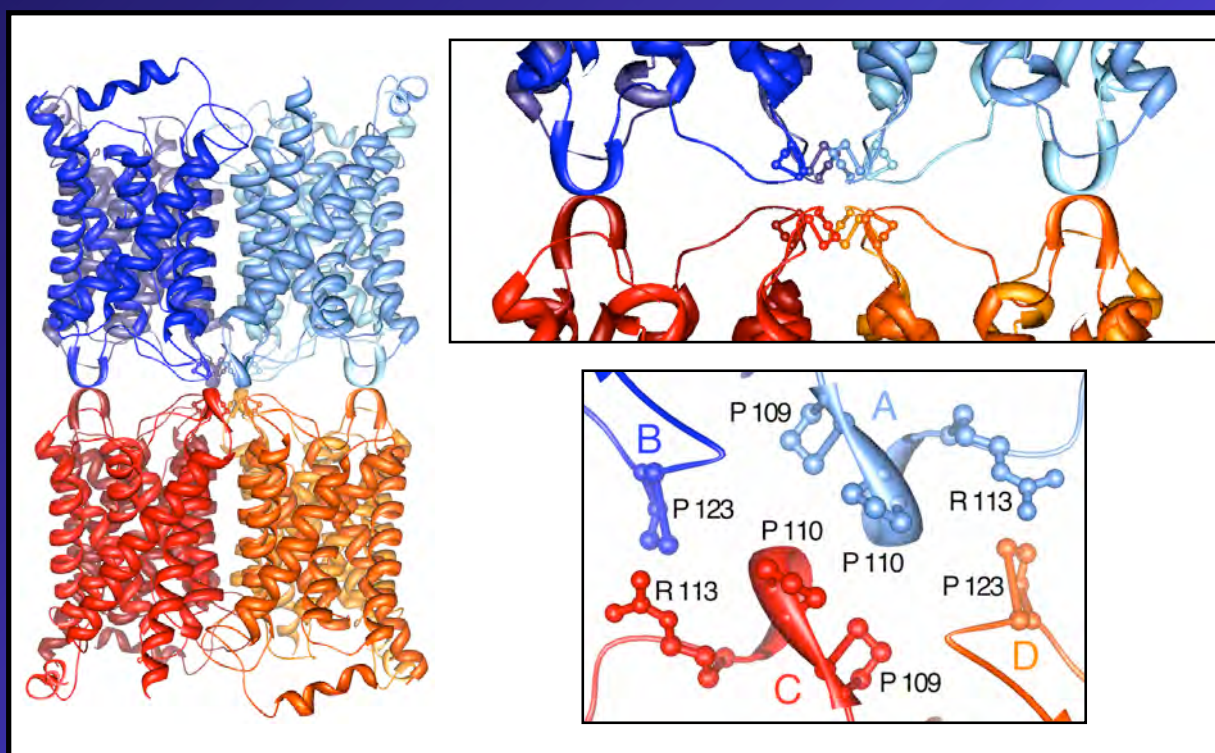
**Electron  
diffraction  
at liquid He  
temperature**



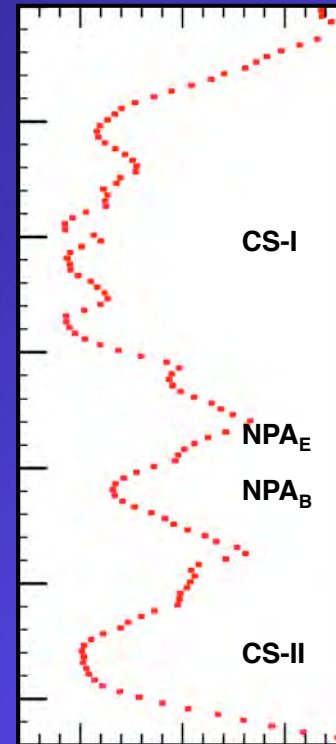
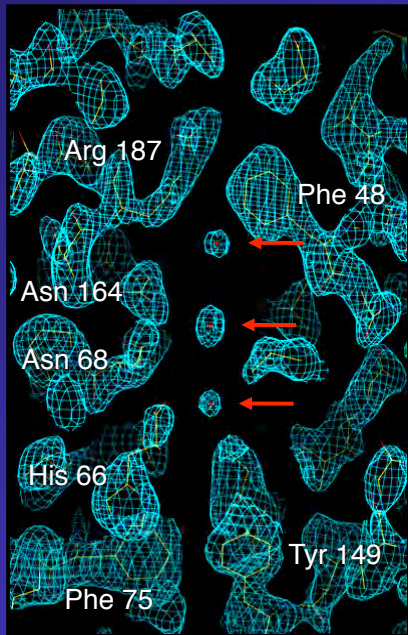
## The 1.9 Å density map



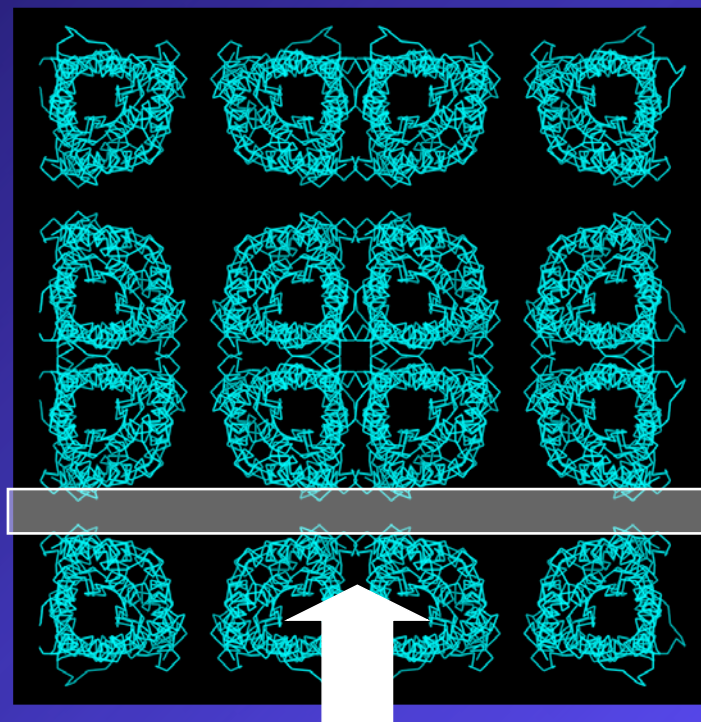
## Junction interactions



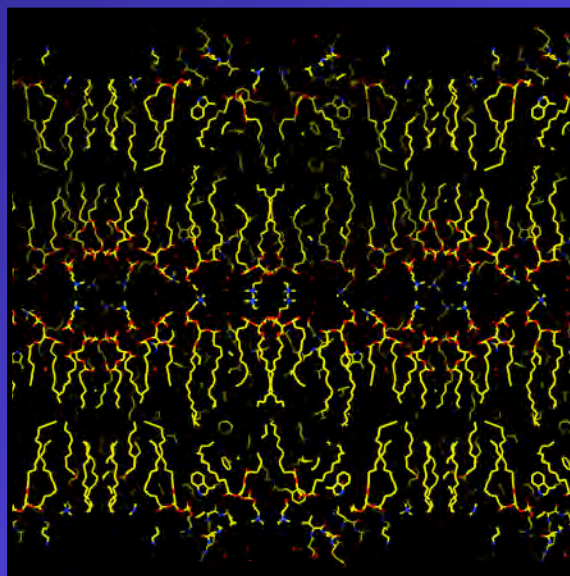
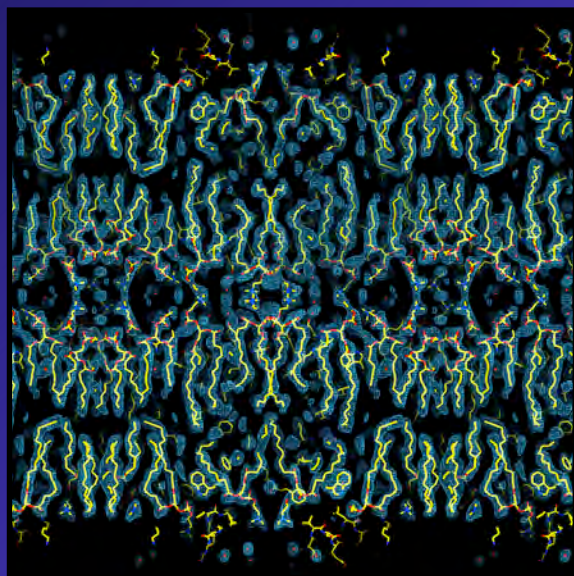
## The AQPO water pore at 1.9 Å resolution



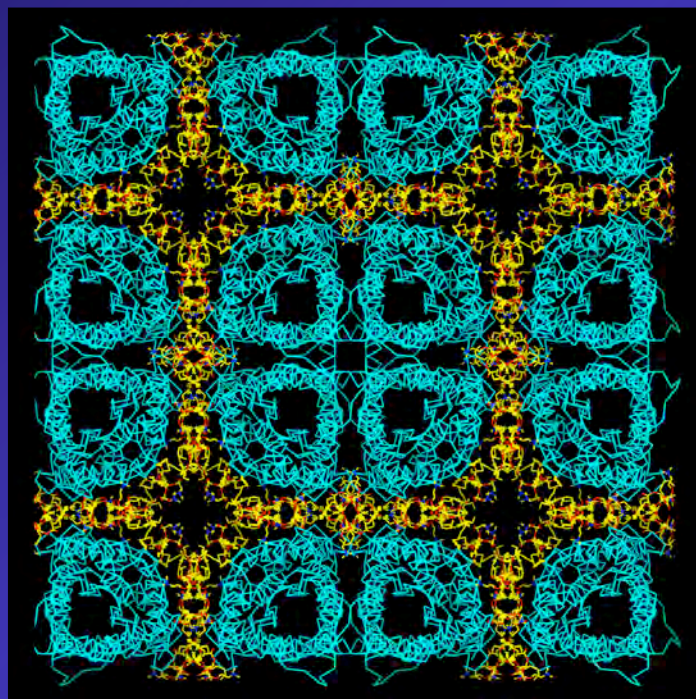
## The packing of AQPO in the 2D crystals



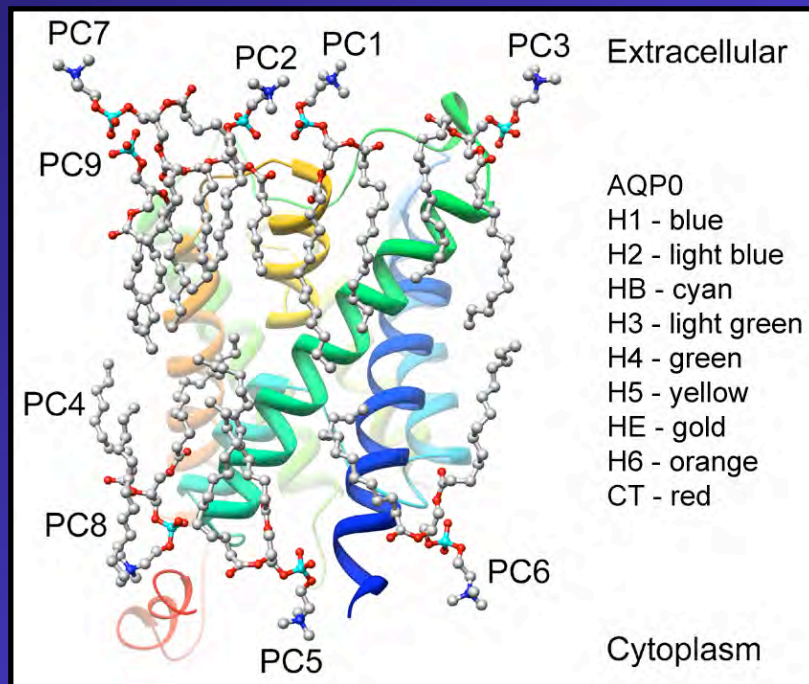
## The packing of AQPO in the 2D crystals



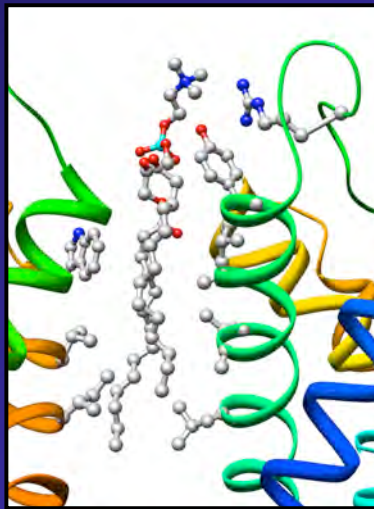
## The packing of AQPO in the 2D crystals



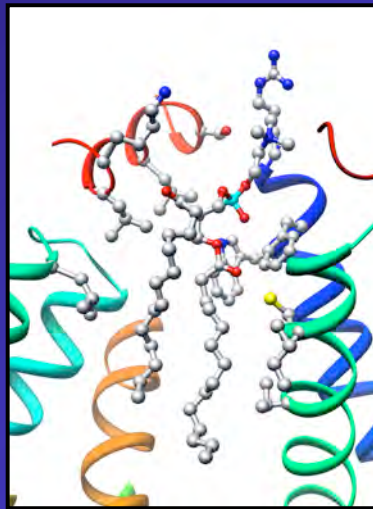
# The lipids surrounding an AQP0 monomer



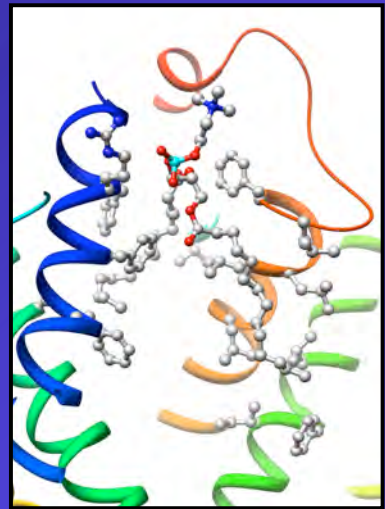
## Protein-lipid interactions



PC 1

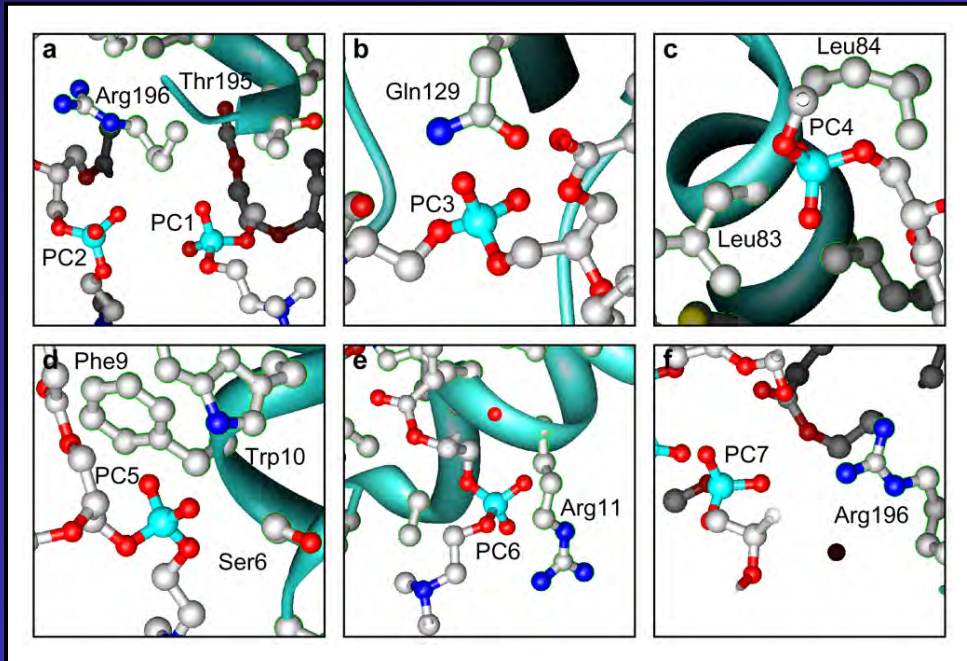


PC 5



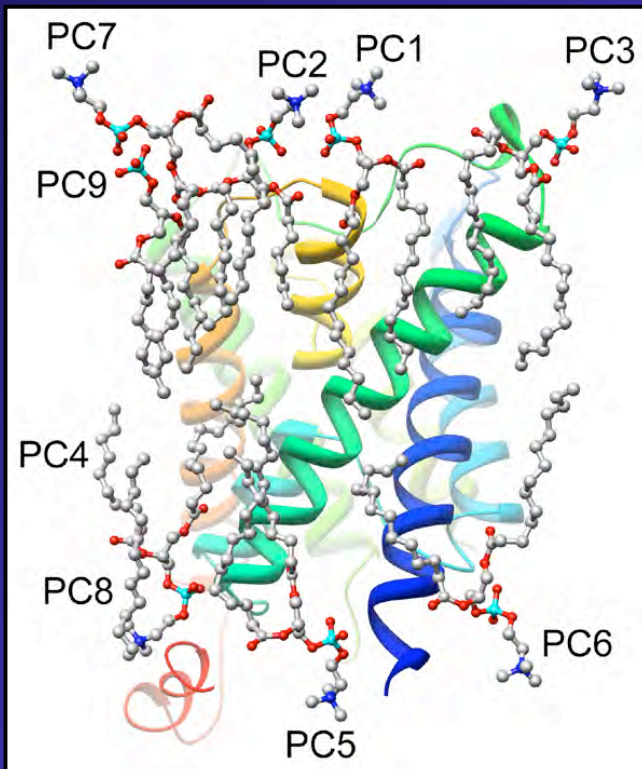
PC 6

# Lipid binding motifs



No obvious binding motif for PC phosphodiester group

# Protein-lipid interactions



## Different lipids

Head group interactions?  
Lipid-binding motifs?

Acyl chain positions?

Bilayer thickness?  
Acyl chain interactions?

Protein conformation?

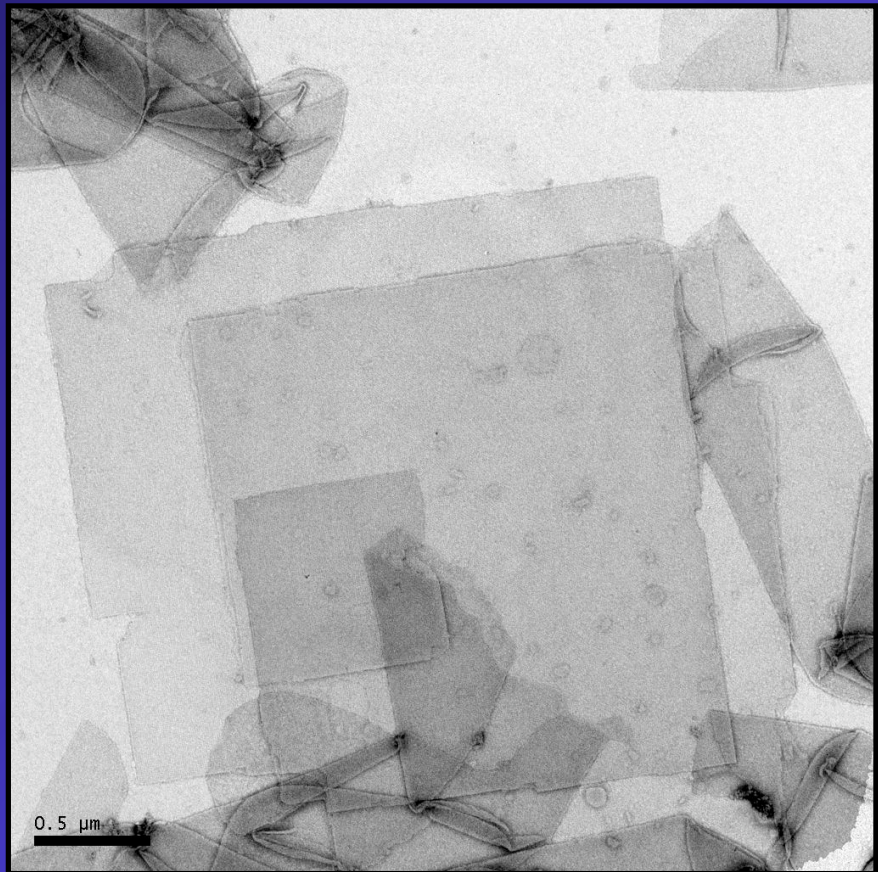


Rich Hite

## Double-layered 2D crystals of AQP0

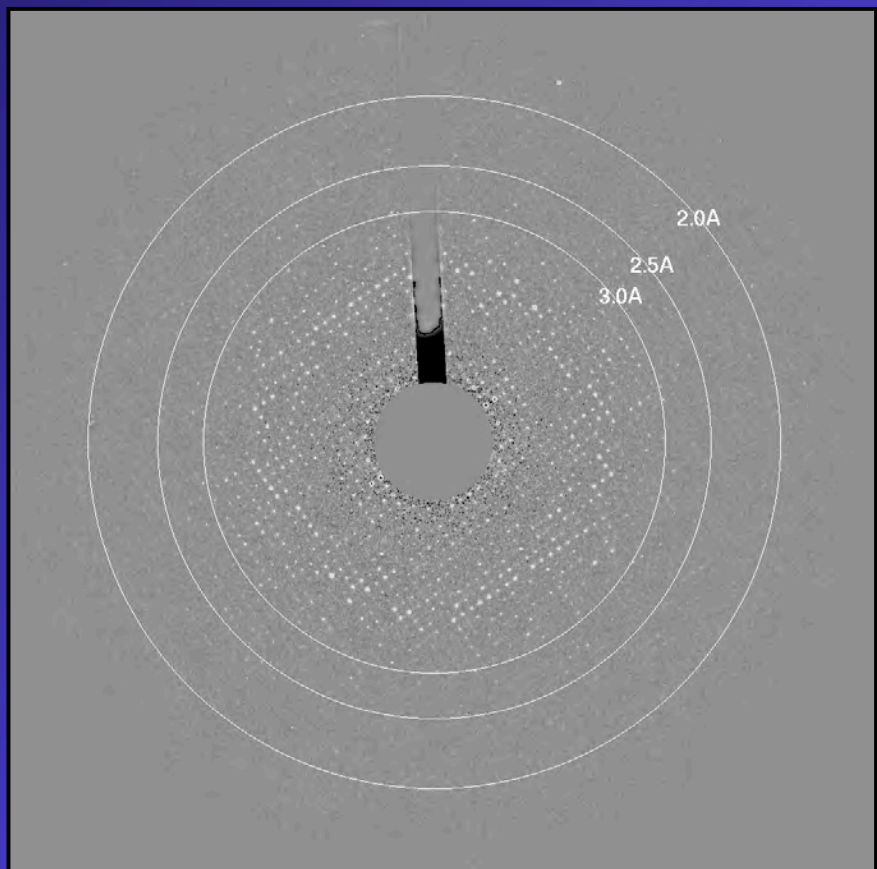
AQP0 in  
*E. coli* polar lipids

67% PE  
23% PG  
10% cardiolipin



## Electron diffraction at liquid He temperature

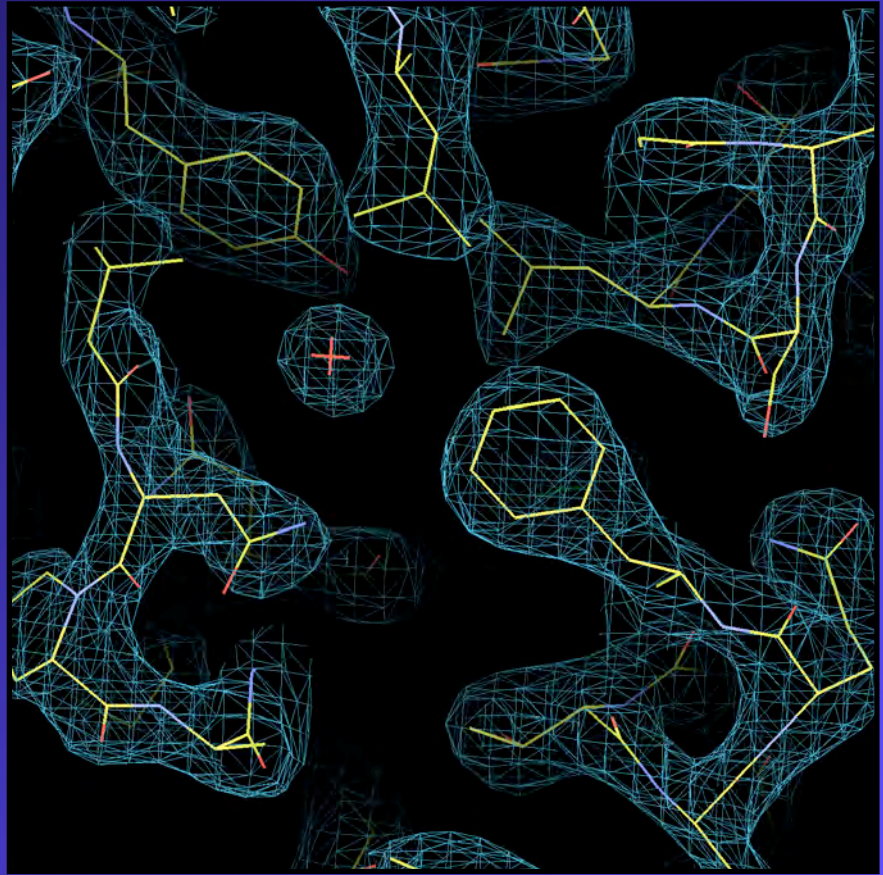
AQP0 in  
*E. coli* polar lipids



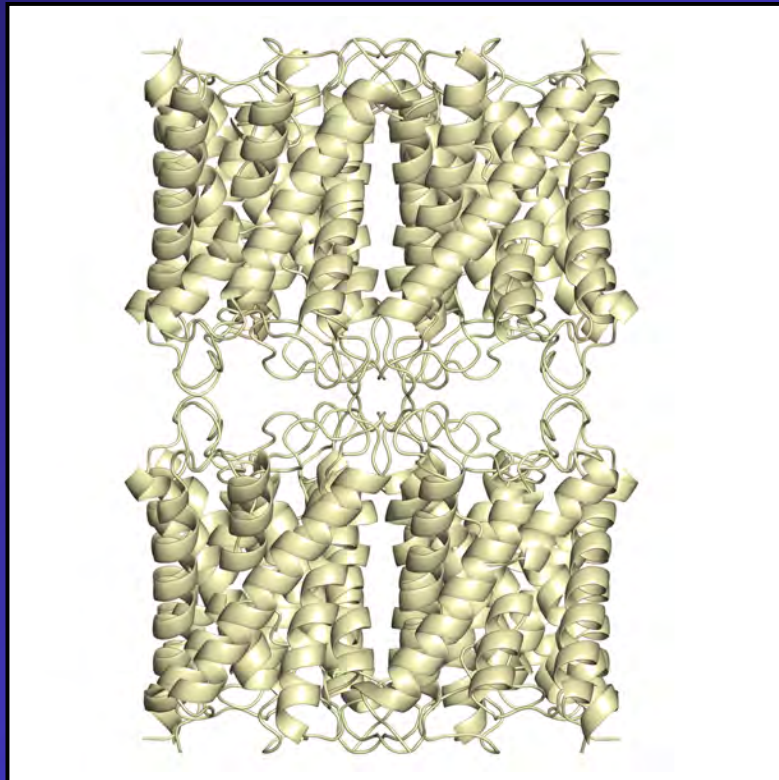


## The 2.5 Å density map

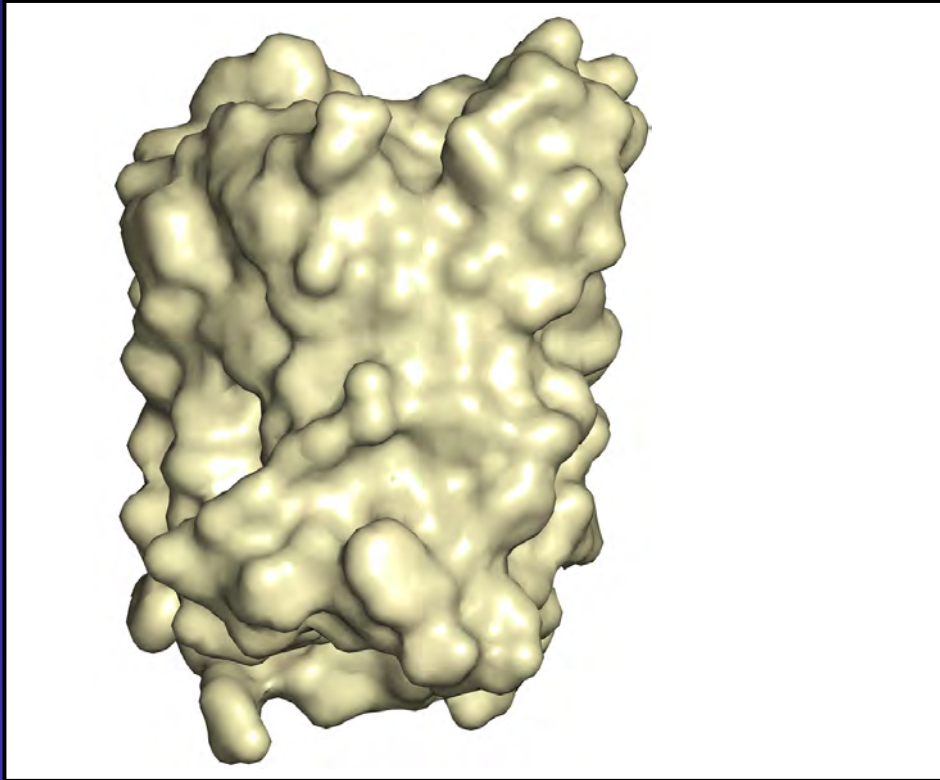
AQP0 in  
*E. coli* polar lipids



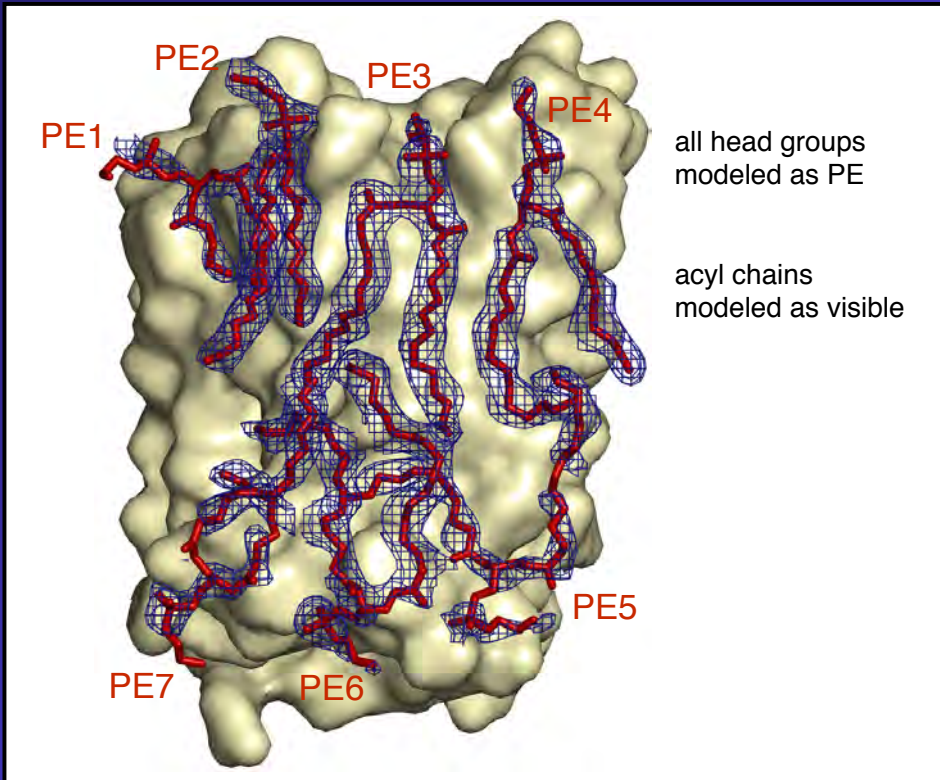
## Model of the AQP0 junction in EPL



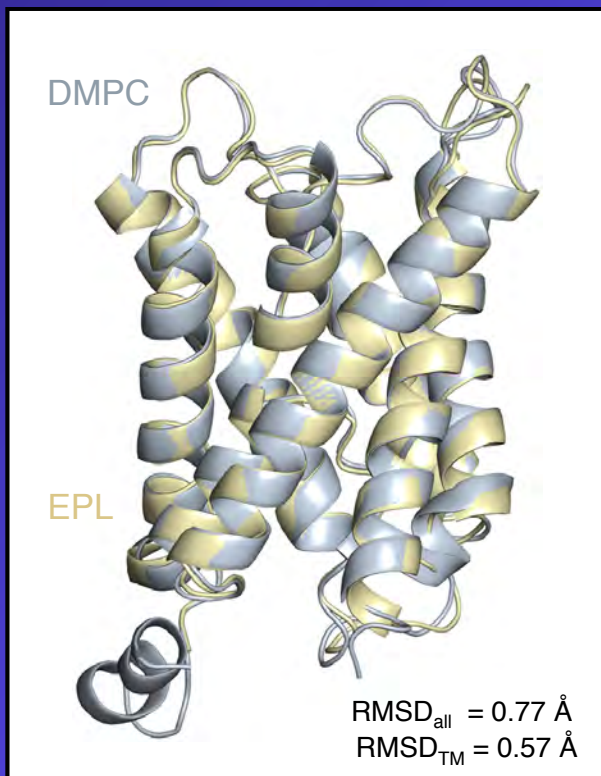
## EPLs surrounding AQPO



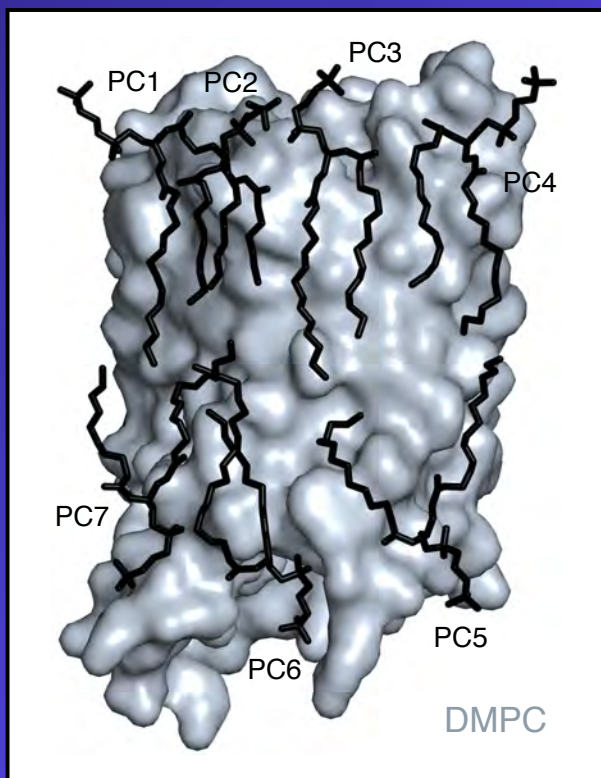
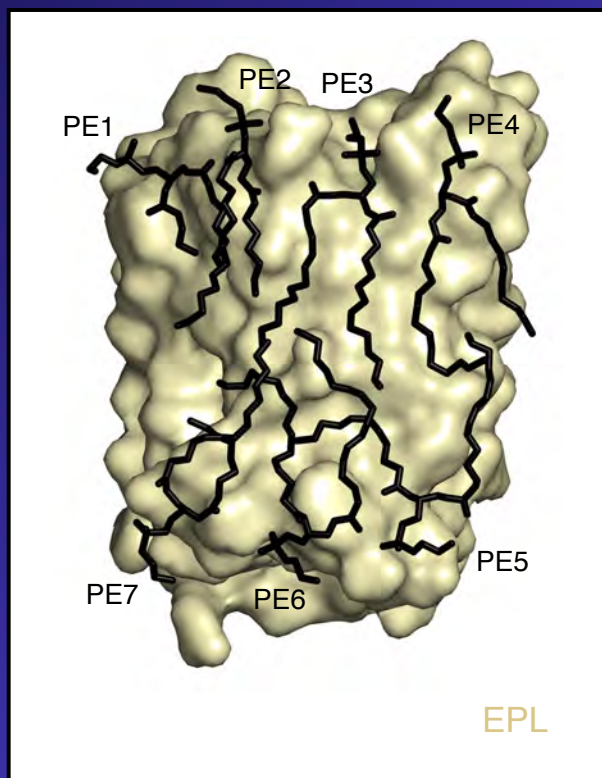
## EPLs surrounding AQPO



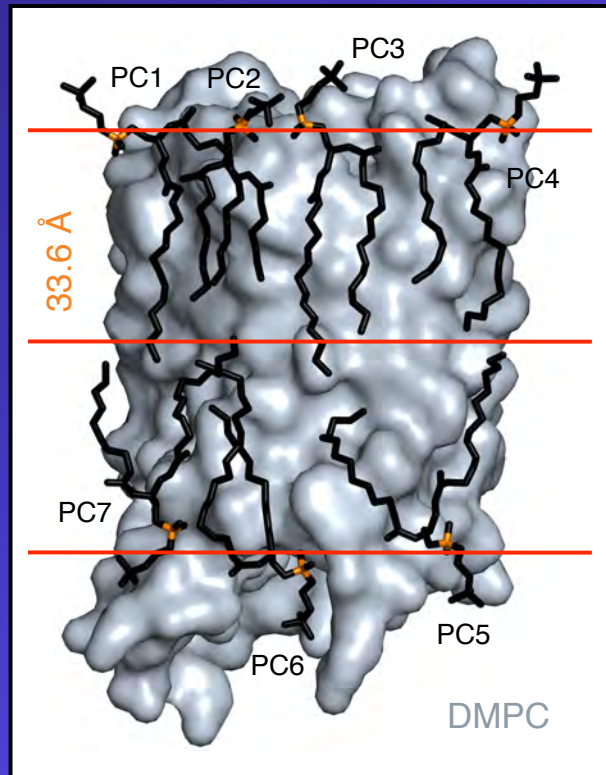
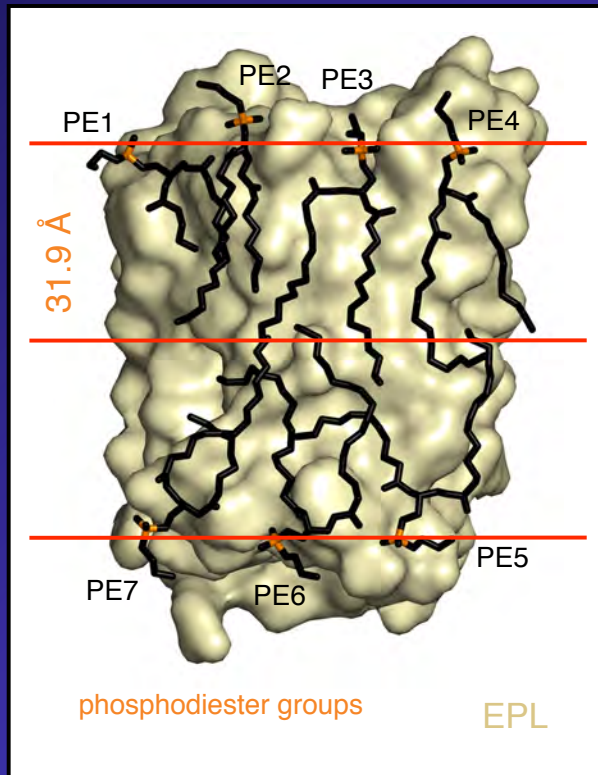
## AQPO in EPL and DMPC



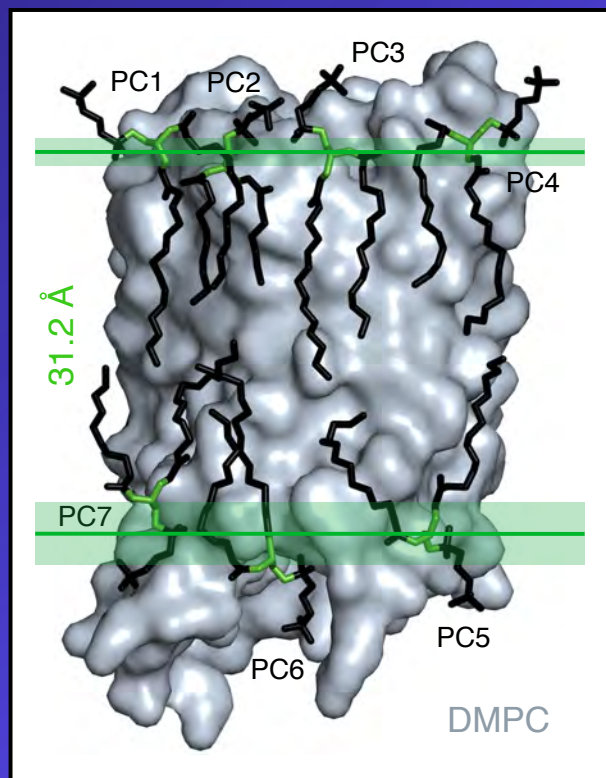
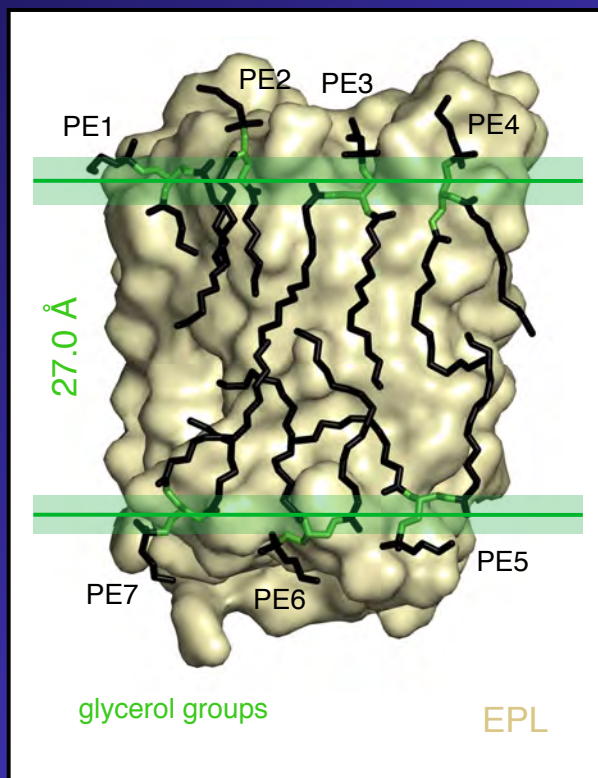
## AQPO interactions with EPL and DMPC



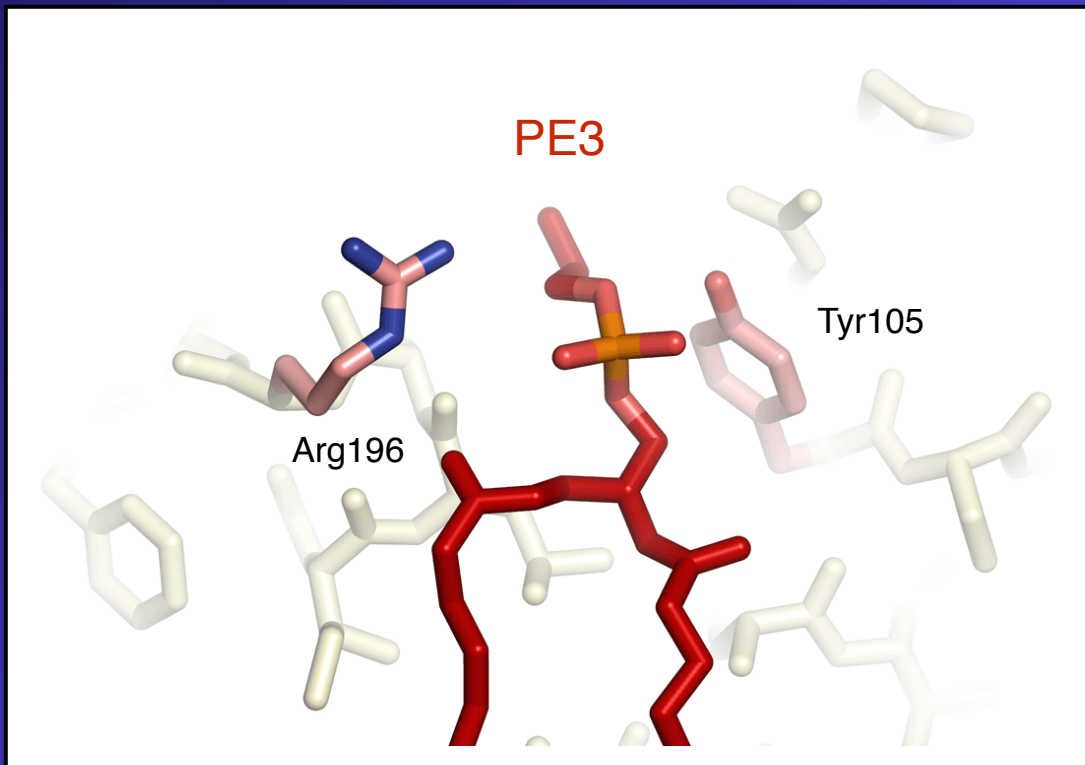
## AQPO interactions with EPL and DMPC



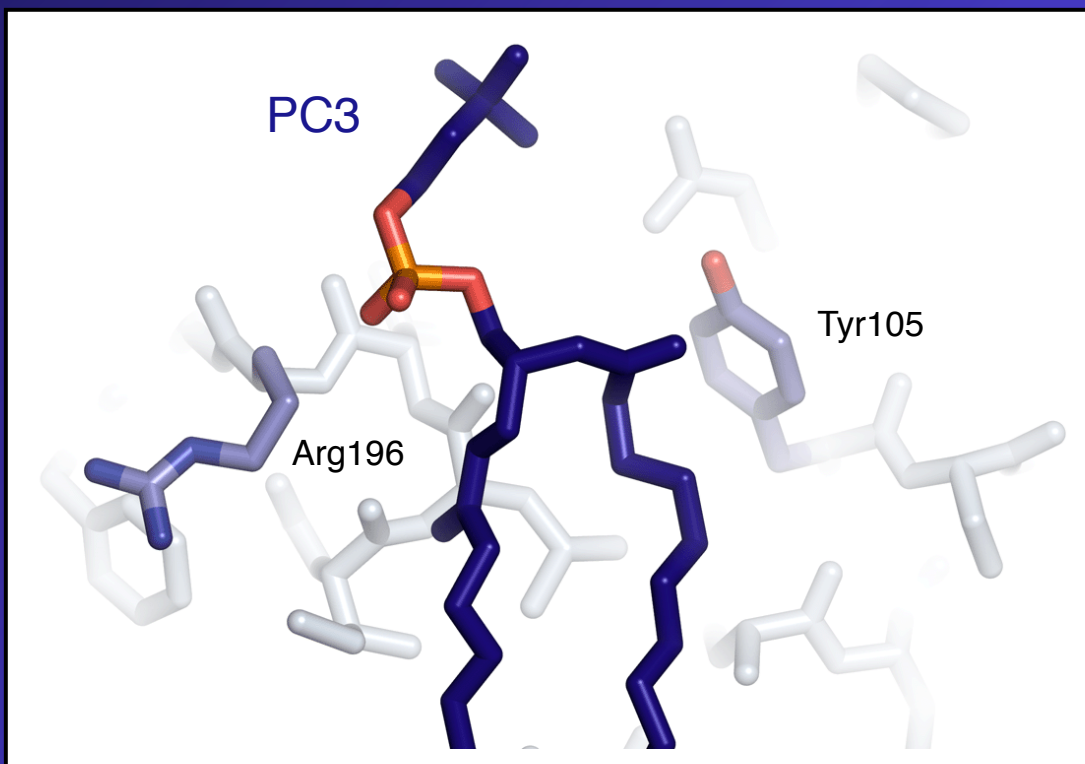
## AQPO interactions with EPL and DMPC



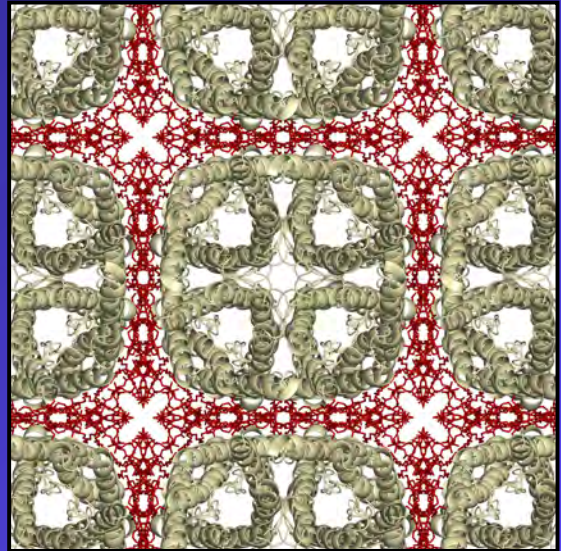
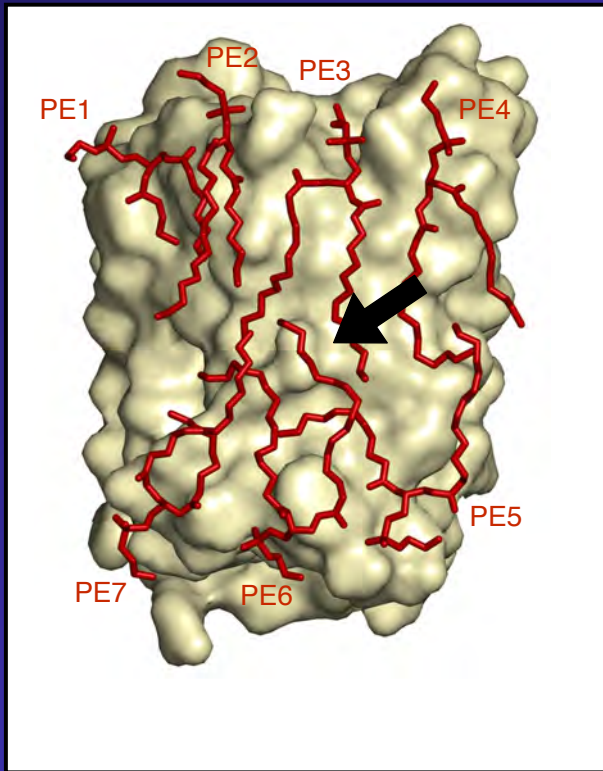
## Head groups and lipid binding motifs



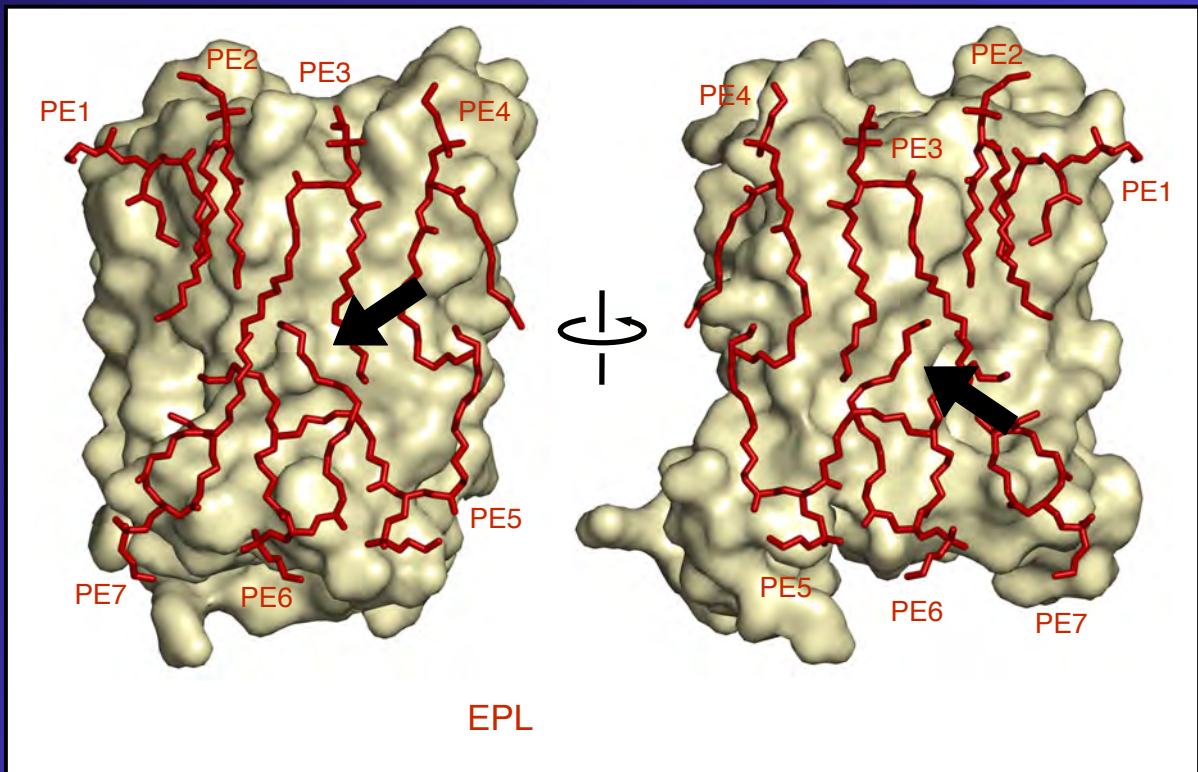
## Head groups and lipid binding motifs



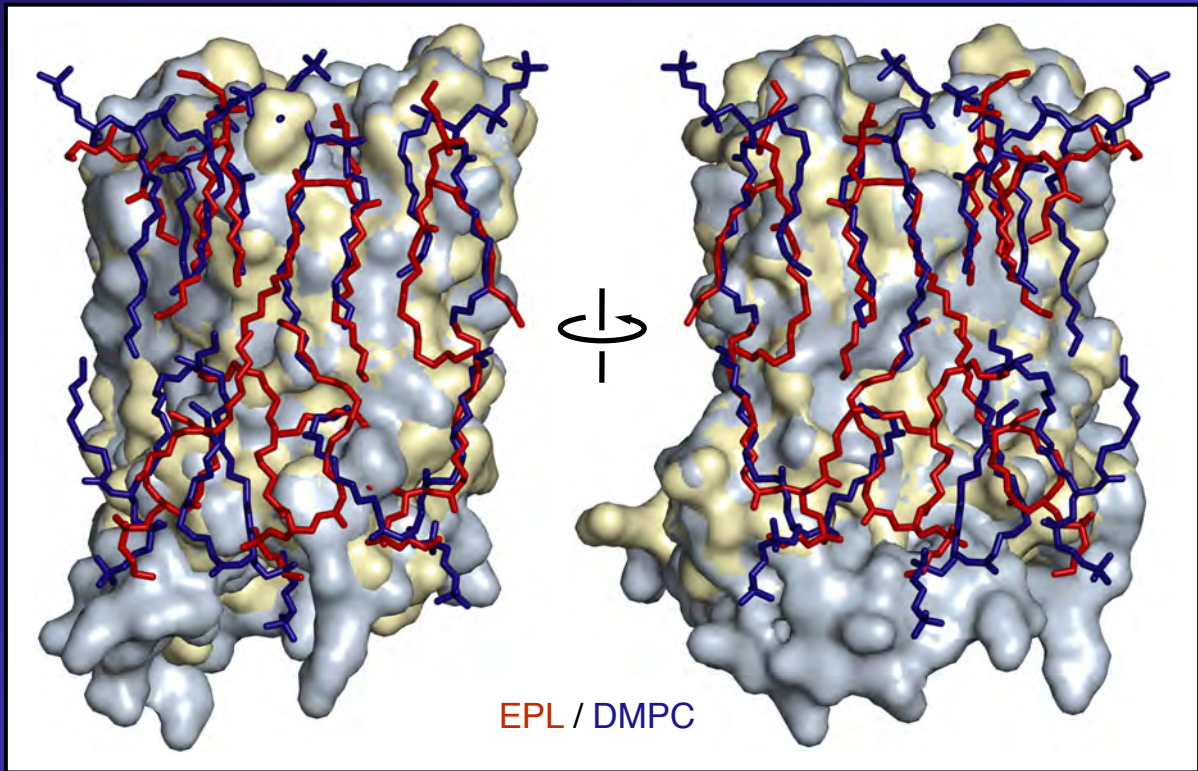
# Acyl chain positions



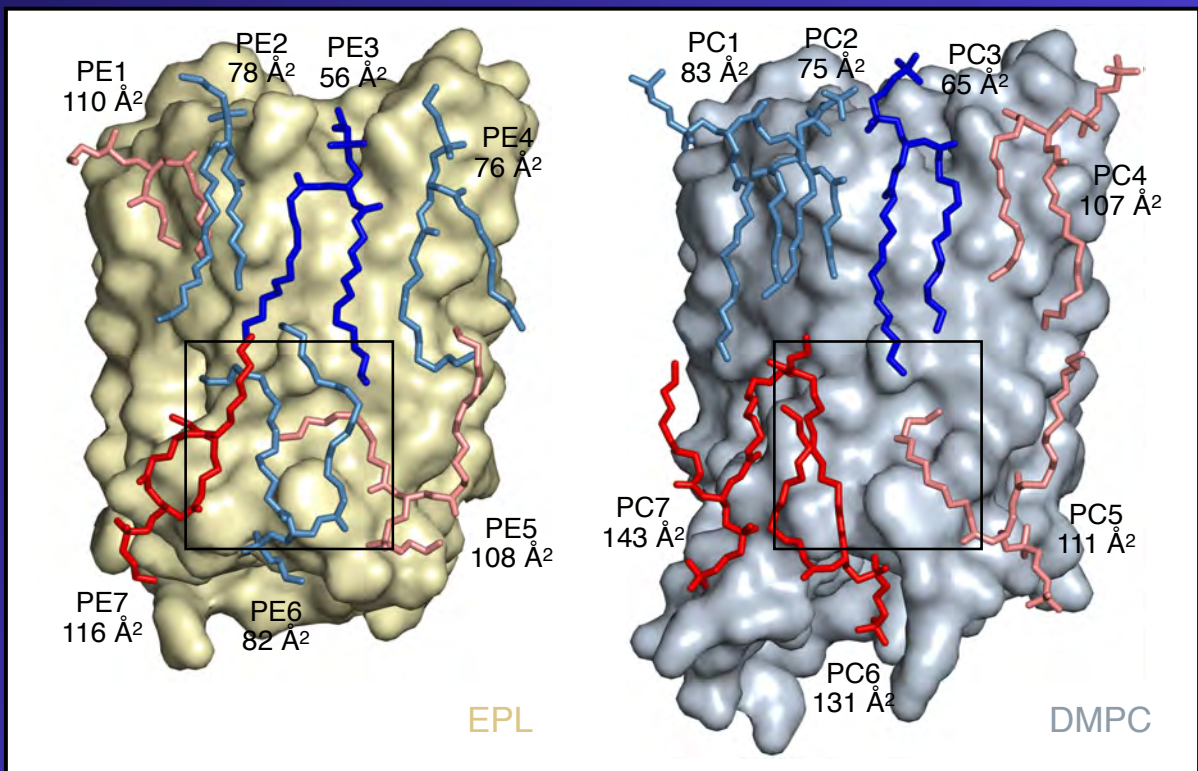
# Acyl chain positions



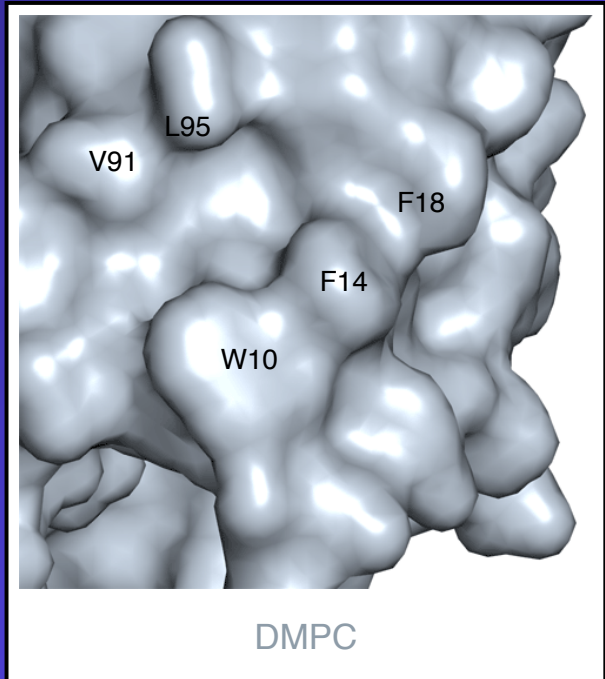
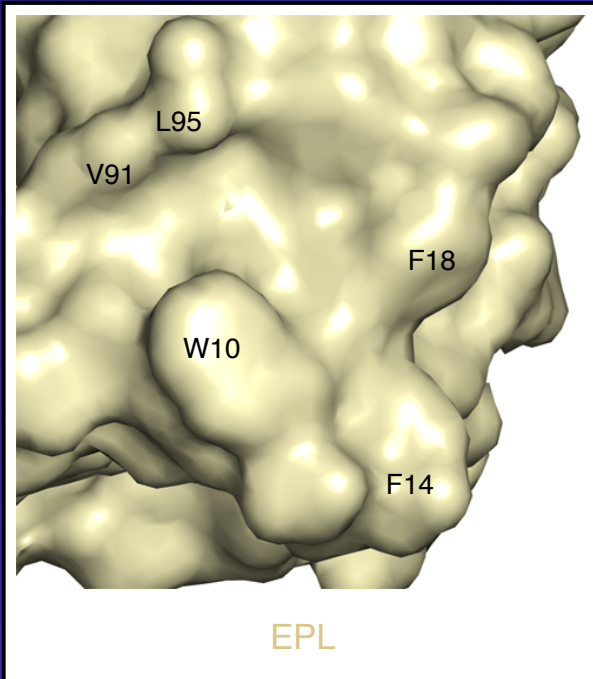
## Acyl chain positions



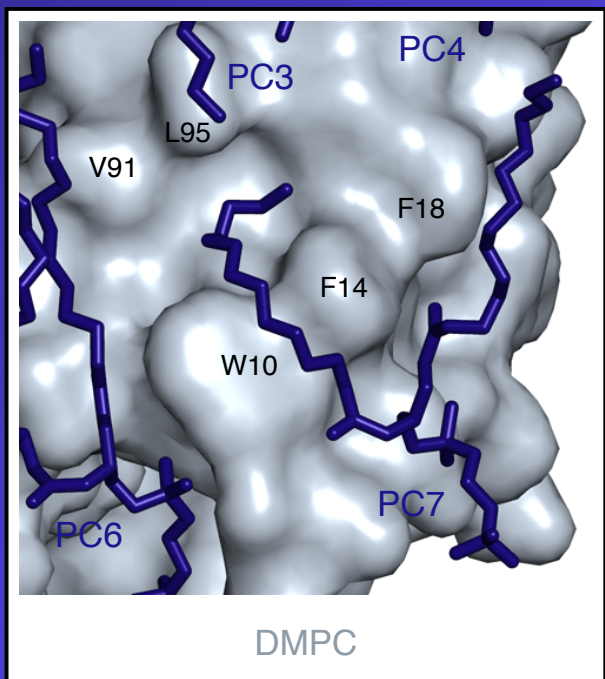
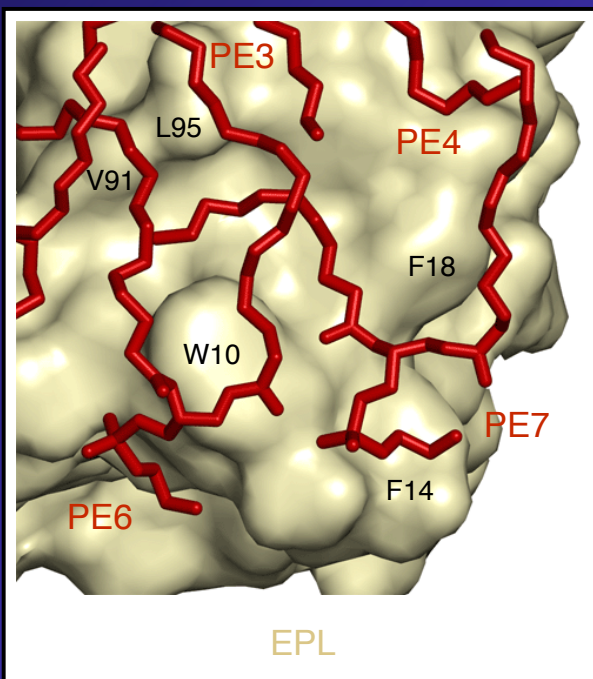
## Acyl chain positions



## Acyl chain positions

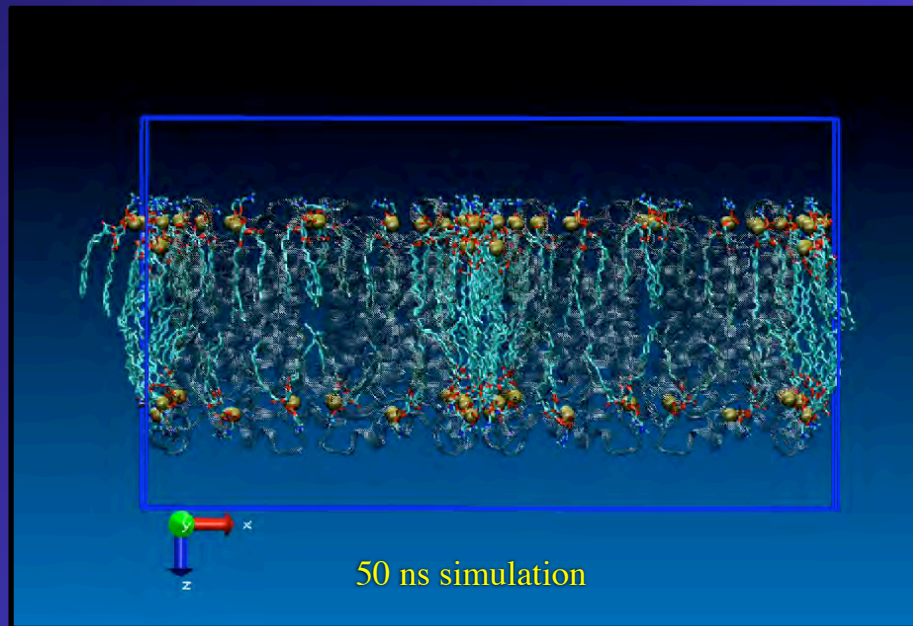


## Acyl chain positions





## Molecular dynamics calculations



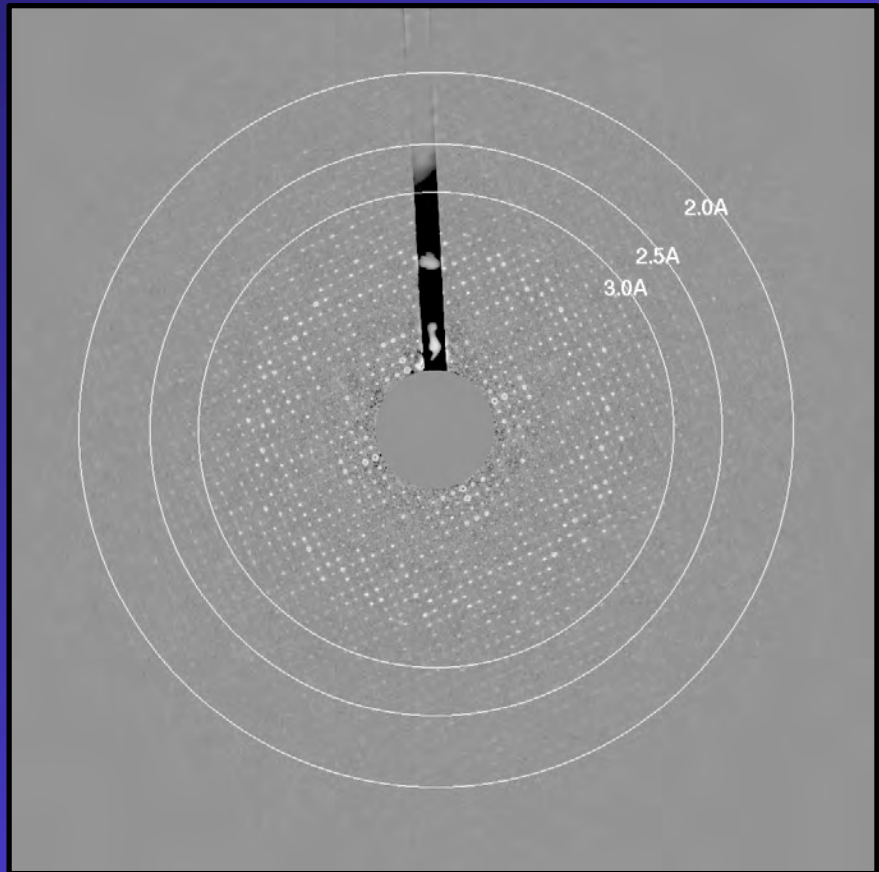
Rodolfo Briones, Camilo Aponte & Bert de Groot  
MPI for Biophysical Chemistry (Göttingen)

## Conclusions

- 1. lipid positions defined by acyl chains**
  - filling in the gaps in protein surface
- 2. further interactions by lipid headgroups**
  - may lead to stronger (specific) binding
  - may define lipid selectivity
- 3. AQP0 forms well-ordered 2D crystals with very different lipids**
  - should allow systematic analysis of lipid-protein interactions

# Electron diffraction at liquid He temperature

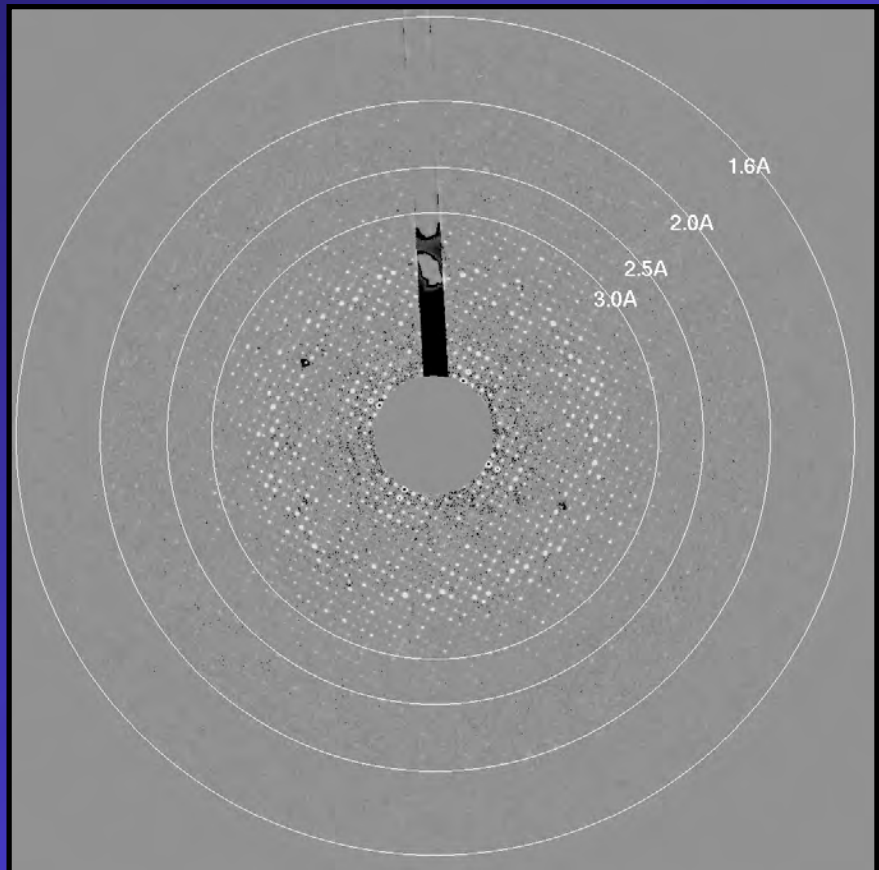
AQP0 in  
SOPE



Andreas Schenk

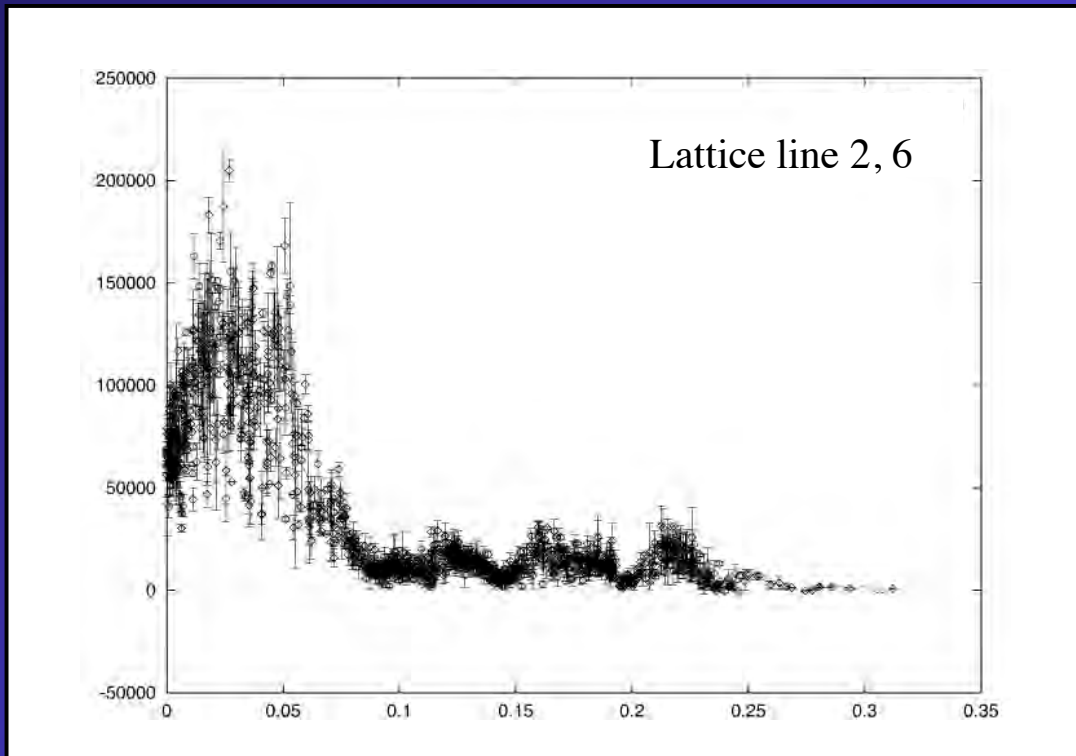
# Electron diffraction at liquid He temperature

AQP0 in  
DMPG

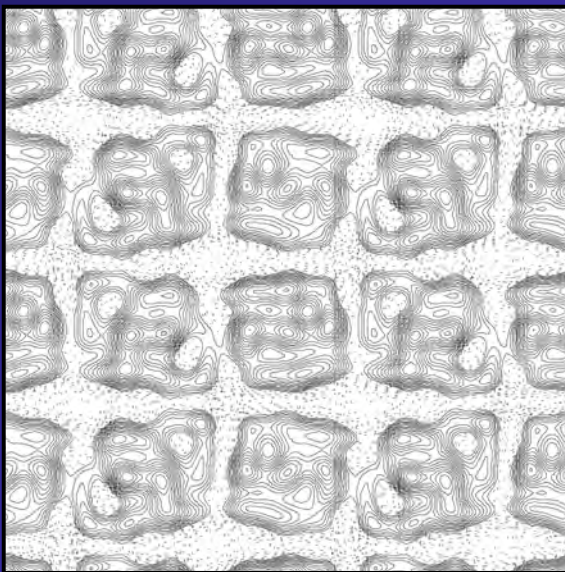


Richard Hite

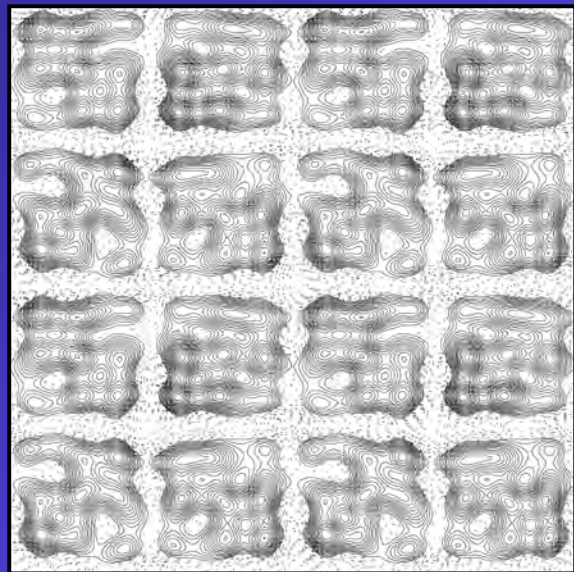
## Merged data for AQPO in DMPG



## AQPO forms different crystals in DMPG

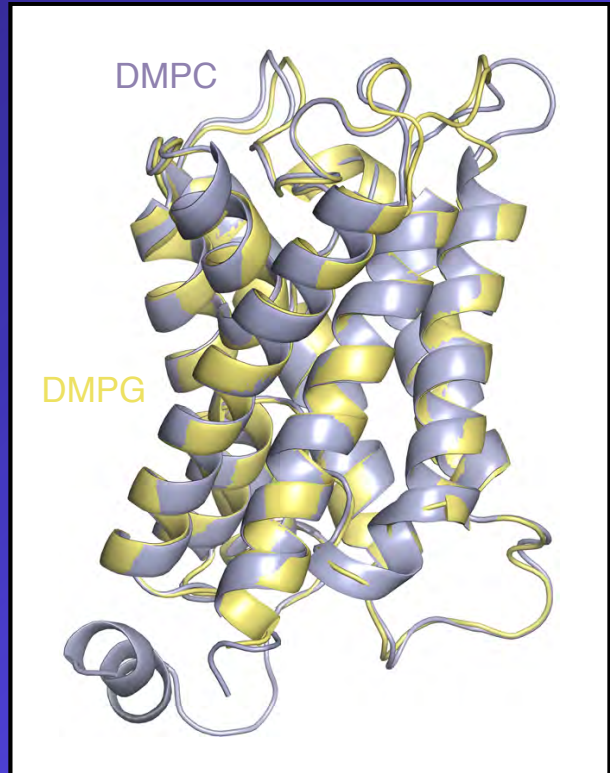
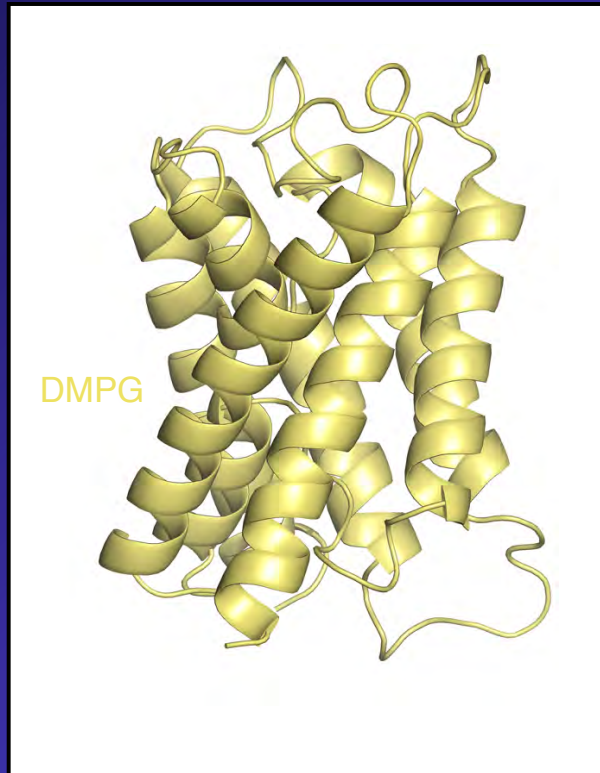


$p12_1$

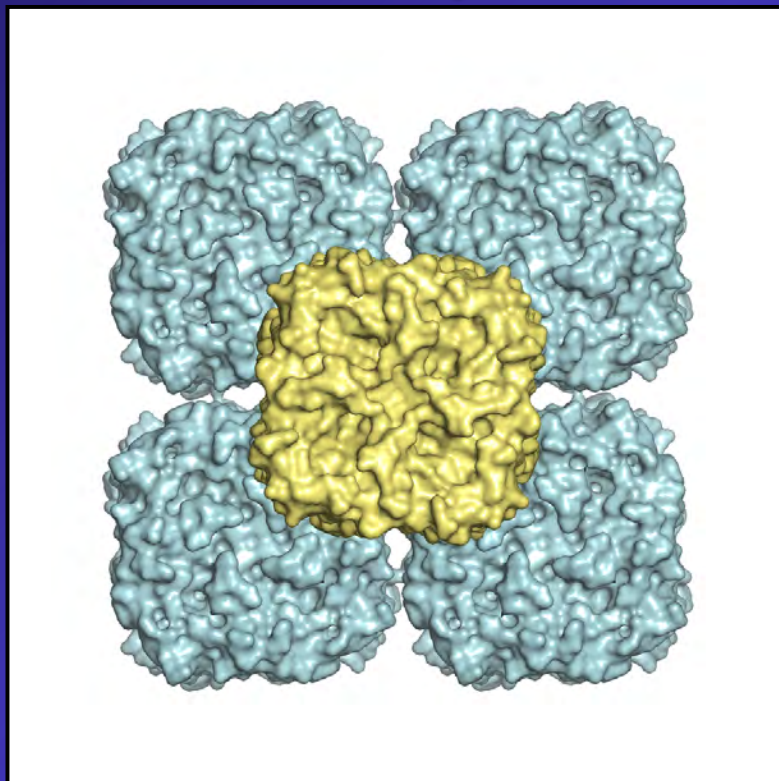


$p42_2$

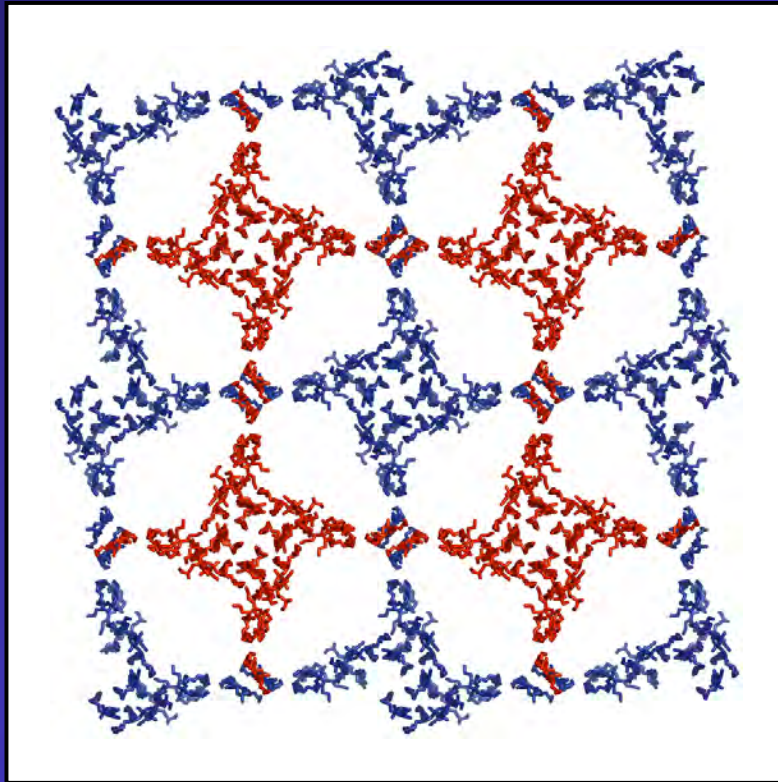
## AQPO in DMPG and DMPC



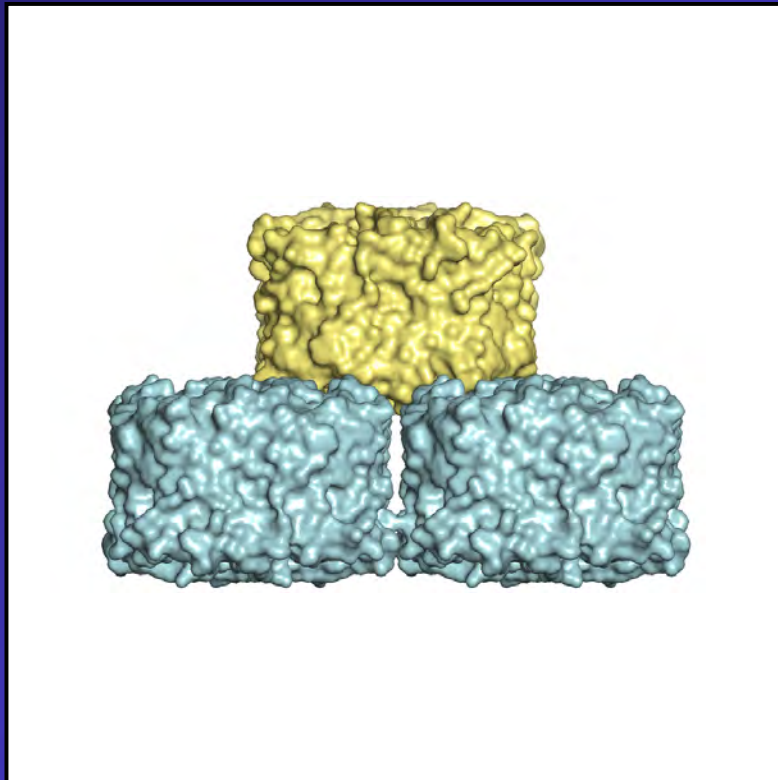
## Model of the AQPO junction in DMPG



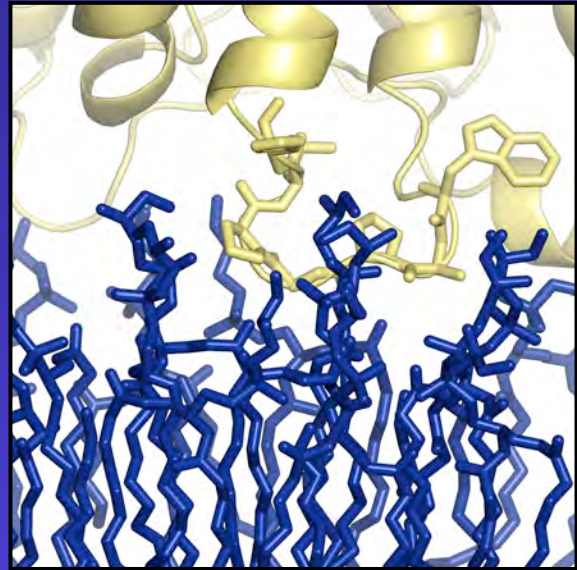
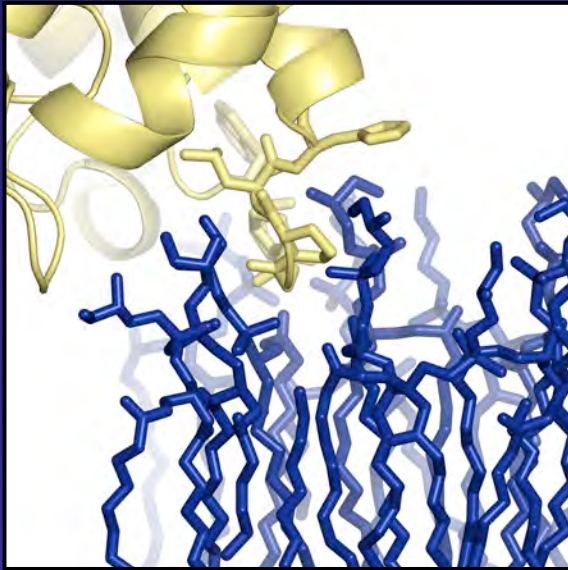
## Model of the AQPO junction in DMPG



## Model of the AQPO junction in DMPG



## Interaction of loop A with lipids



## Collaborators

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Piotr Sliz

University of Auckland

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