

2013 ALS User Meeting
October 9, 2013, Bldg. 15, Room 300
Can Diffuse X-Ray Scattering Reveal Protein Dynamics?

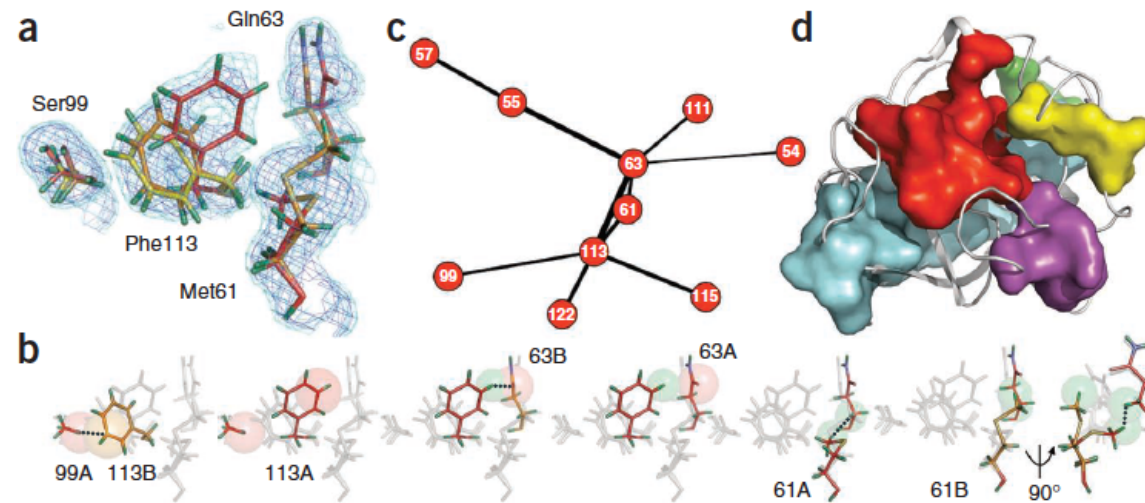
Challenges ahead: What's on the Horizon?

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Workshop: http://cci.lbl.gov/dials/oct_2013_diffuse.htm



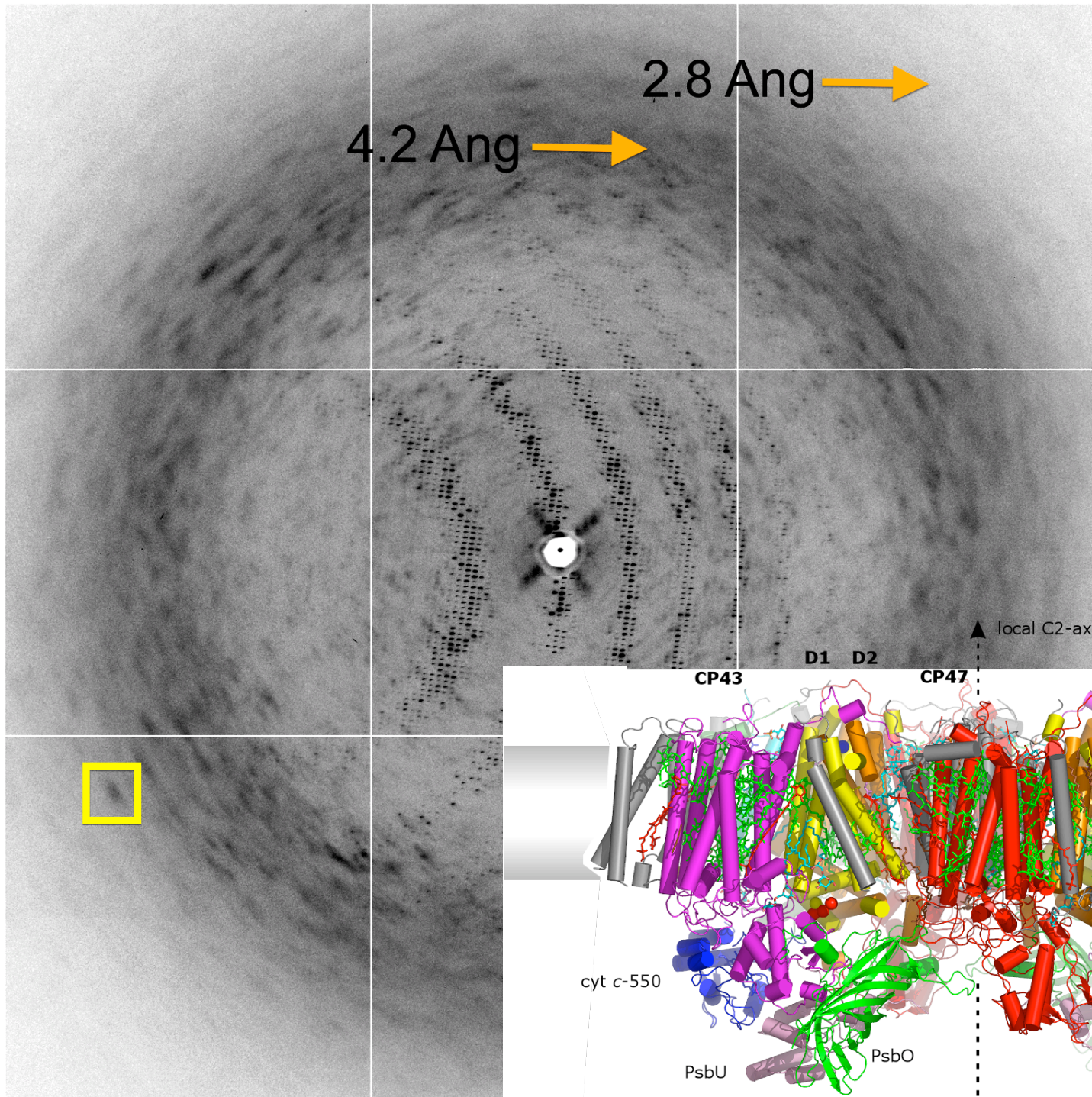
Networks of Dynamic Motion are Crucial for Function



- High resolution density reveals alternate conformers (*Ringer— Lang[2010] Protein Sci 19:1420*)
- Link conformers into networks using hard-sphere stereochemistry (*Contact – van den Bedem[2013] Nat. Methods. 10: 896*)
- Just about anything can perturb the networks: temperature, ligand binding, pH
- Proteins exploit this for regulation. Allostery works by stabilizing transiently populated conformers at distant active sites
- Diffuse scattering offers an experimental window into correlated motion

Thermal Diffuse Scatter from Photosystem II

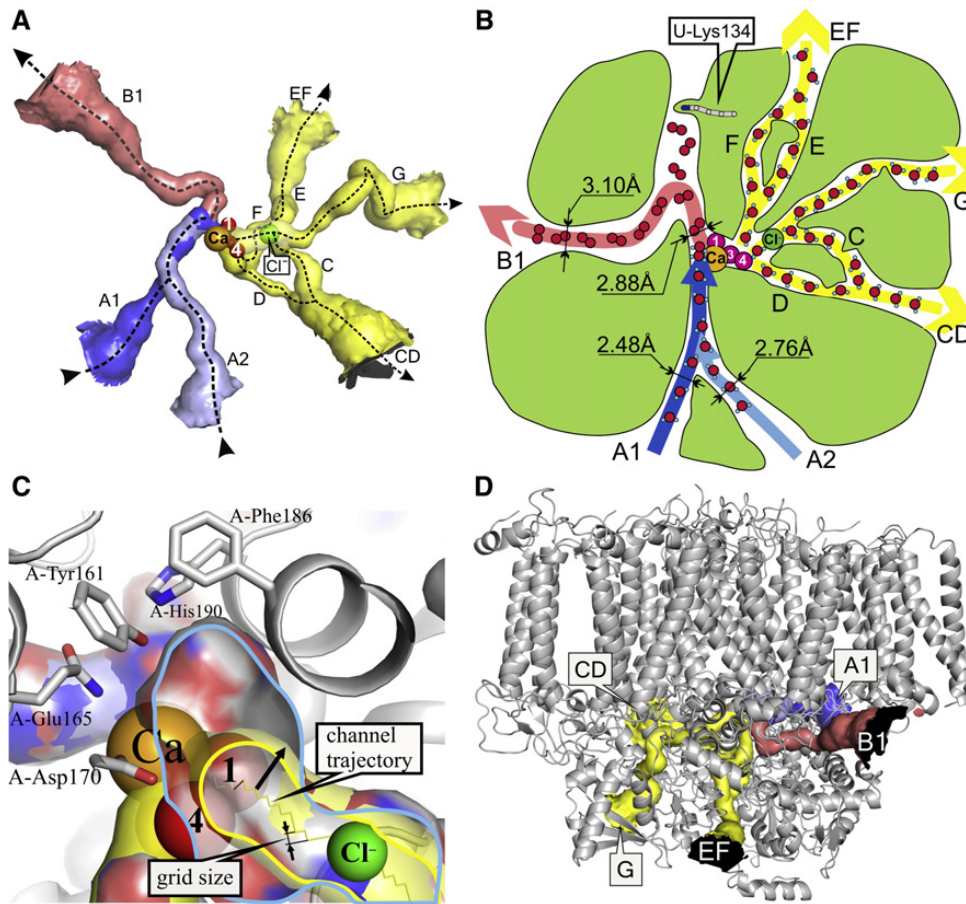
ALS 5.0.2
Dec 2012



Guskov [2009]
Nature Struct. Mol. Biol. (2.9 Å)

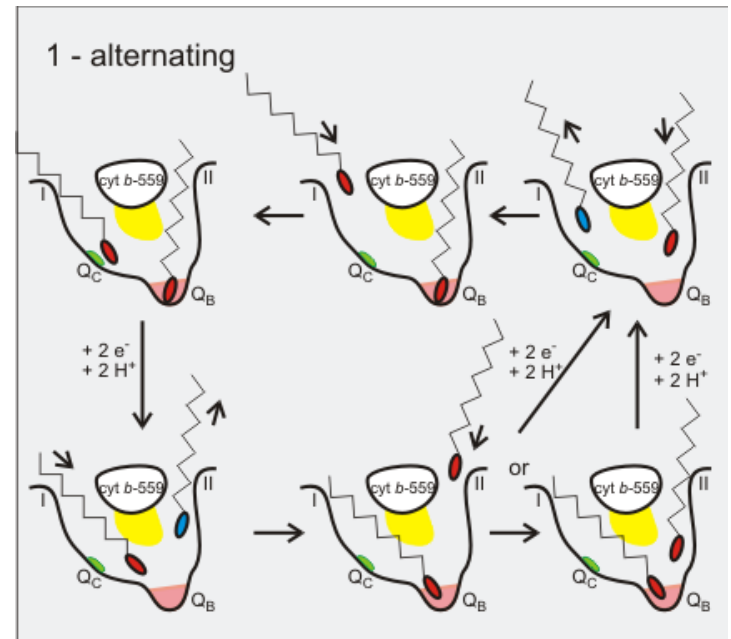
PS II function: need to understand molecular turnover

Water splitting at the Mn_4Ca cluster
Channels for H_2O substrate/ O_2 product



Gabdulkhakov[2009] Structure

Photoexcitation reduces plastoquinone which then exchanges out –
3 proposed mechanisms



2 – wriggling
3 – single channel