

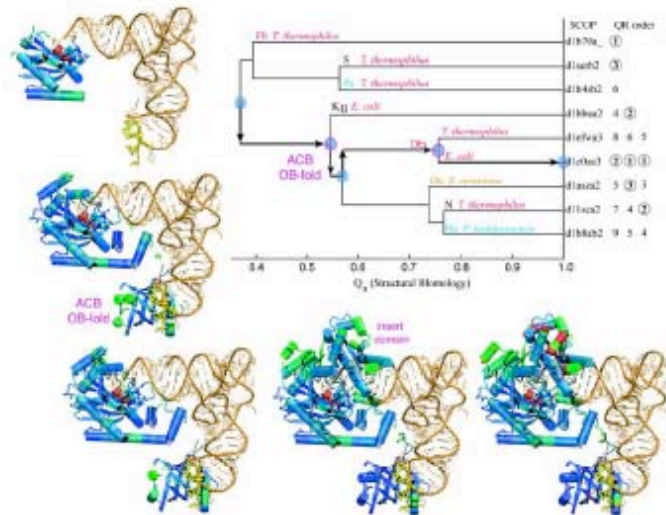
# Part III - Bioinformatics Studies Using Multiseq in VMD

- Aminoacyl tRNA Synthetases
- Aquaporins

San Francisco, 2005, Computational Biology Workshop

# Evolution of Protein Structure

## Aspartyl-tRNA Synthetase



VMD Developers:

Dan Wright

John Eargle

John Stone

Dr. Zan Luthey-Schulten

Brijeet Dhaliwal

Patrick O'Donoghue

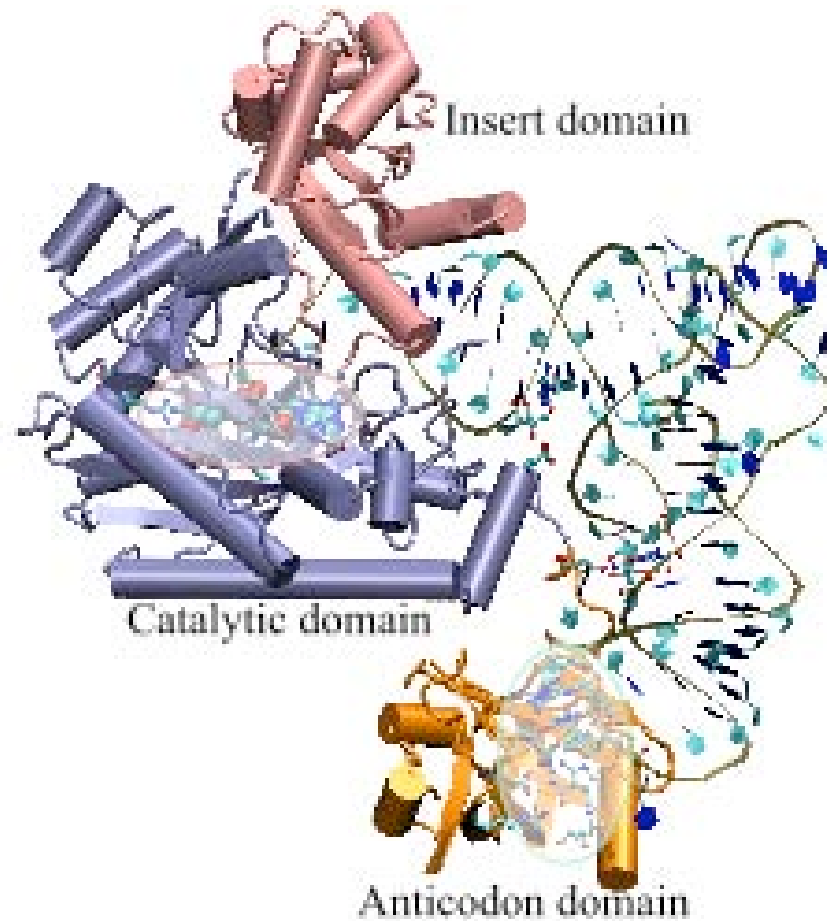
Rommie Amaro

April 2004.

# Multiple Sequence Alignments

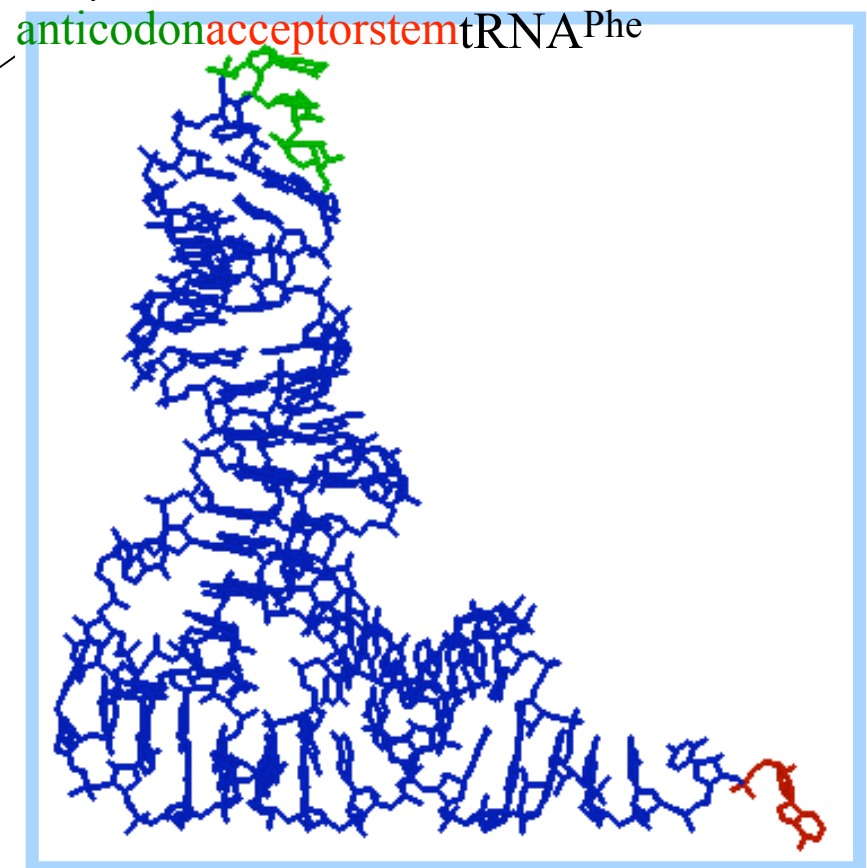
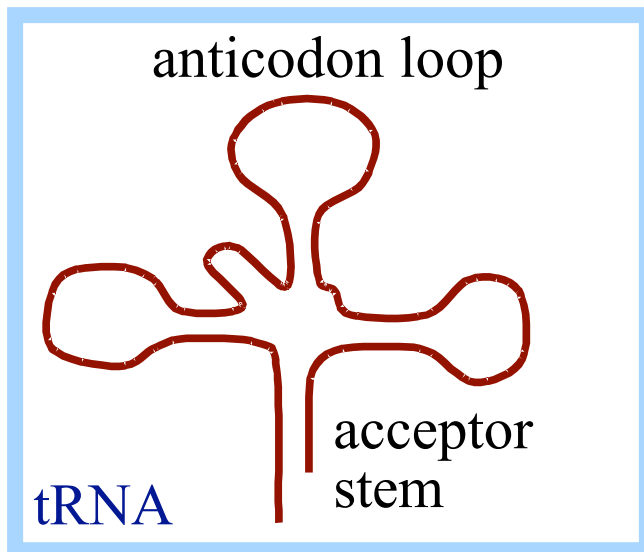
- “The aminoacyl-tRNA synthetases, perhaps better than any other molecules in the cell, optimize the current situation and help to understand (the effects) of HGT” Woese (PNAS, 2000; MMBR 2000)
- Carl Woese - Crafoord Prize 2003

Step 1: Explore active site in catalytic domain and anticodon domain.



# Standard Dogma Molecular Biology

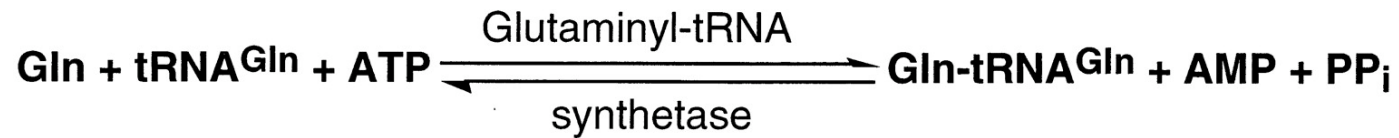
- DNA → RNA → Proteins
- Role of AARS?
- Charging of t-RNA



# Charging the tRNA

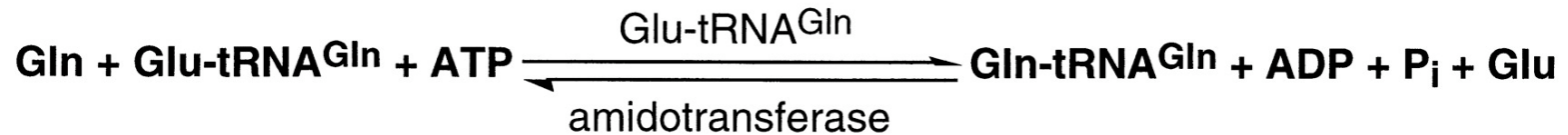
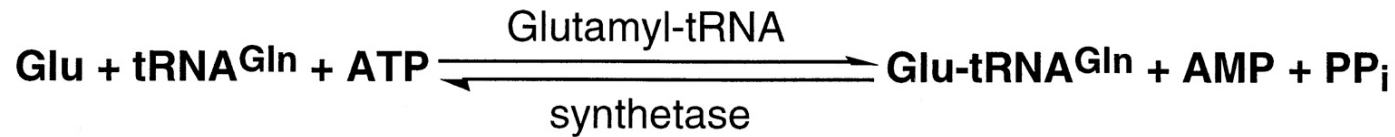
## *Direct acylation*

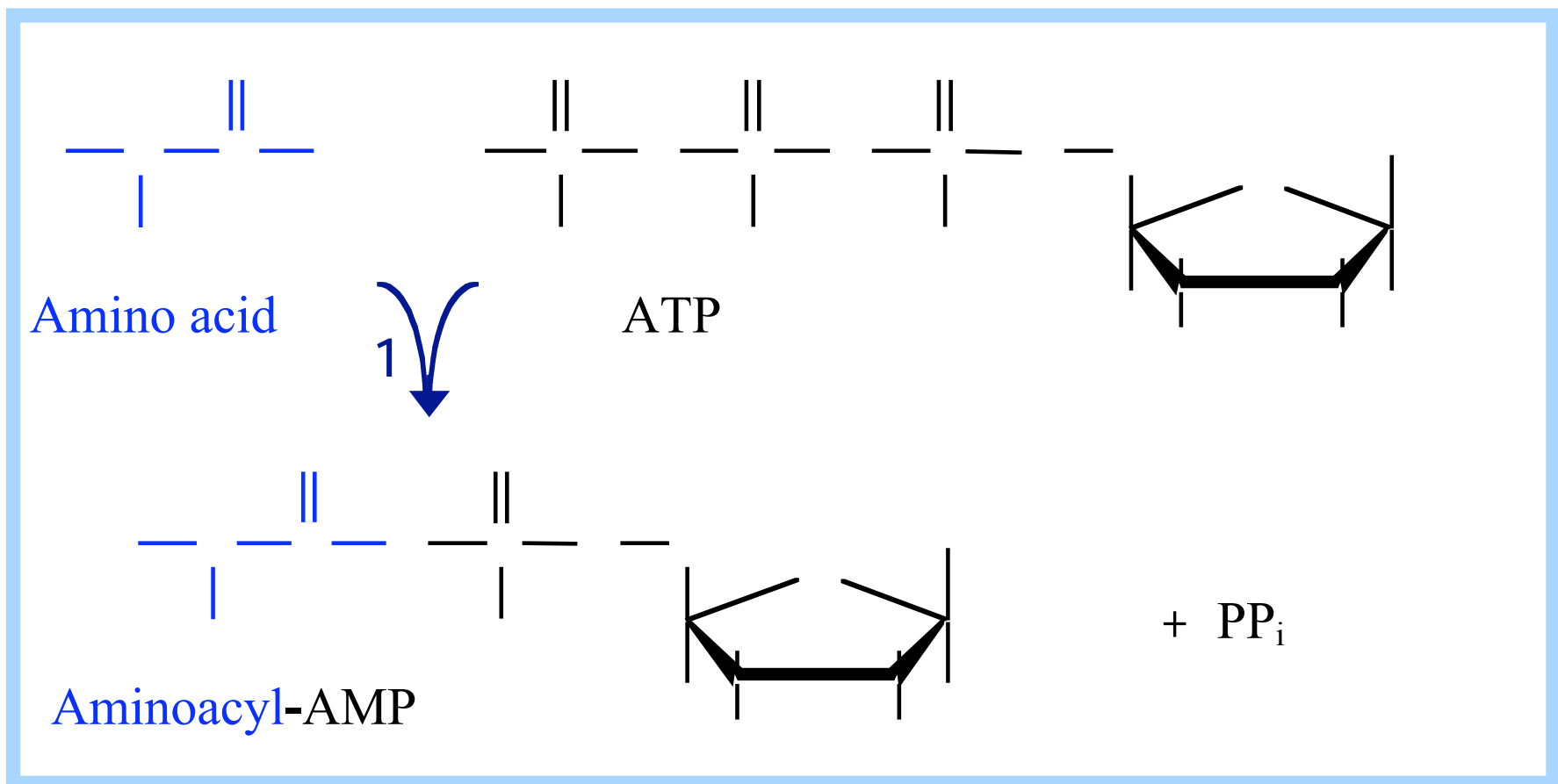
---



## *tRNA-dependent amino acid modification*

---

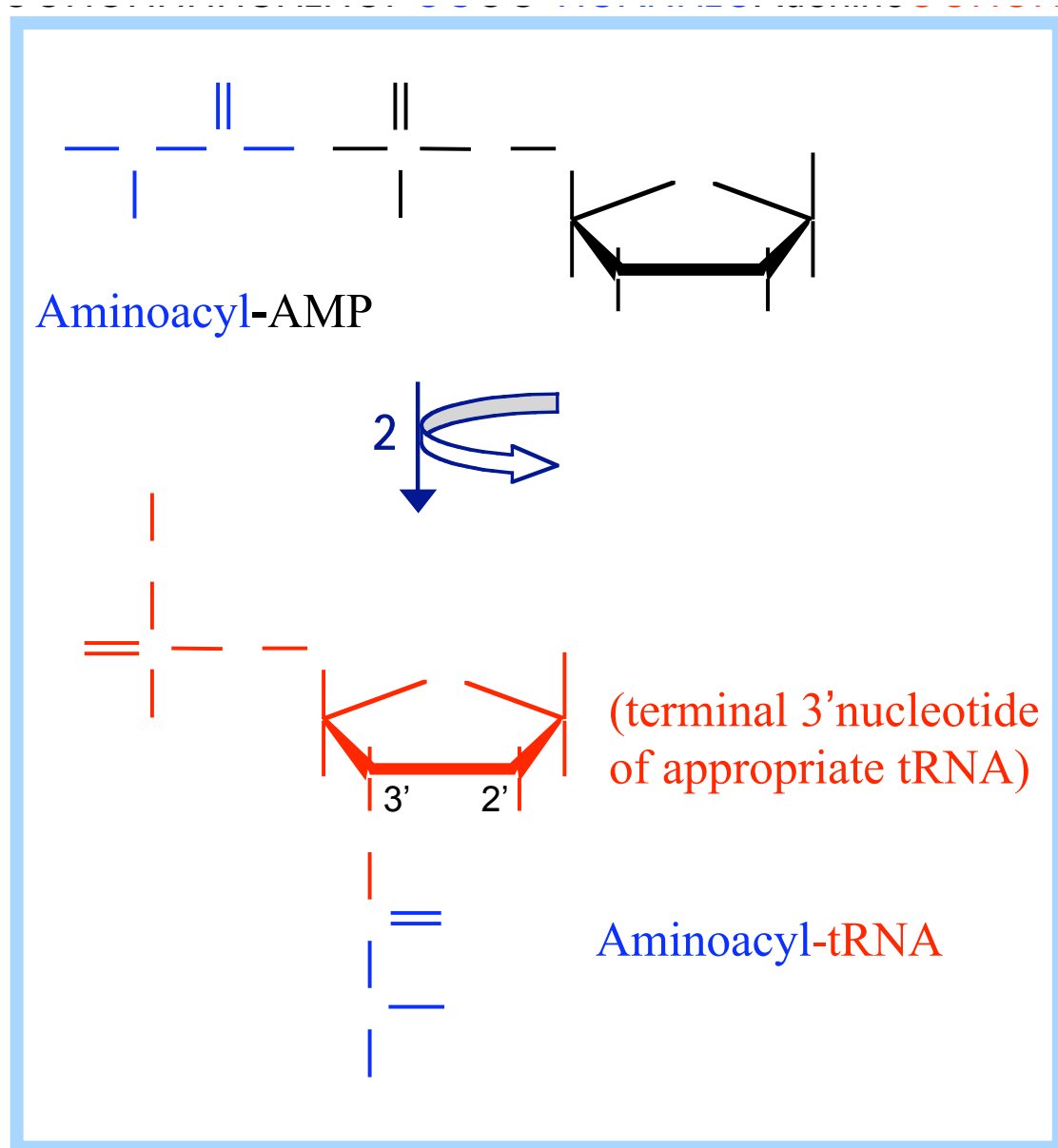




**Aminoacyl-tRNA Synthetases** catalyze linkage of the appropriate amino acid to each tRNA. The reaction occurs in two steps.

In **step 1**, an O atom of the amino acid  $\alpha$ -carboxyl attacks the P atom of the alpha phosphate of ATP.

In **step 2**, the 2' or 3' OH of the terminal adenosine of tRNA attacks the amino acid carbonyl C atom.





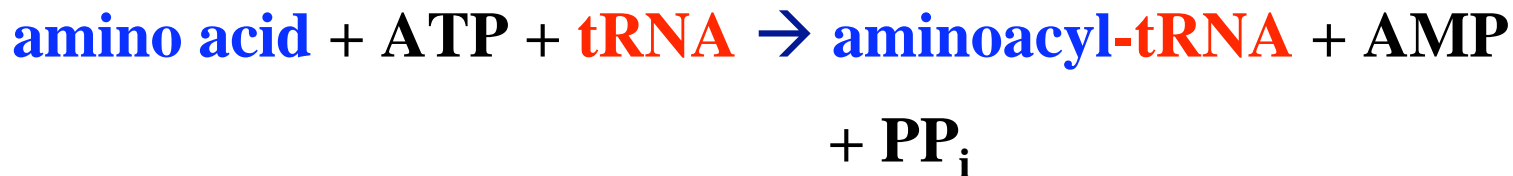
# Aminoacyl-tRNA Synthetase

---

Summary of the 2-step reaction:

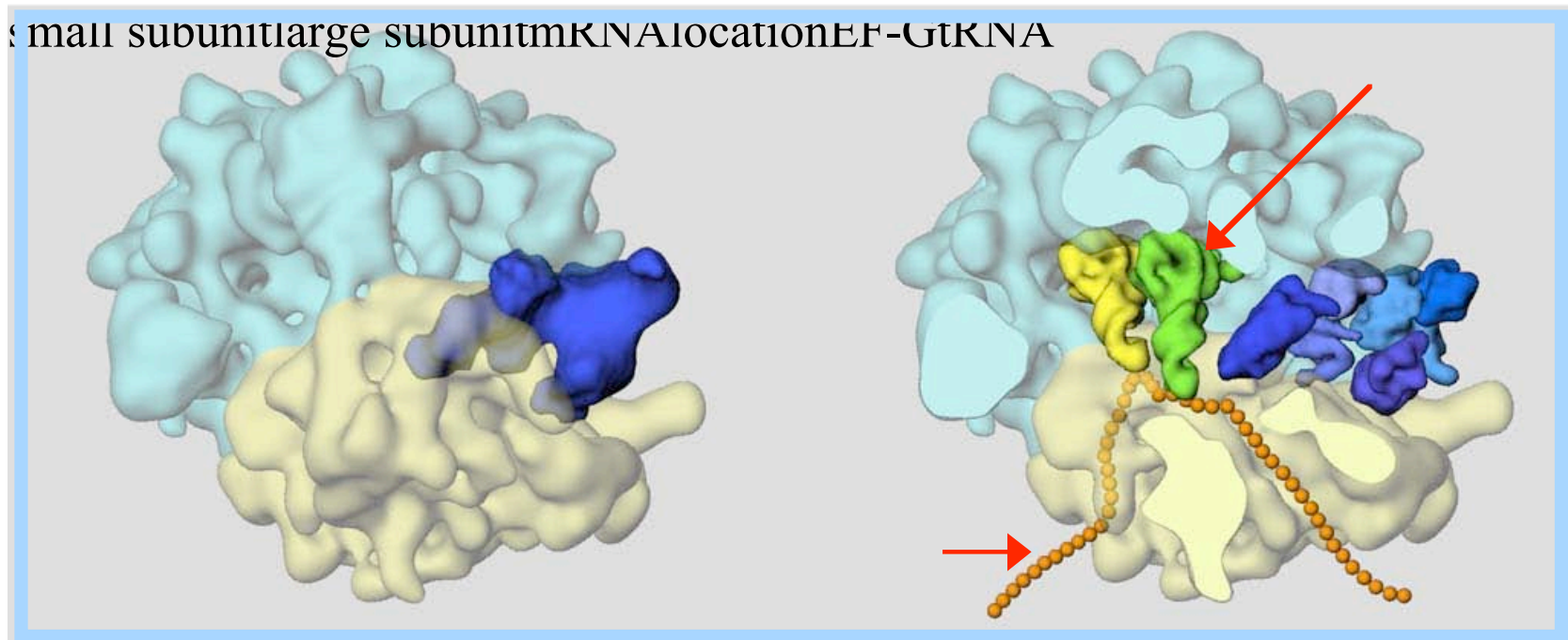


Overall Reaction:



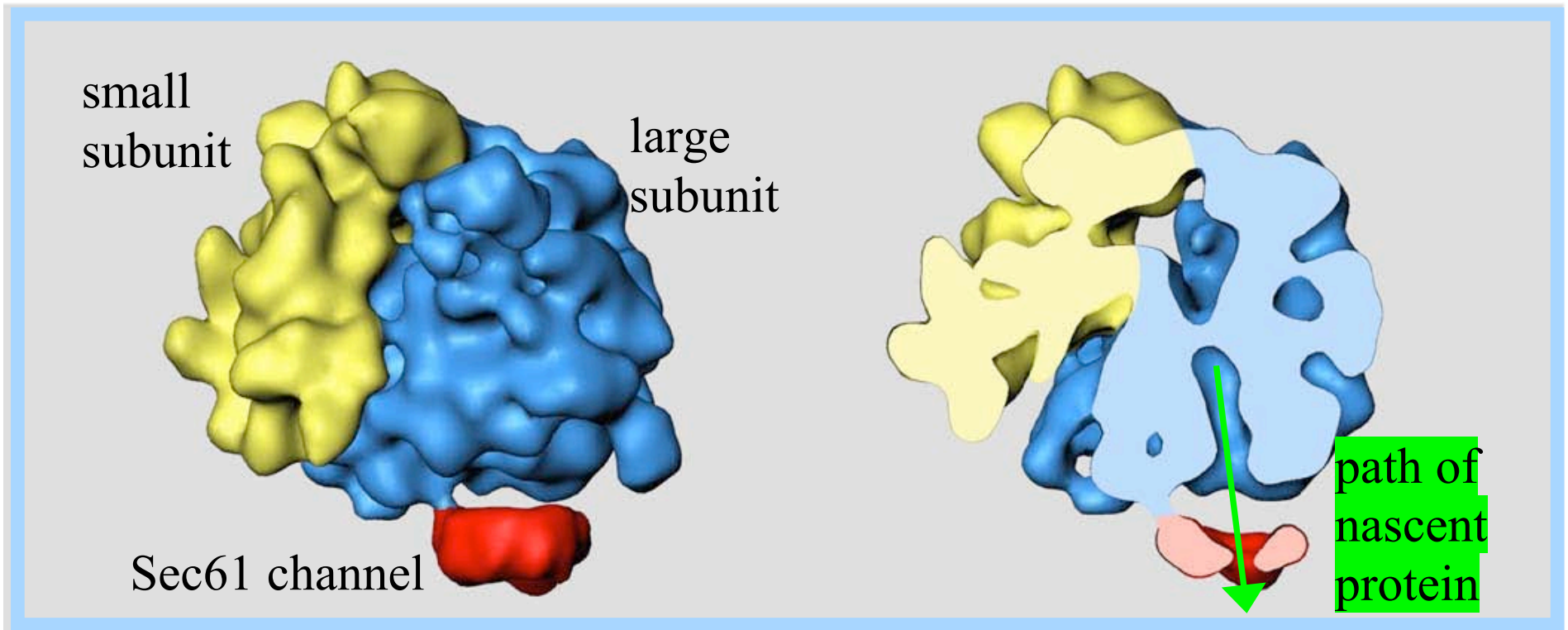
**Next step: EF and Ribosome for Protein Synthesis**

# Structure of the *E. coli* Ribosome



The cutaway view at right shows positions of tRNA (P, E sites) & mRNA (as orange beads).

Figure: Laboratory of Joachim Frank, Wadsworth Center  
cryo-EM and 3D image reconstruction



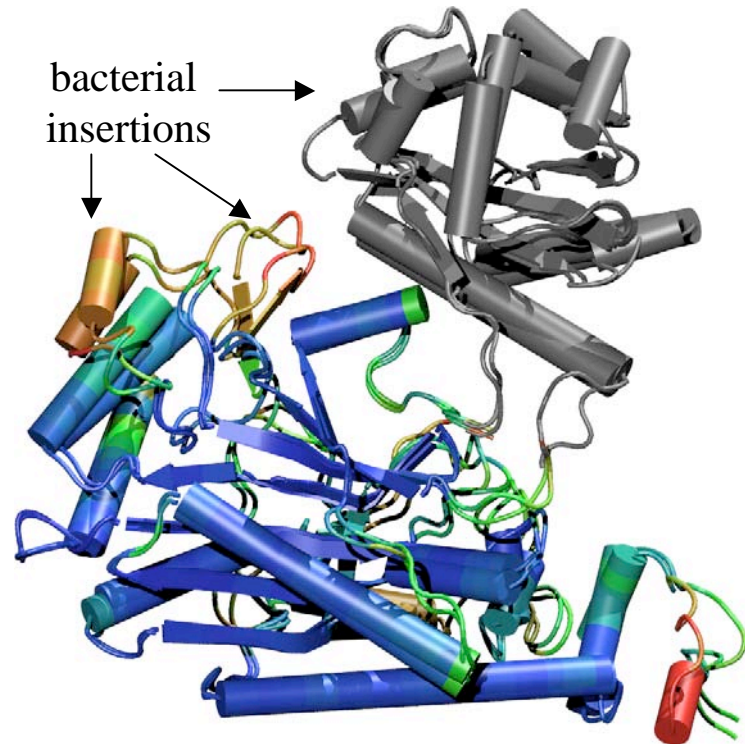
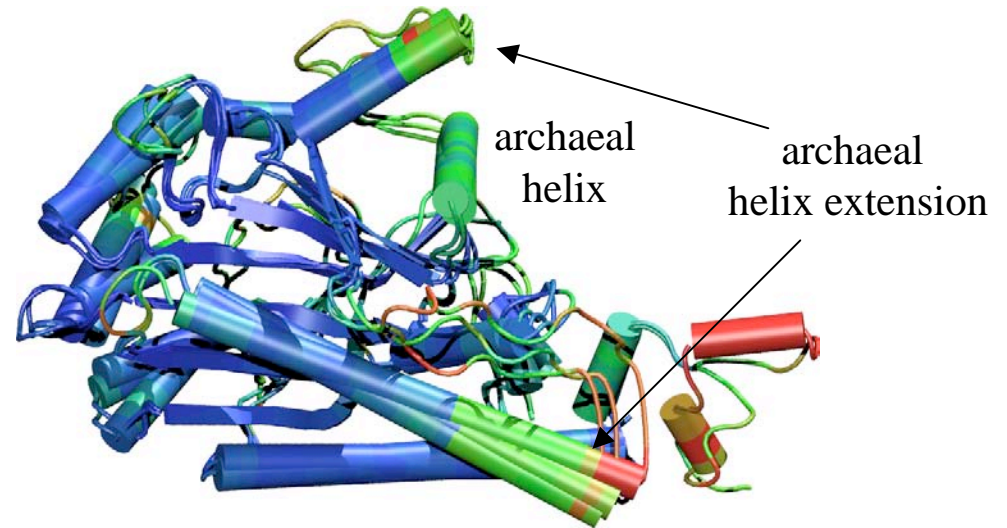
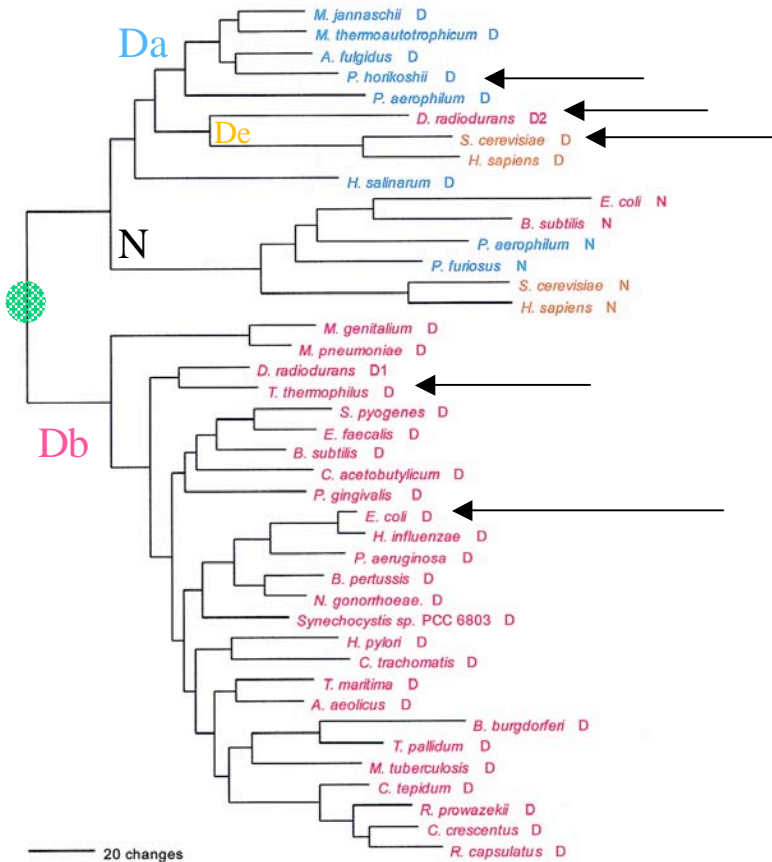
The cutaway view at right shows that the **tunnel** in the yeast large ribosome subunit, through which nascent polypeptides emerge from the ribosome, **lines up** with the lumen of the ER **Sec61 channel**.

Figure provided by Joachim Frank, whose lab carried out the cryo-EM & image reconstruction on which these images are based.

# Horizontal Gene Transfer in Protein Structure

## Sequence Phylogeny

### AspRS-AsnRS Group



# Multiseq extension in VMD

VMD 1.8.3a2 OpenGL Display

**Extensions**

- sequence
- autoimd
- apbsrun
- imd
- contactmap
- pdbtool
- ramaplot
- rmsd
- solvate
- timeline
- multiseq
- tkcon
- vmdmovie

**treeWindow**

Tree

```

graph LR
    A[d1efwa3.ent Thermus thermophilus B] --- B(( ))
    C[d1c0aa3.ent Escherichia coli B] --- B
    B --- D(( ))
    E[d1n9wb1.ent d1n9wb1.ent] --- D
    D --- F(( ))
    G[d1asza2.ent Saccharomyces cerevisiae E] --- F
    H[d1b8aa2.ent Pyrococcus kodakaraensis A] --- F
    
```

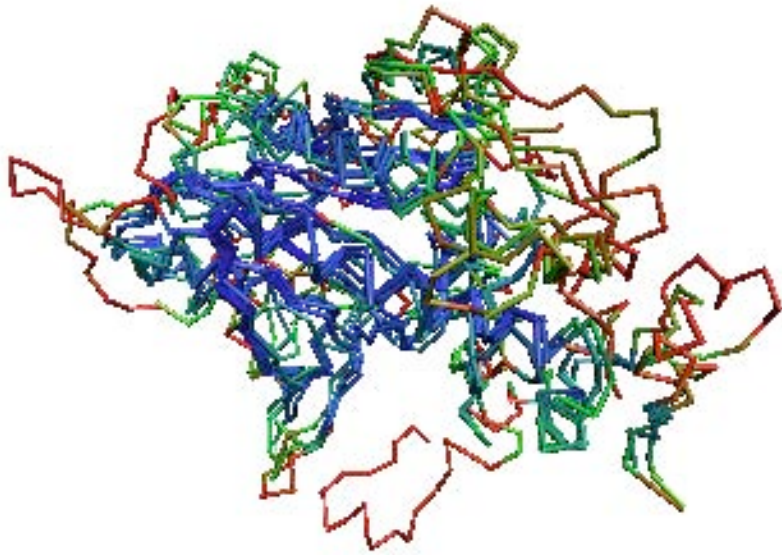
0.56

**Sequence Display**

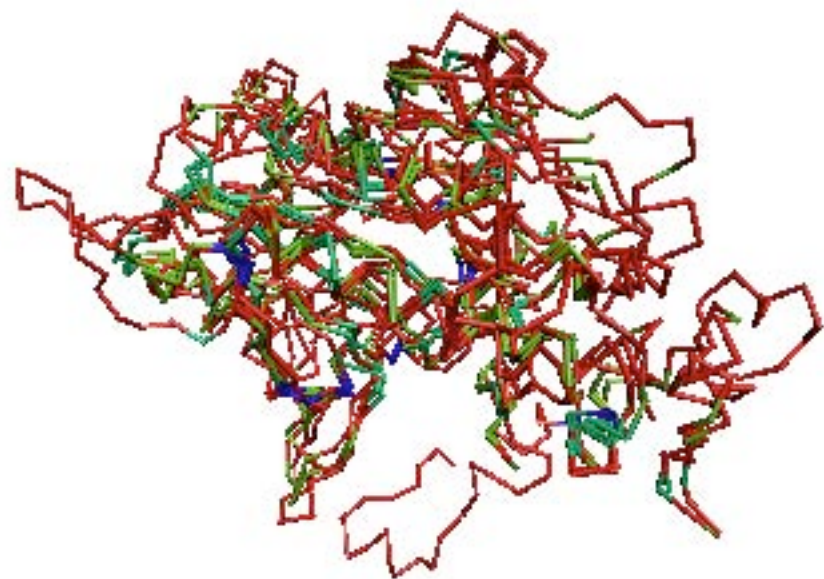
```

d1b8aa2.ent  IDTEGERLLGKYM--MENENAPLYFLYQYPS-----EAKPFYIMKYDN-----K--PEICRAFDLEYRGI
d1asza2.ent  LSTENEKFLGKLV--RDKYDTDFYILDKFPL-----EIRPFYTMPDPA-----N--PKYSNSYDFFMRGEI
d1n9wb1.ent  LSEEAERLLGEYA--KERWGSDFWLVTRYPR-----SVRPFYTYTYP-EE-----DGTTRSFDLLFRGL
d1c0aa3.ent  ---GSD-KP-DLRDE---SKWAPLWVIDFPMFE-DDGEGGLTAMHHPFTSPK-DMTAAELKAAPENAVANAYDMVINGY
d1efwa3.ent  ---GSD-KP-DL-RR---EGFRFLWVVDFP LLEWDEEEEAWTYMHHHPFTSPHPED-LP LLEKDPGRVRLAYDLVLNGVI
    
```

# Conservation

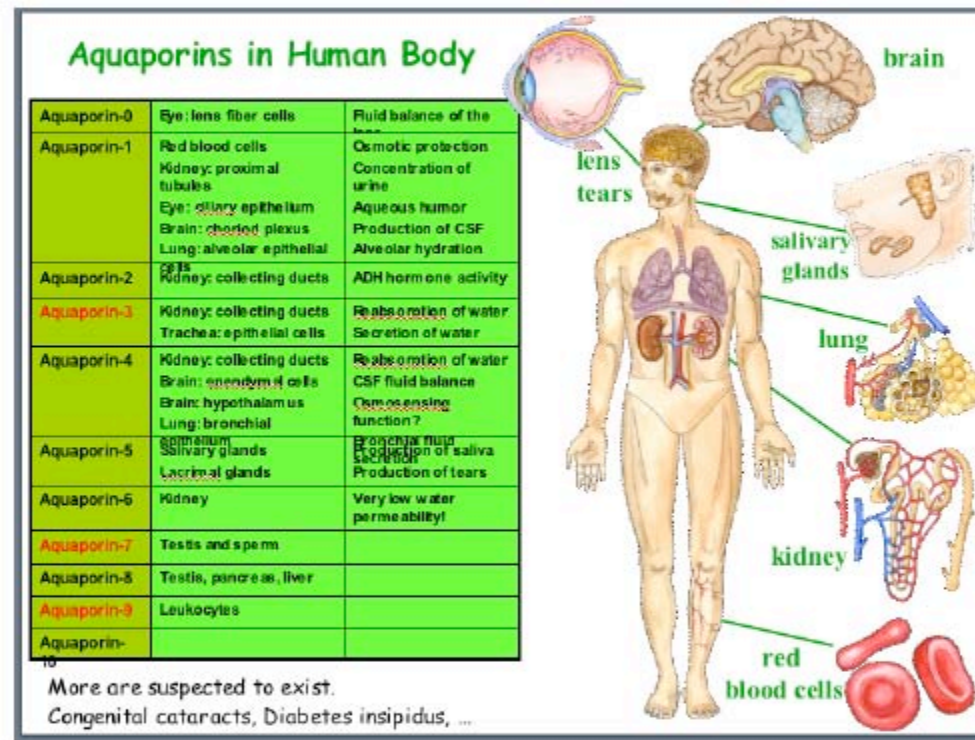


Core Structure Conserved



Sequence Identity of Core  
Less than 15%

# Aquaporins



VMD Developers:

John Stone

Dan Wright

John Eargle

Fatemeh Khalili

Elizabeth Villa

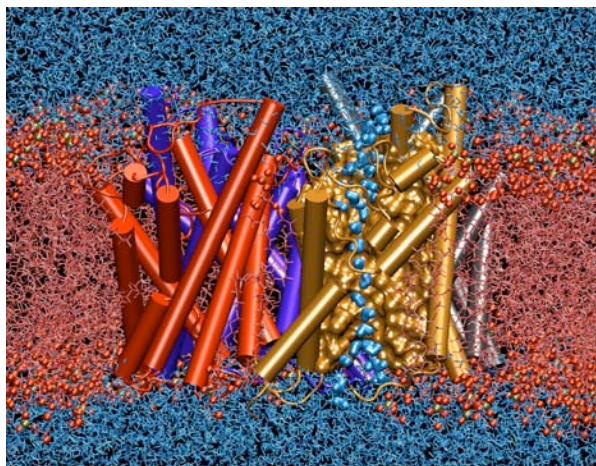
Emad Tajkhorshid

Brijeet Dhaliwal

Zan Luthey-Schulten

# Towards Understanding Membrane Channels

## *The versatile, highly selective and efficient aquaporin*



### **GlpF Structure (Stroud et al)**

NAMD with full electrostatics

Periodic boundary conditions

NpT ensemble at 310 K

1ns equilibration

Protein: ~ 15,000 atoms

Lipids: ~ 40,000 atoms

Water: ~ 51,000 atoms

**Total: ~ 106,000 atoms**

**4 hrs / ns – 1024 TSC CPUs**



### The Nobel Prize in Chemistry 2003

"for discoveries concerning channels in cell membranes"

"for the discovery of water channels"

"for structural and mechanistic studies of ion channels"



**Peter Agre**

🕒 1/2 of the prize

USA

Johns Hopkins University School of Medicine  
Baltimore, MD, USA

b. 1949



**Roderick MacKinnon**

🕒 1/2 of the prize

USA

Rockefeller University, Howard Hughes Medical Institute  
New York, NY, USA

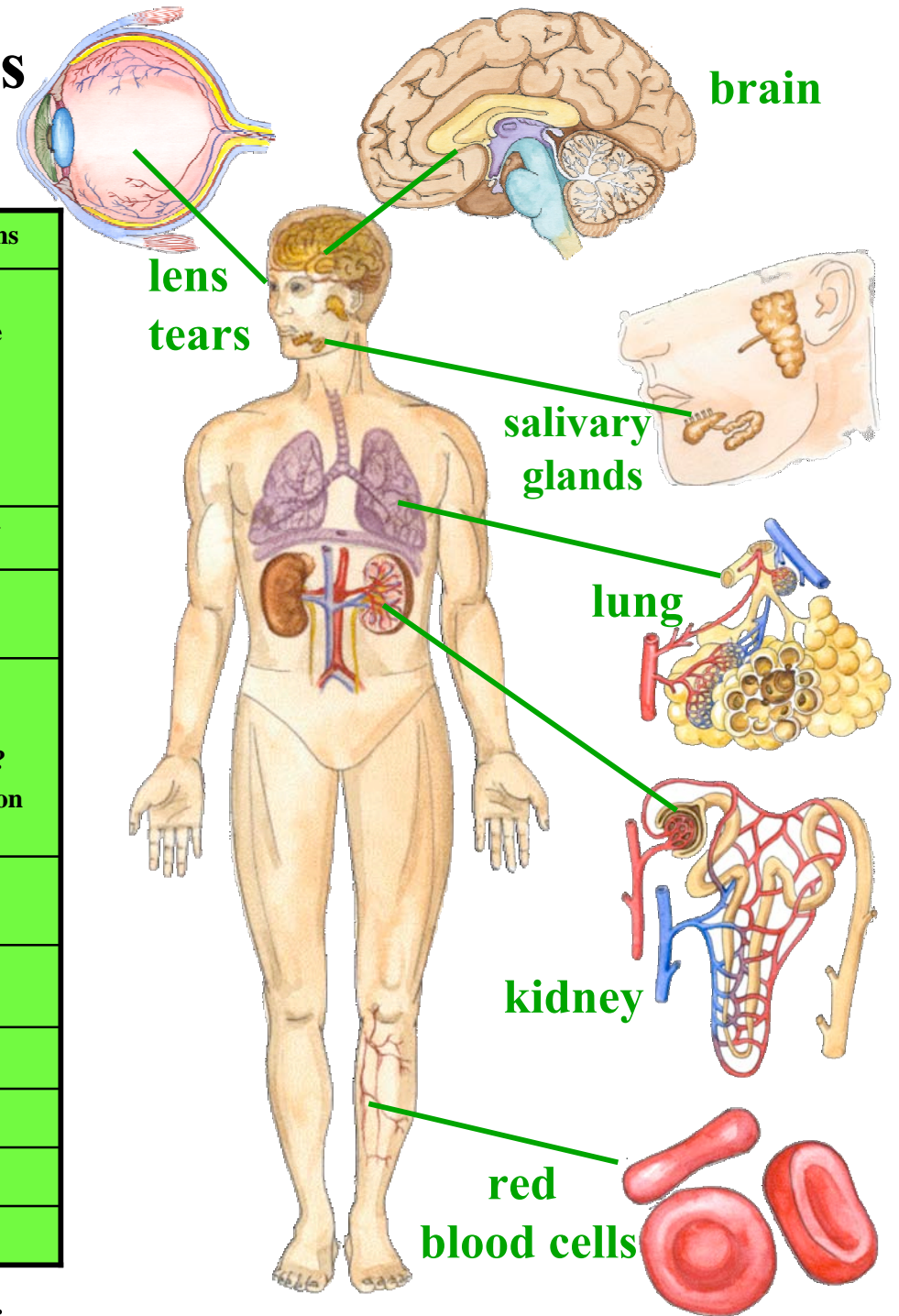
b. 1956





# Water and **Glycerol** Channels in the Human Body

<b>Aquaporin-0</b>	Eye: lens fiber cells	Fluid balance of the lens
<b>Aquaporin-1</b>	Red blood cells Kidney: proximal tubules Eye: ciliary epithelium Brain: choroid plexus Lung: alveolar epithelial cells	Osmotic protection Concentration of urine Aqueous humor Production of CSF Alveolar hydration
<b>Aquaporin-2</b>	Kidney: collecting ducts	ADH hormone activity
<b>Aquaporin-3</b>	Kidney: collecting ducts Trachea: epithelial cells	Reabsorption of water Secretion of water
<b>Aquaporin-4</b>	Kidney: collecting ducts Brain: ependymal cells Brain: hypothalamus Lung: bronchial epithelium	Reabsorption of water CSF fluid balance Osmosensing function? Bronchial fluid secretion
<b>Aquaporin-5</b>	Salivary glands Lacrimal glands	Production of saliva Production of tears
<b>Aquaporin-6</b>	Kidney	Very low water permeability!
<b>Aquaporin-7</b>	Testis and sperm	
<b>Aquaporin-8</b>	Testis, pancreas, liver	
<b>Aquaporin-9</b>	Leukocytes	
<b>Aquaporin-10</b>		



Additional members are suspected to exist.

# Functionally Important Features of Aquaporins

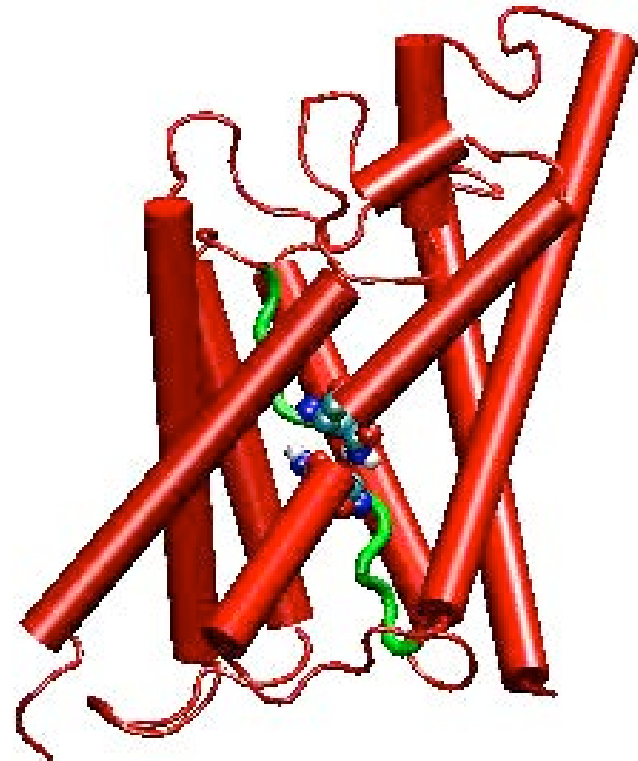
- Water and glycerol transport
- Exclusion of ions and protons
- Tetrameric arrangement in membrane

Aquaporins of known structure:

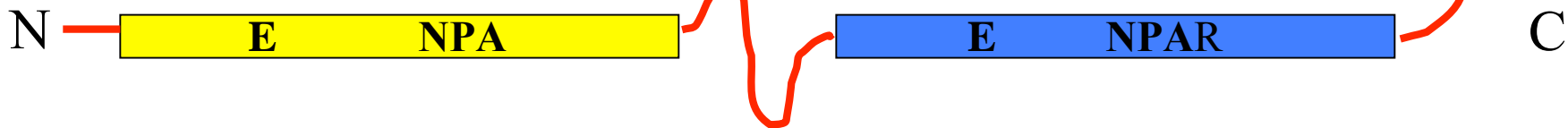
**GlpF** – E. coli glycerol channel (aquaglyceroporin)

– Fu, et al., Science (2000)

**AQP1** – Mammalian aquaporin-1 (pure water channel) -Sui et al, Nature (2001)



**~100% conserved -NPA- signature sequence**



# Load Aquaporin 1J4N into VMD

The image shows the VMD (Visual Molecular Dynamics) interface. The main window, titled "VMD Main", contains a menu bar (File, Molecule, Graphics, Display, Mouse, Extensions, Help) and a table of loaded molecules. The table has columns for ID, T, A, D, F, Molecule, Atoms, Frames, and Vol. The first row shows ID 1, T A D F, Molecule 1J4N, Atoms 2029, Frames 1, and Vol 0. Below the table is a playback control bar with a slider at 0, buttons for zoom, Loop, step (set to 1), and speed.

The "Graphical Representations" window is open, showing the "Selected Molecule" as "1: 1J4N". It has "Create Rep" and "Delete Rep" buttons. A table below shows the representation settings:

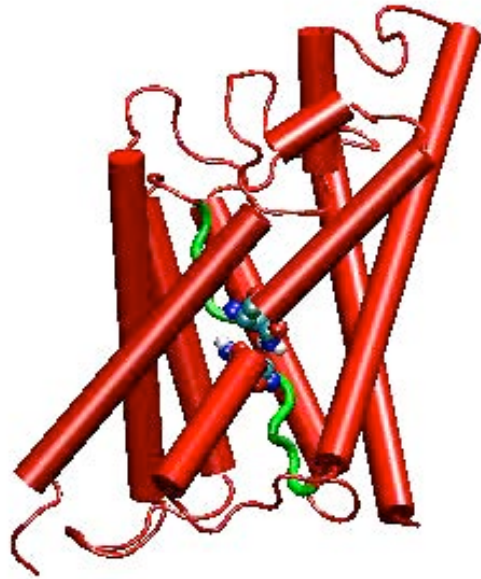
Style	Color	Selection
Tube	Name	all

The "Selected Atoms" field contains "all". The "Draw style" tab is active, showing "Coloring Method" set to "Name" and "Material" set to "Opaque". The "Drawing Method" is set to "Tube". At the bottom, the "Radius" is set to 0.5 and "Resolution" is set to 11. There are "Apply Changes Automatically" and "Apply" buttons.

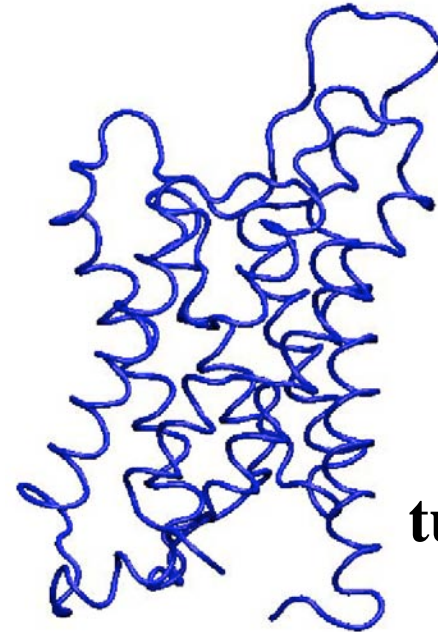
The "VMD 1.8.2b7 OpenGL Display" window shows a 3D ribbon representation of the Aquaporin 1J4N protein structure, colored in a light blue/cyan. The structure is a complex, multi-domain protein with several alpha-helices and beta-strands. The system tray at the bottom right shows icons for VMD, a task manager, and a clock.

# VMD Permits Different Rendering Styles

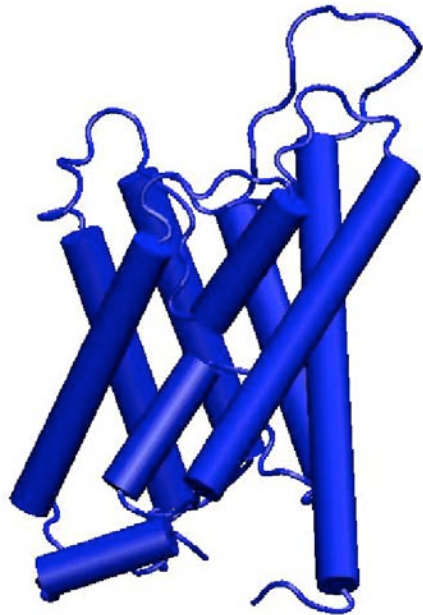
**movie**



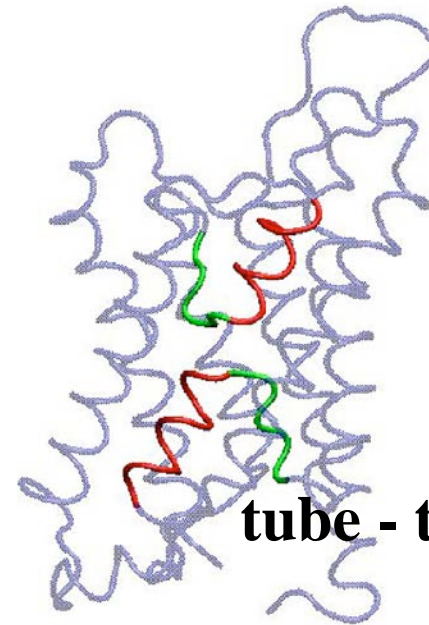
**tube**



**cartoon**



**tube - transparent**





# Load Aquaporins 1j4n, 1fqy, 1lda, 1rc2 into VMD

The screenshot displays the VMD (Visual Molecular Dynamics) software interface. The main window shows a 3D rendering of four aquaporin structures (1j4n, 1fqy, 1lda, 1rc2) in different colors (grey, red, blue, and yellow). The interface includes several panels:

- VMD Main:** A menu bar (File, Molecule, Graphics, Display, Mouse, Extensions, Help) and a table listing loaded molecules.
- Graphical Representations:** A panel for configuring the selected molecule (5: 1rc2), including style (Tube), color (ColorID 3), and selection (chain A) options.
- Multiple Sequence Alignment:** A window showing sequence alignment for the four proteins.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	A	D	F		1J4N	2029	1	0
2	A	D	F		1FQY	1661	1	0
3	A	D	F		1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

PDB code	Description
1j4n	Bovine AQP1
1fqy	Human AQP1
1lda	E. coli Glycerol Facilitator (GlpF)
1r2c	E. coli AqpZ

```

d1fqya_.ent  KLPWRVAVAEFLATTLFVFIISIGSALGFKYPVGNWQTAVQDNVKSLSLAFGLSIATLA
d1j4na_.ent  HASEFKKKLFWRAVVAEFLAHILFIFISIGSALGFHYPIKSNQTTGAVQDNVKSLSLA
d1lda_.ent   TLFGQCIAEFLGTGLLIFFGVGVAALKVAGASFGQWEISVINGLGVAMATYLTAGV
d1rc2a_.ent  HFRKLAACEFGTFWLVFGGCSAVLAAGFPFELIGFAGVALAFGLTLVLTMAFVGH
    
```

# Aligning Structures and Sequences

The image displays the VMD (Visual Molecular Dynamics) software interface, illustrating the process of aligning structures and sequences. The main window, titled "VMD 1.8.2b7 OpenGL Display", shows a 3D ribbon representation of a protein structure, colored by residue type (blue for helix, red for sheet, yellow for loop). The "VMD Main" window at the top left provides a summary of loaded molecules:

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1		A	D	F	1J4N	2029	1	0
2		A	D	F	1FQY	1661	1	0
3		A	D	F	1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

The "Graphical Representations" window on the left shows the configuration for the selected molecule "5: 1rc2". The "Style" is set to "Tube", "Color" is "ColorID 3", and "Selection" is "chain A". The "Drawing Method" is also set to "Tube". The "Radius" is 0.5 and the "Resolution" is 11. The "Multiple Sequence Alignment" window at the bottom right displays a sequence alignment of four proteins: 1fgy, 1j4n, 1lda, and 1rc2. The alignment shows conserved regions across the sequences, with gaps represented by dashes.

```
1fgy  -----KLFWRVAVAEFLATTLFVFFISIGSAL-GF-KY---PVGNNQTAVDNPKVSLAPGLSIATLAQS-VGHISGAHLNPAVTLGILLSCQISIF-RAI
1j4n  MASEFKKKLFWRAVVAEFLAMILFIFISIGSAL-GF-HYPIKSNQT-TGAVQDNVKVSLAPGLSIATLAQSVGH-ISGAHLNPAVTLGILLSCQ-ISVLRAI
1lda  -----TLKGQCIAEFLGTGLLIFFGVGCVV-ALKVA-----G-A-SFGQWEISVIWGLGVAMATYLTG-VVSGAHLNPAVTIALWLFA-CFDKRVV
1rc2  -----MFRKLAECFPTFWLVFGCGSAVLA-AG-----FPE-LGIGFAGVALAPGLTVLTMFAVVG-HISGGHFNPAVTIGLWAGG-RFPAREVV
```



# Comparing Structures by Similarity - Q Value

The image displays the VMD (Visual Molecular Dynamics) software interface, illustrating the process of comparing protein structures by similarity using the Q Value.

**VMD Main Window:** Shows a table of loaded molecules and playback controls.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	A	D	F		1J4N	2029	1	0
2	A	D	F		1FQY	1661	1	0
3	A	D	F		1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

**Graphical Representations Window:** Shows the configuration for the selected molecule (5: 1rc2).

- Selected Molecule: 5: 1rc2
- Buttons: Create Rep, Delete Rep
- Table:

Style	Color	Selection
Tube	ColorID 3	chain A
- Selected Atoms: chain A
- Draw style: Selections, Trajectory, Periodic
- Coloring Method: ColorID 3, Material: Opaque
- Drawing Method: Tube, Default
- Radius: 0.5
- Resolution: 11
- Buttons: Apply Changes Automatically, Apply

**VMD 1.8.2b7 OpenGL Display Window:** Shows a 3D ribbon representation of the protein structure (1rc2) colored by residue.

**Multiple Sequence Alignment Window:** Shows a sequence alignment interface with a context menu open.

- Buttons: Align Molecules..., FASTA, Highlight PDB, Pairwise RMSD
- Context Menu:
  - RMSD Per Residue
  - Tree
  - STAMP Parameters
  - Bulk Residue Selection
  - Molecule Coloring
    - Q per residue (checked)
  - Highlight Style
    - Sequence Identity per residue

The sequence alignment window displays the following sequences:

```
1fgy -----KLFWAQVADFLATLLEVFSTIGSAL-GF-FY---PVQRIQAVQINVKVSLAFGLSATLAQS-VGHSGAHLNFAVTLGLLLSQGISIF-RAI
1j4n MASEFKKLFWRARVAEFLAMILFIFISIGSAL-GF-HYPIKSNQT-TGAVQDNVKVSLAFGLSATLAQSVGH-ISGAHLNFAVTLGLLLSQGI-ISVLRRI
1lda -----TLRGQCIAEPLGTGLLIPFGVGCVA-ALKVA-----G-A-SFGQWEISVIWGLGVAMAIYLTG-VVSGAHLNFAVTLALWLFQ-CFDKRRV
1rc2 -----MFRKLAACEPGTFLVLFVGGCGSAVLA-AG-----FPE-LGIGFAGVALAPGLTTLTMAFAVG-HISGGHPNFAVTLGLWAGG-RFPAKEV
```

# Comparing Structures by Similarity - Q Value

The image displays the VMD (Visual Molecular Dynamics) software interface, illustrating the process of comparing protein structures by similarity using the Q Value.

**VMD Main Window:** Shows a list of loaded molecules:

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	A	D	F		1J4N	2029	1	0
2	A	D	F		1FQY	1661	1	0
3	A	D	F		1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

**Graphical Representations Window:** Shows the configuration for the selected molecule (5: 1rc2):

- Selected Molecule: 5: 1rc2
- Style: Tube
- Color: ColorID 3
- Selection: chain A
- Coloring Method: ColorID
- Material: Opaque
- Drawing Method: Tube
- Radius: 0.5
- Resolution: 11
- Apply Changes Automatically:

**VMD 1.8.2b7 OpenGL Display Window:** Shows a 3D ribbon representation of the protein structure (1rc2) colored by the Q Value, with different colors representing different similarity levels.

**Multiple Sequence Alignment Window:** Shows a sequence alignment of four proteins (1f4y, 1j4n, 1lda, 1rc2) with a context menu open over the alignment. The menu options include:

- RMSD Per Residue
- Tree
- STAMP Parameters
- Bulk Residue Selection
- Molecule Coloring
  - Q per residue
  - Sequence Identity per residue
- Highlight Style

The alignment text is as follows:

```
1f4y  -----KLFWAQVADFLATLFLVFTSIGSAL-GF-FY---PVQRIQAVQNVKVSLEAFGLSATLAQS-VGHSGAHLNFAVTLGLLLSQGISIF-RAI
1j4n  MASEFKKLFWRARVAEFLAMILFIFISIGSAL-GF-HYPIKSNQT-TCQVQDNVKSLEAFGLSATLAQSVGH-ISGAHLNFAVTLGLLLSQGI-ISVLRRI
1lda  -----TLRGQCIAEPLGTGLLIFPGVGCVA-ALKVA-----G-A-SFGQWEISVIWGLGVAMAIYLTG-VVSGAHLNFAVTLALWLFQ-CFDKRRV
1rc2  -----MFRKLAACEPGTFLVLFVGGCGSAVLA-AG-----FPE-LGIGFAGVALPGLTTLTMAFAVG-HISGGHPNFAVTLGLWAGG-RFPAKEV
```

# Exhibiting Sequence Identity - Side View

The image displays the VMD (Visual Molecular Dynamics) software interface, illustrating how to exhibit sequence identity in a side view. The main window, titled "VMD 1.8.2b7 OpenGL Display", shows a 3D ribbon representation of a protein structure, colored by sequence identity. The structure is composed of multiple chains, with colors ranging from red to blue, indicating varying degrees of identity. The "VMD Main" window shows a list of loaded molecules:

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	A	D	F		1J4N	2029	1	0
2	A	D	F		1FQY	1661	1	0
3	A	D	F		1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

The "Graphical Representations" window shows the configuration for the selected molecule "5: 1rc2". The "Style" is set to "Tube", the "Color" is "ColorID 3", and the "Selection" is "chain A". The "Drawing Method" is also set to "Tube". The "Multiple Sequence Alignment" window shows a sequence alignment of four proteins: 1fqy, 1j4n, 1lda, and 1rc2. The alignment is displayed in a side view, with sequence identity highlighted in yellow. The alignment shows that the sequences are highly similar, with many residues conserved across all four proteins.

```
1fqy  -----KLFWRVVAEFLATTLFVFIISIGSAL-GF-KY---FVGNQTVQDNVKVSLAFGLSIATLAQS-VGHSIGAHLPNPAVTLGLLSCOISIF-RV
1j4n  MASEFKKLFWRVVAEFLAMILFIFISIGSAL-GF-HYP IKSNOT-TGAVQDNVKVSLAFGLSIATLAQSVGH-I SGAHLPNPAVTLGLLSCO-ISVLRV
1lda  -----TLRGQCIAEFLGTGLLFFGVGVVA-ALKVA-----G-A-SFGQWEISVIWGLGVMAIYLTA-GVSGAHLPNPAVTLALWLFV-CFDKRV
1rc2  -----MFRKLAECFGTFWLVFGCCSAVLA-AG-----FPE-LGIGPAGVALAFGLTVLTMFAVVG-HISGGHFNPAVTIGLWAGG-RFPAREV
```

# Exhibiting Sequence Identity - Top View

The image displays the VMD (Visual Molecular Dynamics) software interface. The main window, titled "VMD Main", contains a menu bar (File, Molecule, Graphics, Display, Mouse, Extensions, Help) and a table of loaded molecules:

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	A	D	F		1J4N	2029	1	0
2	A	D	F		1FQY	1661	1	0
3	A	D	F		1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

Below the table is a playback control bar with a slider at 0, buttons for zoom, Loop, step (set to 1), and speed.

The "Graphical Representations" window shows the configuration for the selected molecule "5: 1rc2". It includes a table for the representation:

Style	Color	Selection
Tube	ColorID 3	chain A

Other settings include "Selected Atoms" (chain A), "Coloring Method" (ColorID 3), "Material" (Opaque), and "Drawing Method" (Tube). Controls for Radius (0.5) and Resolution (11) are also present.

The "Multiple Sequence Alignment" window displays a sequence alignment of four proteins: 1fqy, 1j4n, 1lda, and 1rc2. The alignment shows conserved regions highlighted in yellow:

```
1fqy  -----KLFWRVVAEFLATTLFVFIISIGSAL-GF-KY---FVGNQTAVDNWKVSLAFGLSIATLAQS-VGHSAGHLNPAVTLGLLLSCOISIF-RV
1j4n  MASEFKKLLFWRAVVAEFLAMILFIFISIGSAL-GF-HYP IKSNOT-TGAVQDNVKVSLAFGLSIATLAQSVGH-I SGAHLNPAVTLGLLLSCO-ISVLRV
1lda  -----TLRGQCIAEFLGTGLLFFGVGVA-ALKVA-----G-A-SFGQWEISVIWGLGVMAIYLTA-GVSGAHLNPAVTIALWLFV-CFDKRV
1rc2  -----MFRKLAECFQTFWLVFGCCSAVLA-AG-----FPE-LGIGFAGVALAFGLTVLTMFAFVG-HISGGHFNPAVTIGLWAGG-RFPAREV
```

# Showing Conserved Residues - Monomer

The screenshot displays the VMD (Visual Molecular Dynamics) software interface. The main window, titled 'VMD 1.8.2b7 OpenGL Display', shows a 3D ribbon representation of a protein monomer. The protein is colored by residue type: red for alpha-helices, green for beta-strands, and yellow for loops and turns. The 'VMD Main' window shows a table of loaded molecules:

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	A	D	F		1J4N	2029	1	0
2	A	D	F		1FQY	1661	1	0
3	A	D	F		1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

The 'Graphical Representations' window is configured for molecule '5: 1rc2'. The 'Selected Molecule' is '5: 1rc2'. The 'Style' is 'Tube', 'Color' is 'ColorID 3', and 'Selection' is 'chain A'. The 'Drawing Method' is 'Tube'. The 'Coloring Method' is 'ColorID' with a value of '3'. The 'Material' is 'Opaque'. The 'Drawing Method' is 'Tube'. The 'Radius' is set to 0.5 and the 'Resolution' is set to 11. The 'Apply Changes Automatically' checkbox is checked.

The 'Multiple Sequence Alignment' window shows a sequence alignment of four proteins: 1fqy, 1j4n, 1lda, and 1rc2. The alignment is displayed as follows:

```

1fqy  -----KLFWRVVAEFLATTLFVFIISIGSAL-GF-KY---FVGNQTVQDNVKVSLAFGLSIATLAQS-VGHSIGAHLPNPAVTLGLLLSCOISIF-RV
1j4n  MASEFKKLFWRVVAEFLAMILFIFISIGSAL-GF-HYPIKSNQ-TGAVQDNVKVSLAFGLSIATLAQSVGH-ISGAHLPNPAVTLGLLLSCO-ISVLRV
1lda  -----TLRGQCIAEFLGTGLLFFGVGVVA-ALKVA-----G-A-SFGQWEISVIWGLGVMAIYLTA-GVSGAHLPNPAVTLALWLFV-CFDKRV
1rc2  -----MFRKLAECFQTFWLVFGCCSAVLA-AG-----FPE-LGIGPAGVALAFGLTVLTMFAVVG-HISGGHNPNAVTLGLWAGG-RFPAREV
  
```

The conserved residues are highlighted in yellow in the original image.

# Showing Conserved Residues - Tetramer

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
1	A	D	F		1J4N	2029	1	0
2	A	D	F		1FQY	1661	1	0
3	A	D	F		1lda	1997	1	0
5	T	A	D	F	1rc2	3530	1	0

0

zoom  Loop step 1 speed

Graphical Representations

Selected Molecule

5: 1rc2

Create Rep Delete Rep

Style	Color	Selection
Tube	ColorID 3	chain A

Selected Atoms

chain A

Draw style Selections Trajectory Periodic

Coloring Method Material

ColorID 3 Opaque

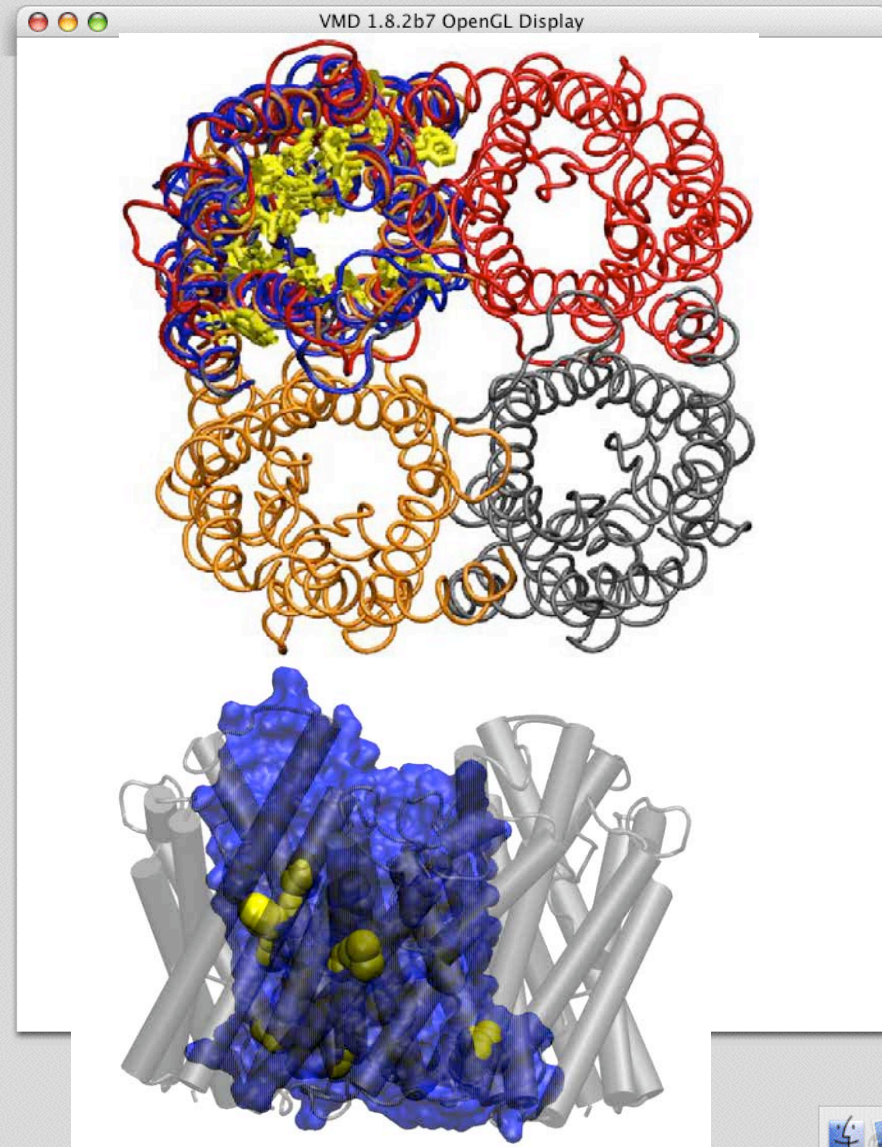
Drawing Method

Tube Default

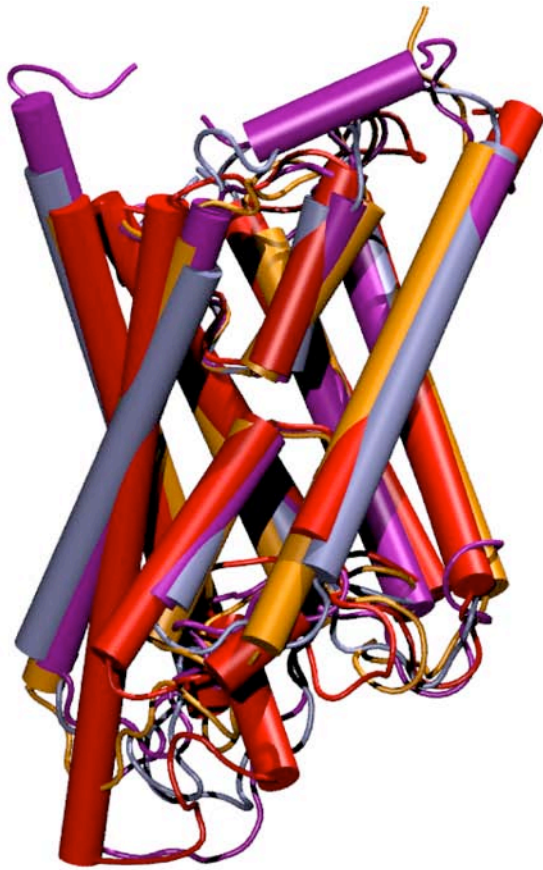
Radius 0.5

Resolution 11

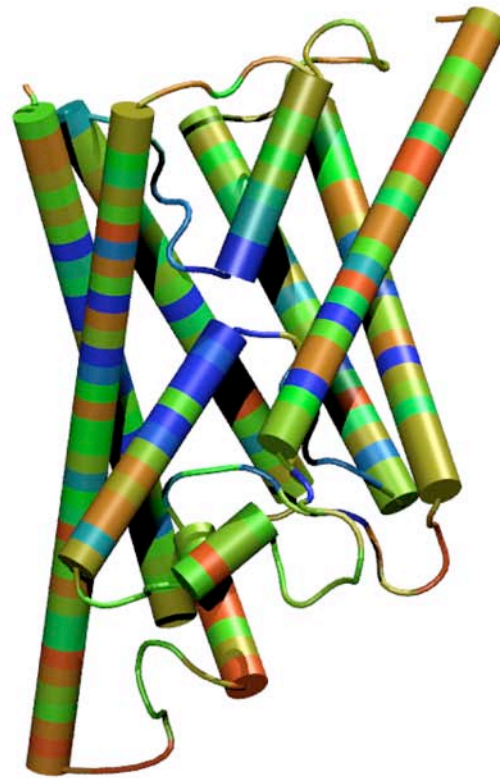
Apply Changes Automatically Apply



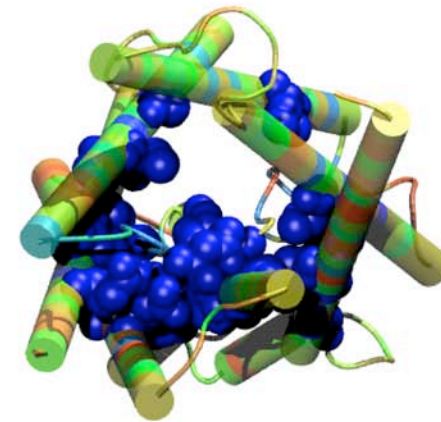
# Structure and Sequence Comparisons Water/Glycerol Channels



2 AQP1, GLPF, AQPZ  
from animal and bacteria



GLPF Sequence Conservation



Top view

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