

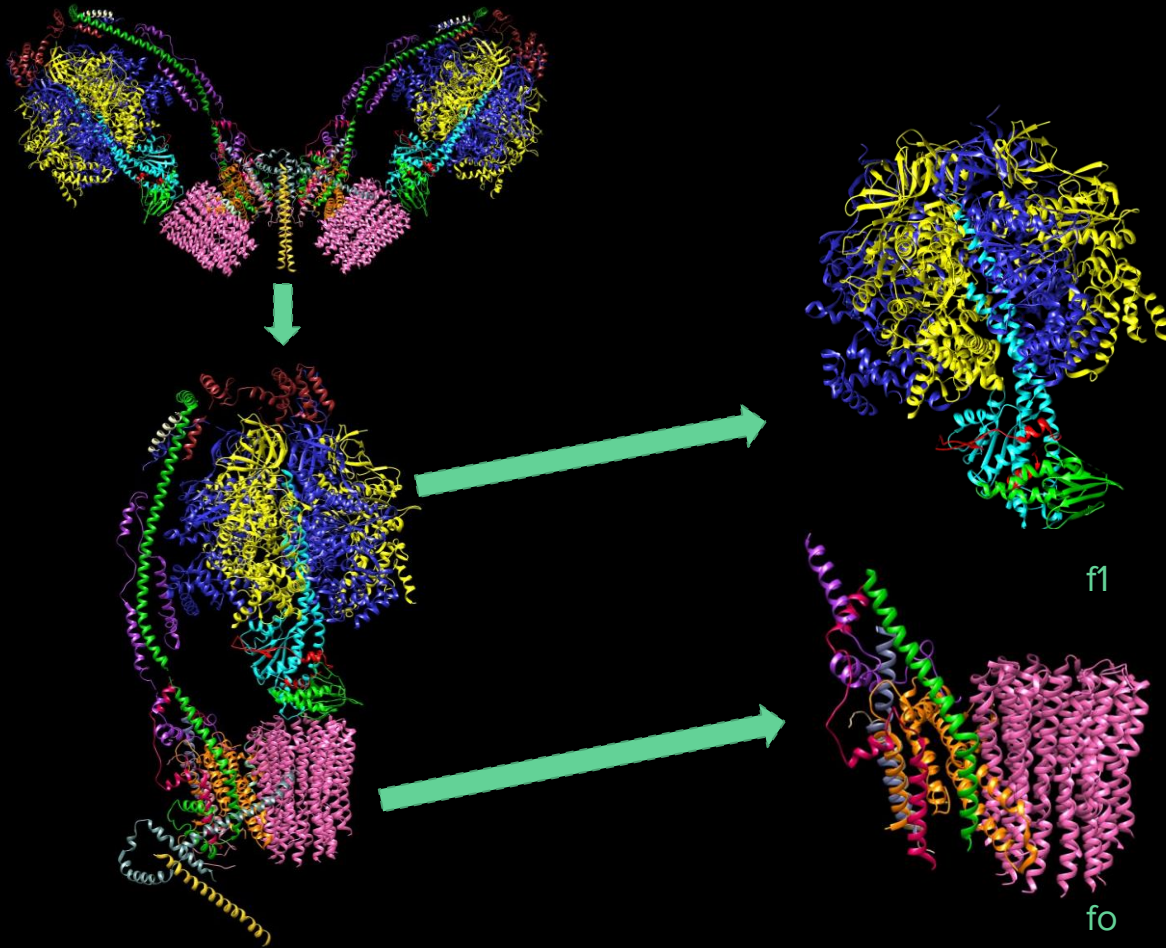


ATP SYNTHASE COMPLEX

Structural Biology - Group 11

Víctor Herrera, Socayna Jouide, Xavier Marimon, Rebeca Sánchez and Ana Yagüe

Index



Interactions
+
Comparisons

ATPase CLASSIFICATION

- V-ATPases: located in vacuoles in eukaryotic cells.
- E-ATPases: located in the cellular surface
- P-ATPases: located in bacteria, organelles and eukaryote plasmatic membranes
- F-ATPases: located in the mitochondria, chloroplast and bacterial plasmatic membrane.
- A-ATPases: located in Archaea

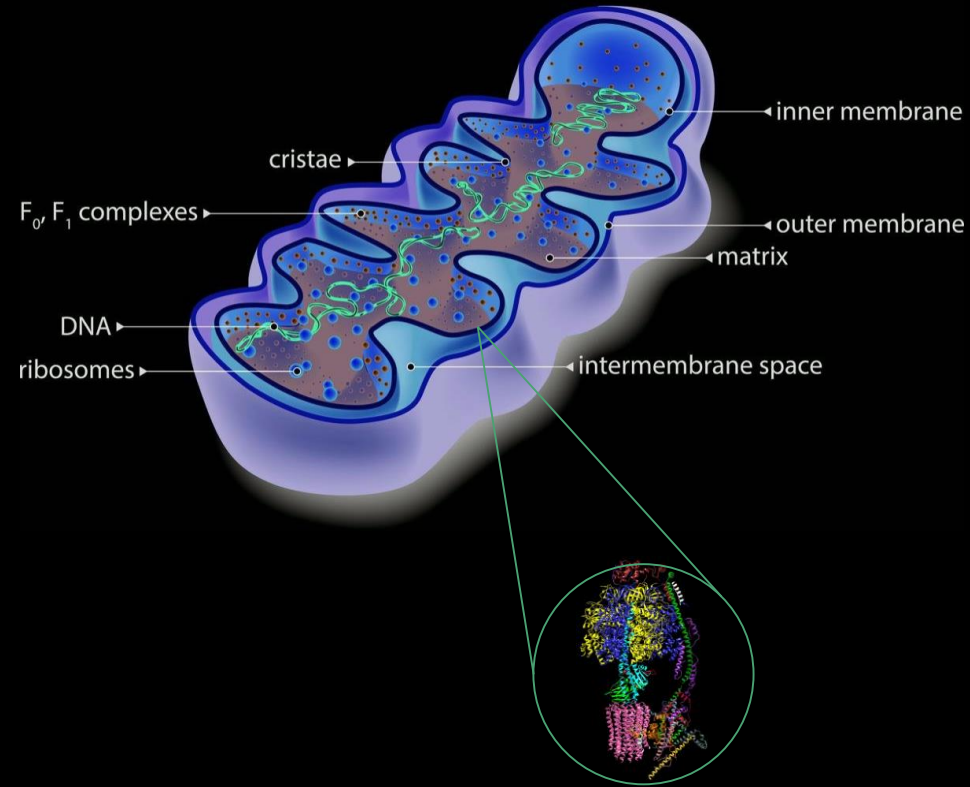


ATP hydrolysis

ATP synthesis

ATP SYNTHASE

- Located in the mitochondrial membrane, chloroplasts and bacterial plasmatic membrane
- 10nm diameter
- Almost 100% effectivity
- Two functional domains: F1 and Fo



Proton gradient



Protons pass
through Fo



F1 coupled

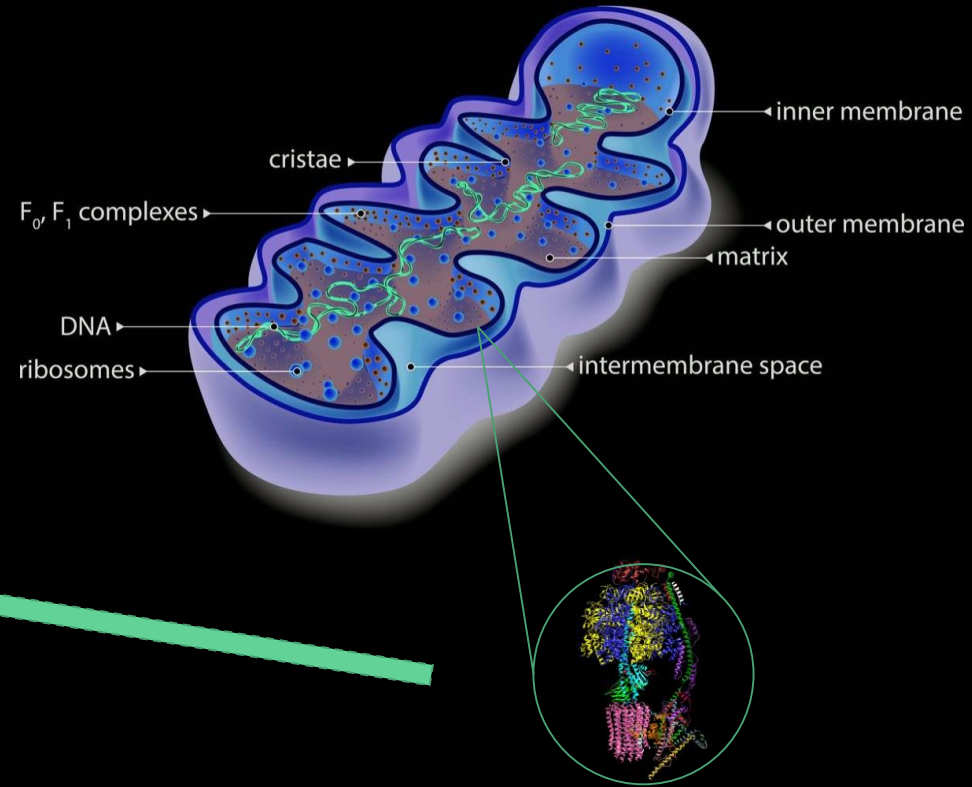


ADP + P



ATP

ATP SYNTHASE



Proton gradient



Protons pass
through F_0



F_1 coupled



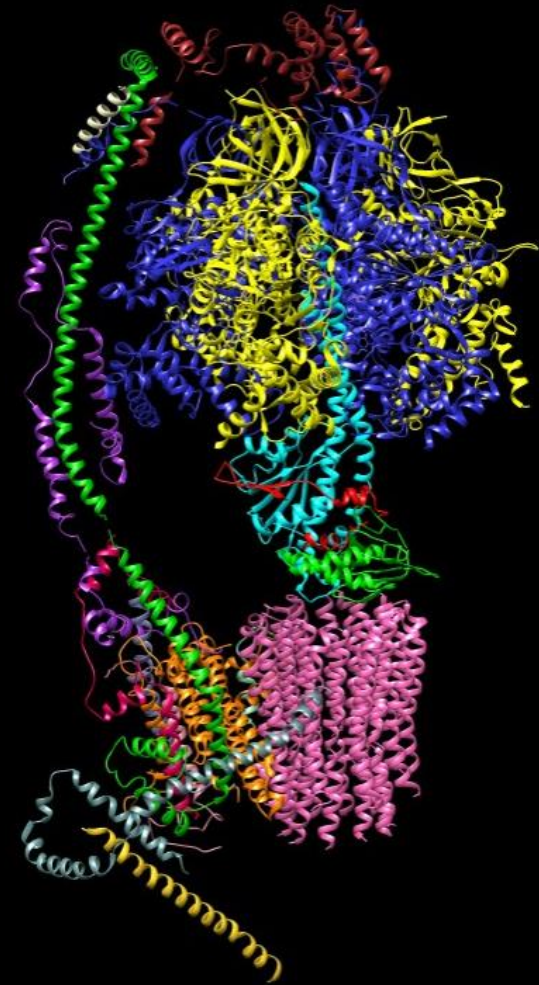
ADP + P



ATP

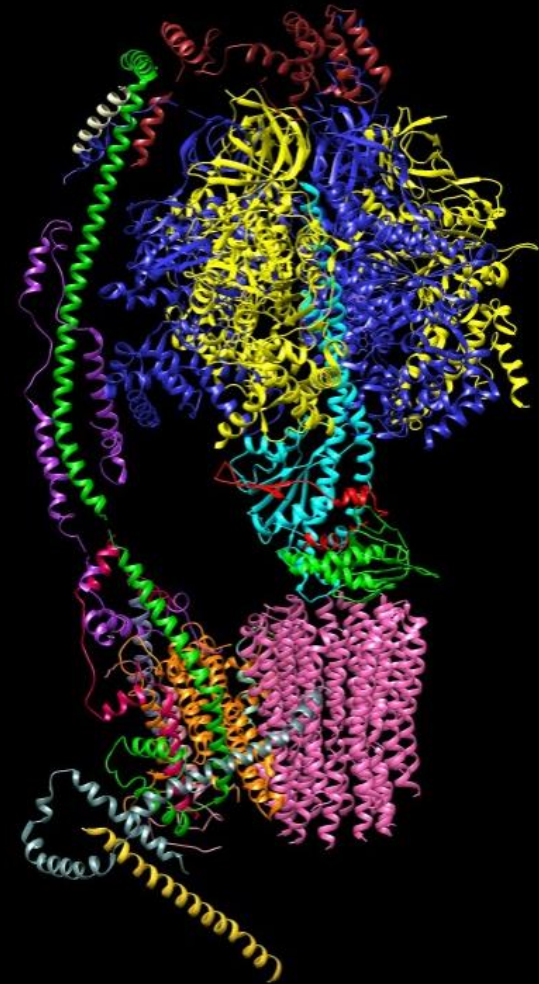
YEAST F1-F₀ ATP SYNTHASE

F1		F ₀		
Catalytic head	Central stalk	Peripheral Stalk	Rotor	Supernumerary subunits
α	γ	b	a	f
β	δ	OSCP	8	i/j
	ϵ	d	c (ring)	k
		h		g
				e

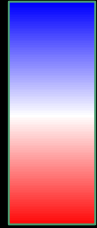


YEAST F1-F₀ ATP SYNTHASE

- SUBUNIT ALPHA
- SUBUNIT BETA
- SUBUNIT GAMMA
- SUBUNIT DELTA
- SUBUNIT EPSILON
- SUBUNIT c
- SUBUNIT a
- SUBUNIT b
- SUBUNIT 8
- SUBUNIT f
- SUBUNIT d
- SUBUNIT OSCP
- SUBUNIT h
- SUBUNIT e
- SUBUNIT g
- SUBUNIT k
- SUBUNIT i/j



YEAST F1-F₀ ATP SYNTHASE: hydrophobicity



HYDROPHILIC

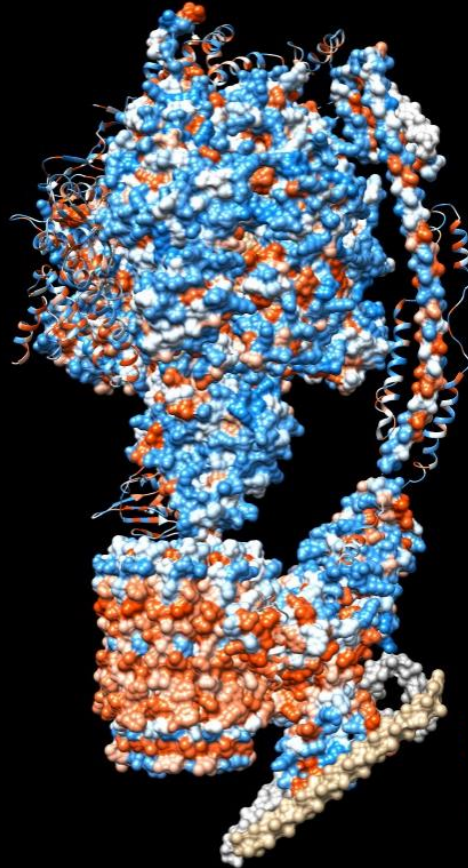
HYDROPHOBIC

Matrix regions

- Total residues = 2183
- **Polar residues = 1190 - Percentage: 54.5**
- Nonpolar residues = 993 - Percentage: 45.5
- Acidic residues = 270 - Percentage: 12.4
- Basic residues = 259 - Percentage: 11.9
- Basic residues with His = 286 - Percentage: 13.1

Membrane-embedded regions

- Total residues = 573
- Polar residues = 225 - Percentage: 39.3
- **Nonpolar residues = 348 - Percentage: 60.7**
- Acidic residues = 24 - Percentage: 4.2
- Basic residues = 42 - Percentage: 7.3
- Basic residues with His = 55 - Percentage: 9.6

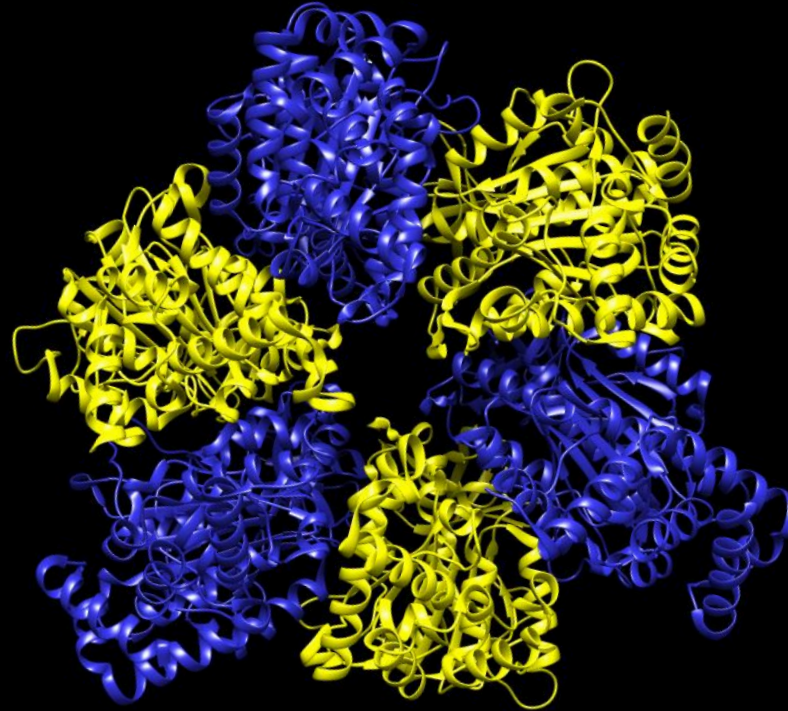


F1 ATP SYNTHASE



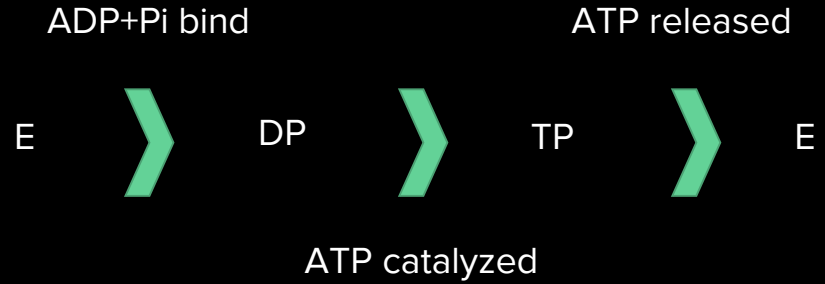
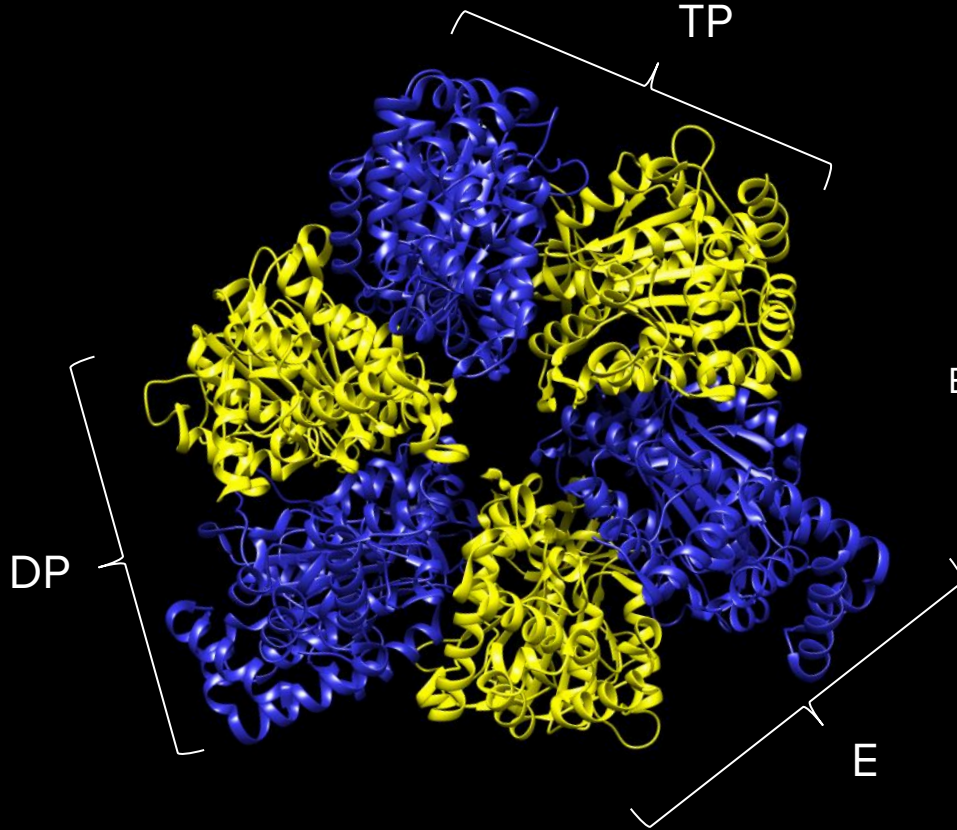
- ALPHA
- BETA
- GAMMA
- DELTA
- EPSILON

ALPHA AND BETA COMPLEX



- ALPHA
- BETA

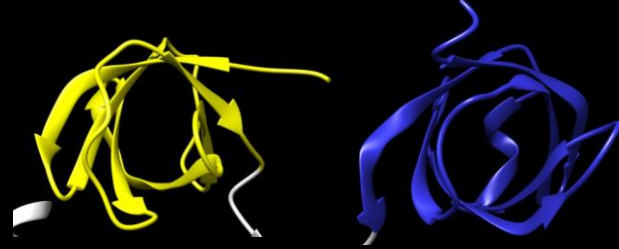
ALPHA AND BETA COMPLEX



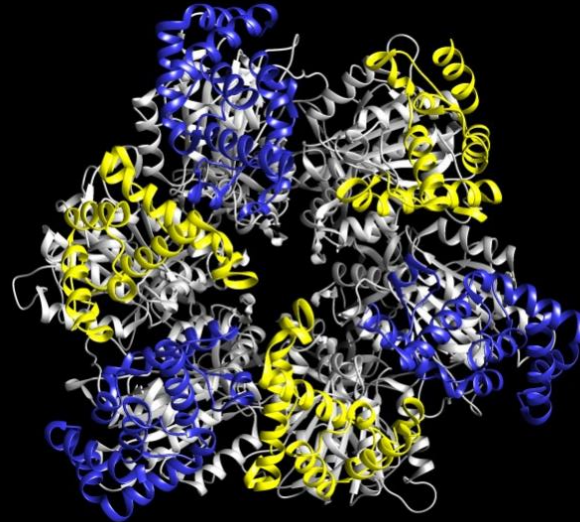
- ALPHA
- BETA

ALPHA AND BETA COMPLEX

Beta barrel

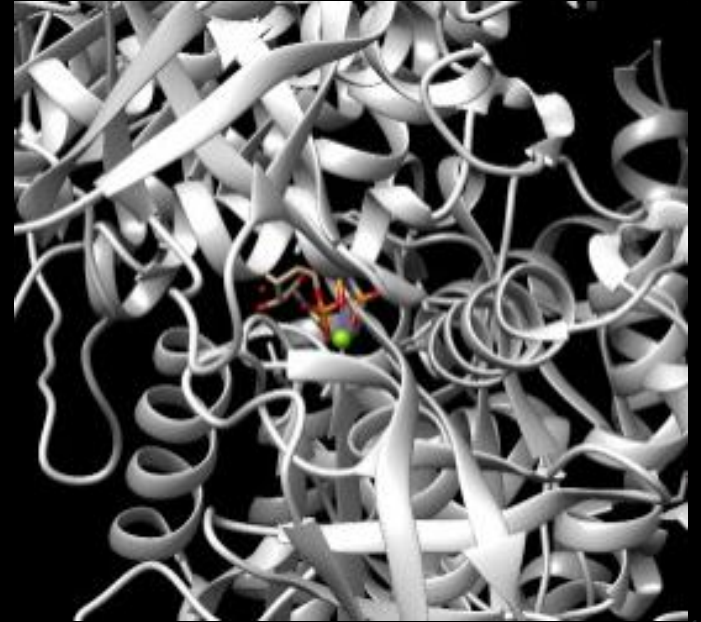


Alpha helix bundle

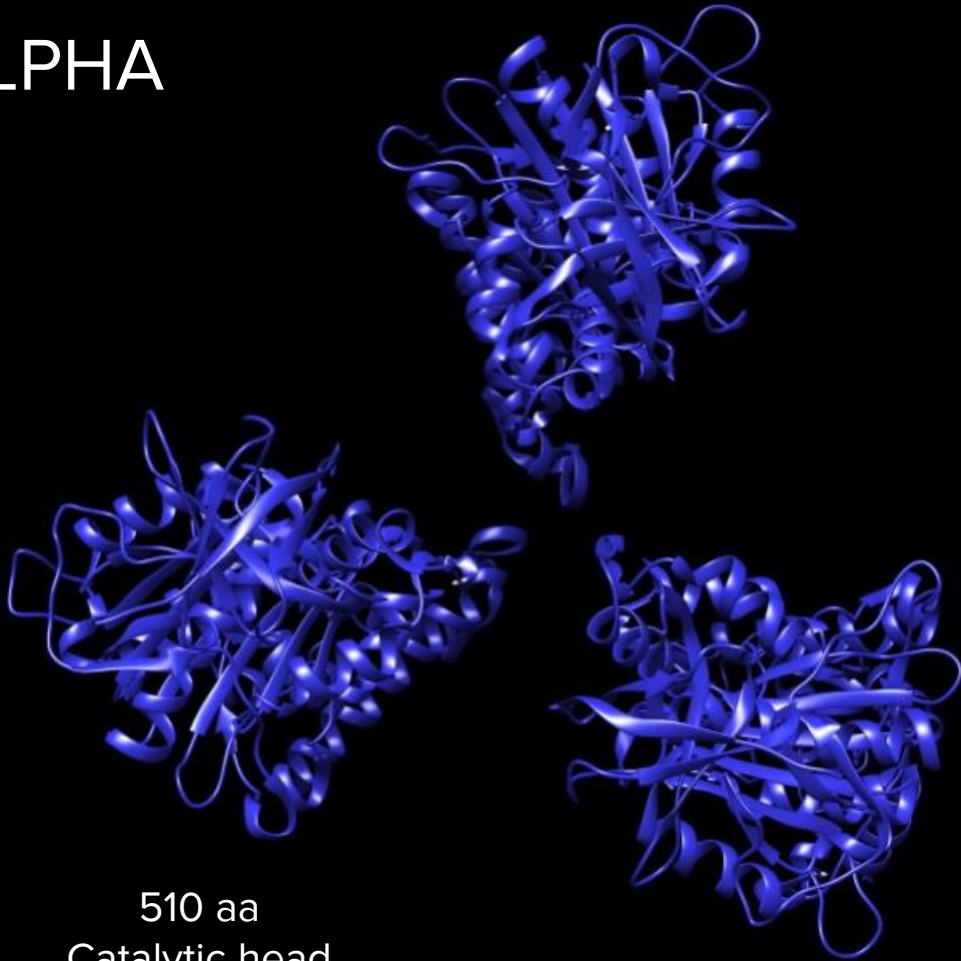


● ALPHA
● BETA

ALPHA AND BETA COMPLEX



ALPHA



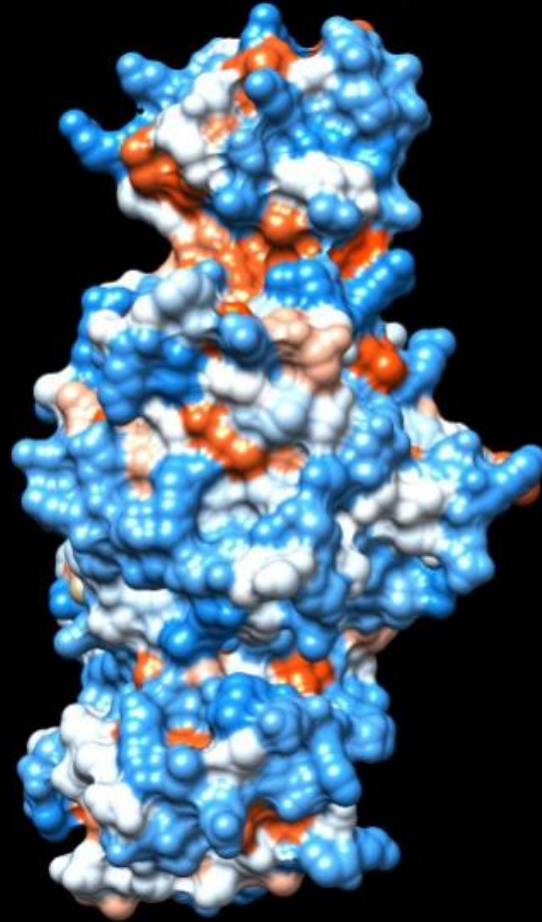
510 aa
Catalytic head



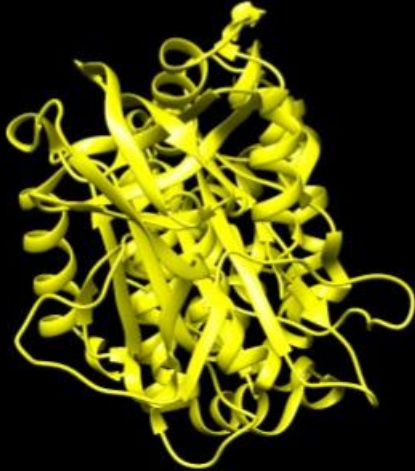
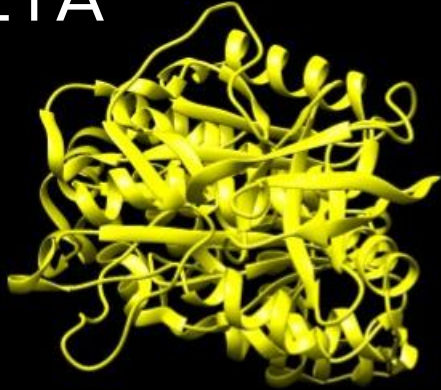
Beta barrel and alpha helix bundle

ALPHA

- Total residues = 510
- **Polar residues = 274 - Percentage: 53.7**
- Nonpolar residues = 236 - Percentage: 46.3
- Acidic residues = 58 - Percentage: 11.4
- Basic residues = 57 - Percentage: 11.2
- Basic residues with His = 63 - Percentage: 12.4



BETA



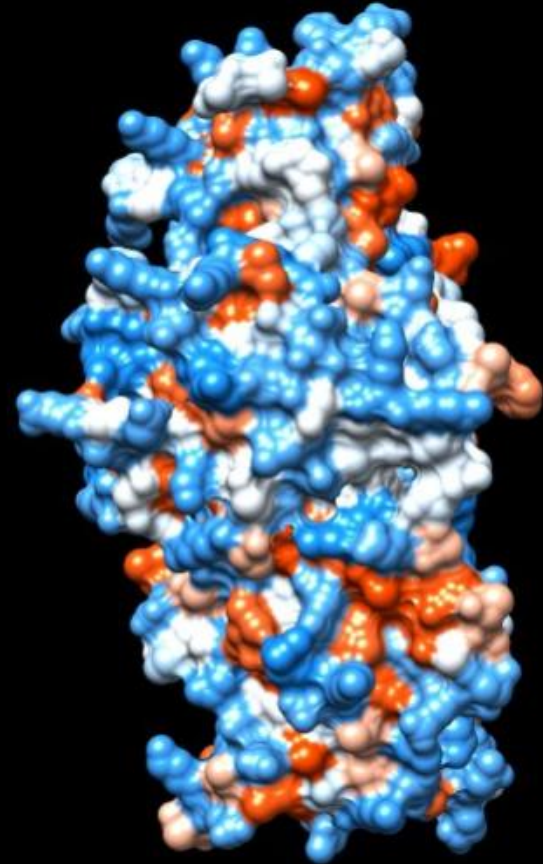
478 aa
Catalytic head



Beta barrel and alpha helix bundle

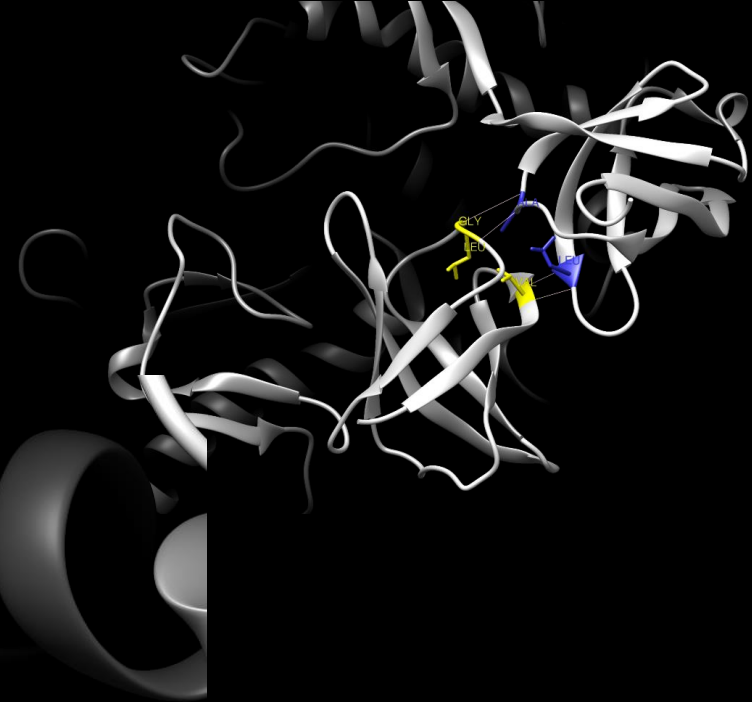
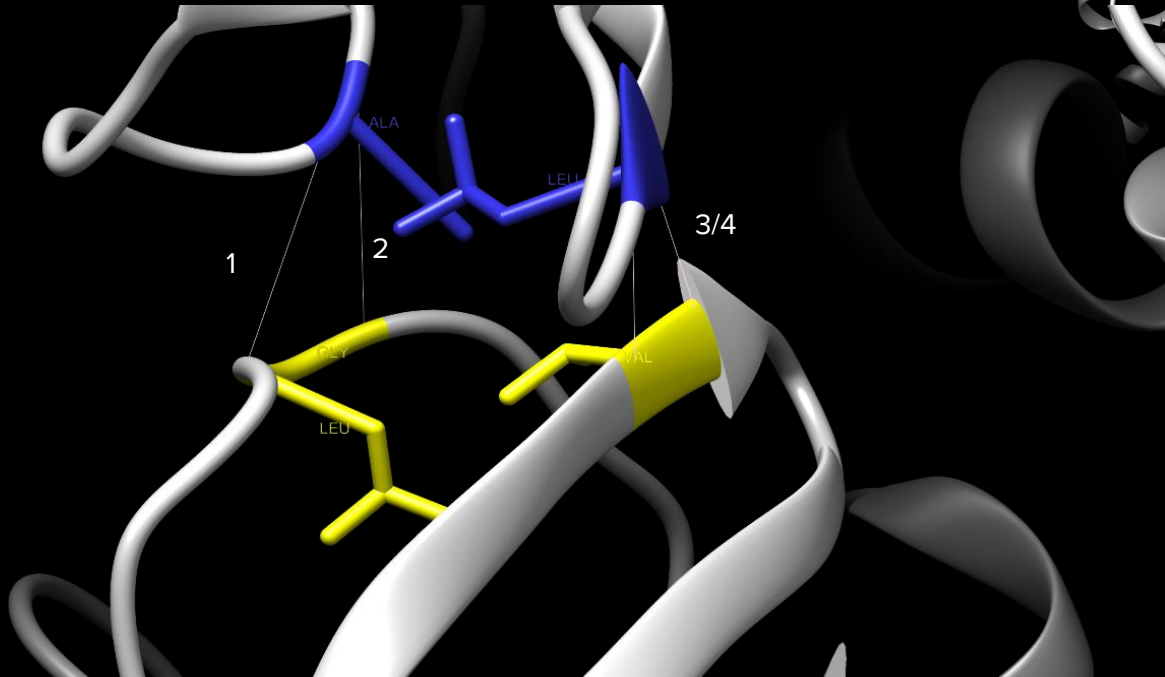
BETA

- Total residues = 478
- **Polar residues = 252 - Percentage: 52.8**
- Nonpolar residues = 226 - Percentage: 47.3
- Acidic residues = 63 - Percentage: 13.2
- Basic residues = 48 - Percentage: 10
- Basic residues with His = 55 - Percentage: 11.5



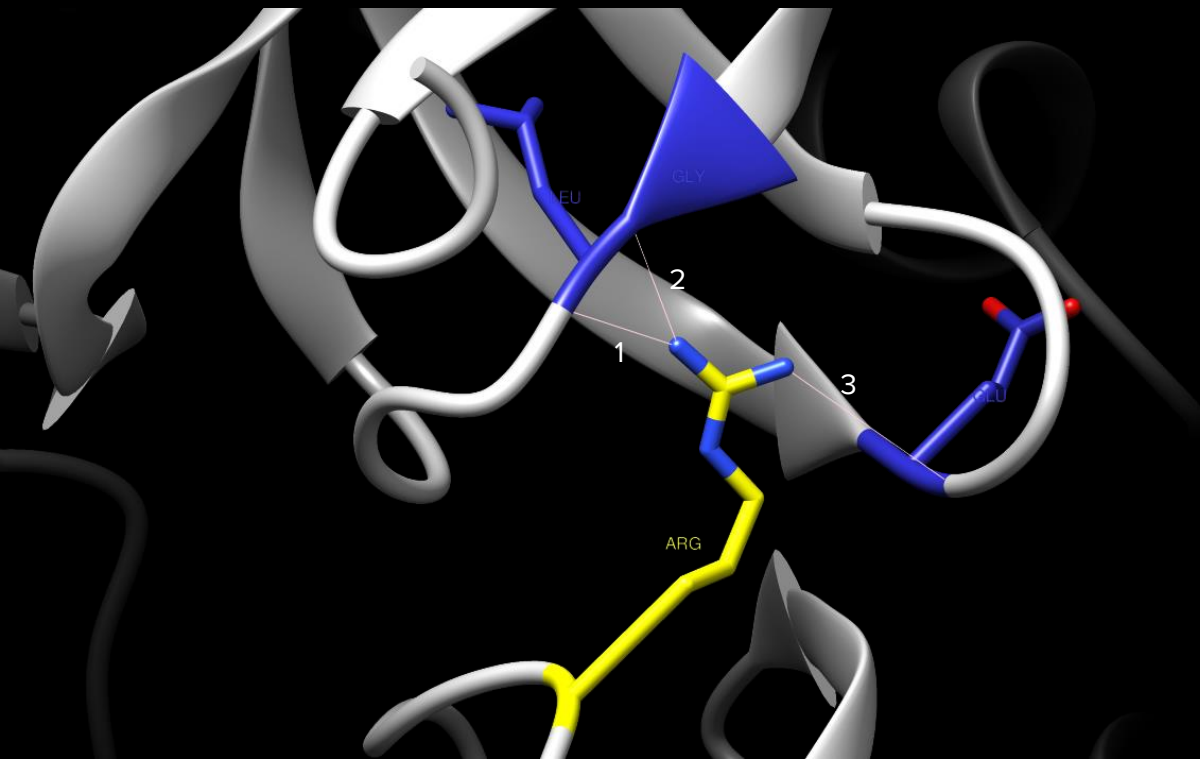
ALPHA-BETA INTERACTIONS

- | | | |
|---------------|------------|--------|
| 1. ALA 51.A N | LEU 70.E O | 2.661Å |
| 2. GLY 69.E N | ALA 51.A O | 3.047Å |
| 3. LEU 68.A N | VAL 16.E O | 2.741Å |
| 4. VAL 16.E N | LEU 68.A O | 2.718Å |



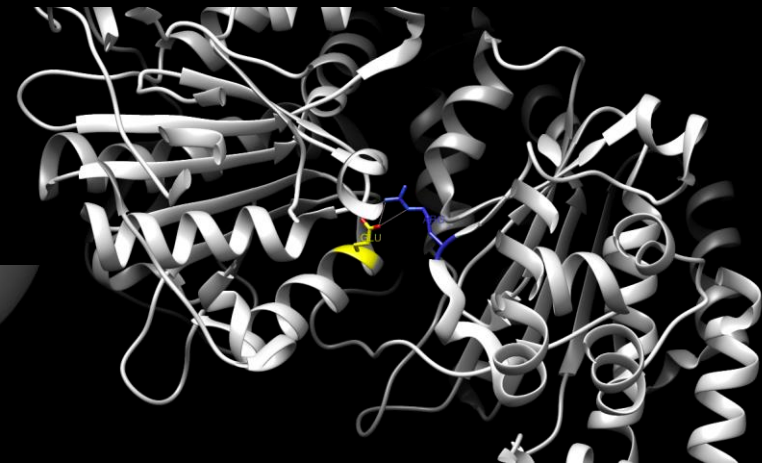
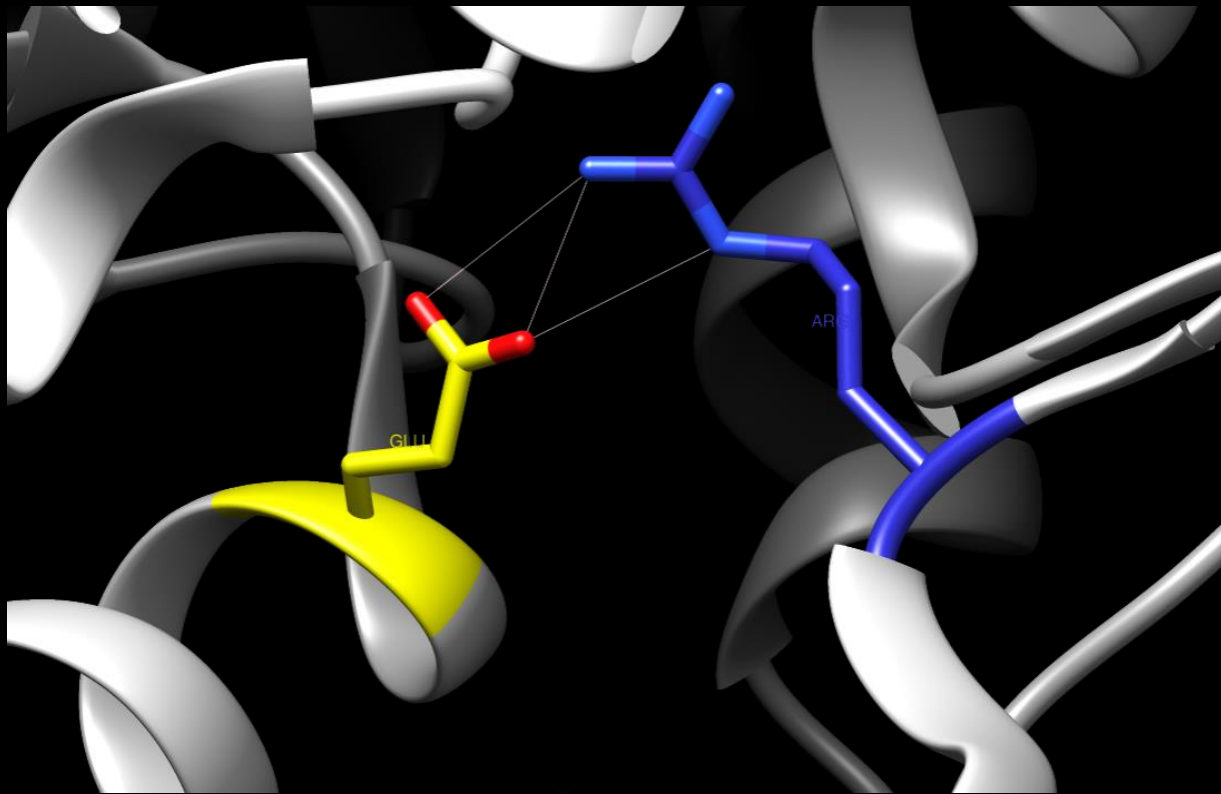
ALPHA-BETA INTERACTIONS

ARG 72.E N HOH 826.A O 2.876Å
ARG 72.E NE HOH 826.A O 3.075Å
ARG 72.E NH2 HOH 826.A O 3.852Å



1. ARG 72.E NH2 LEU 46.A O 2.910Å
2. ARG 72.E NH2 GLY 45.A O 2.798 Å
3. ARG 72.E NH1 GLU 69.A O 2.866Å

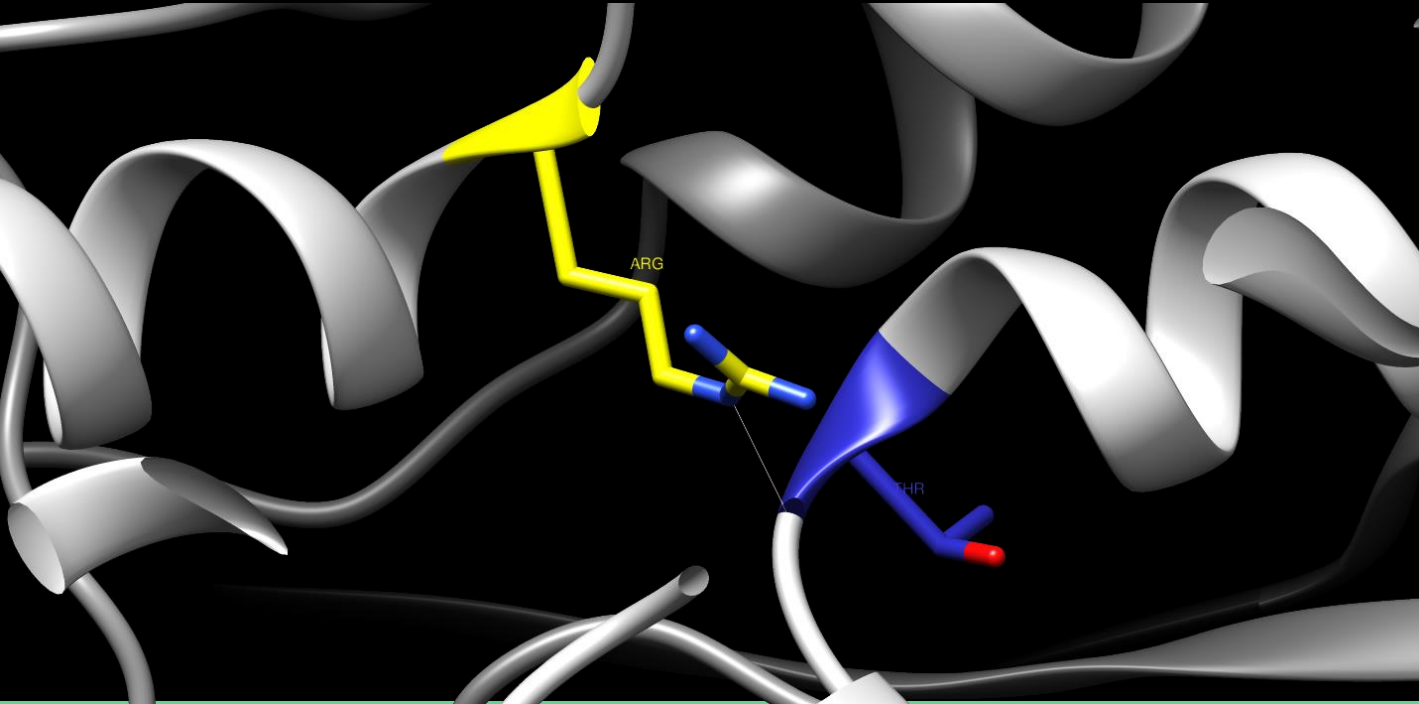
ALPHA-BETA INTERACTIONS



ARG 375.A NE GLU 193.E OE2 3.483Å
ARG 375.A NH2 GLU 193.E OE1 4.064Å
ARG 375.A NH2 GLU 193.E OE2 3.006Å

ALPHA-BETA INTERACTIONS

ARG 190.E NE THR 348.A O 3.228Å

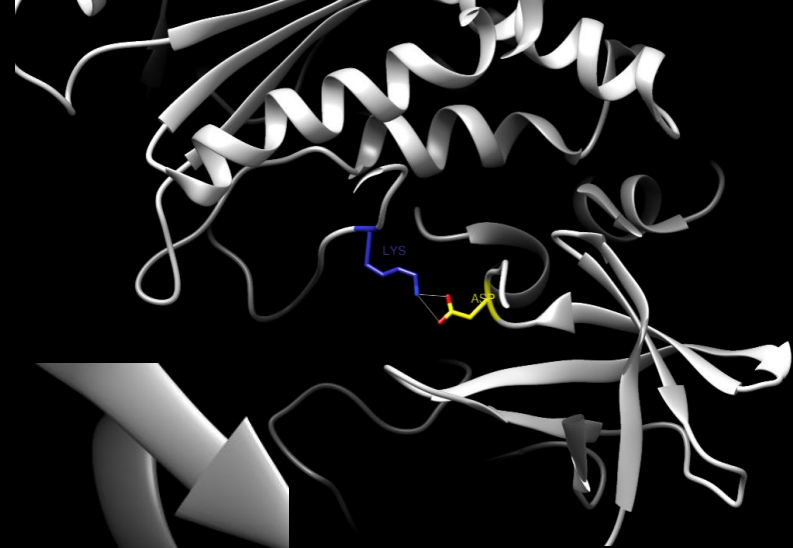
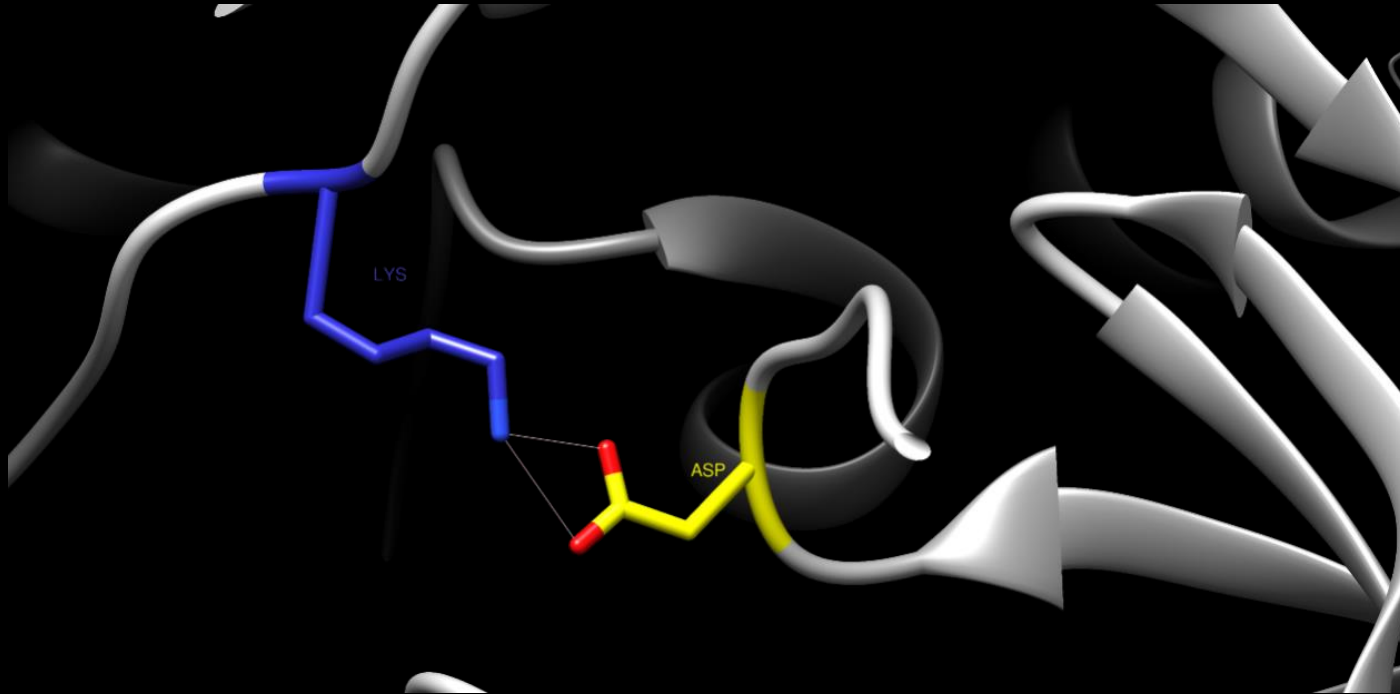


ALPHA-BETA INTERACTIONS

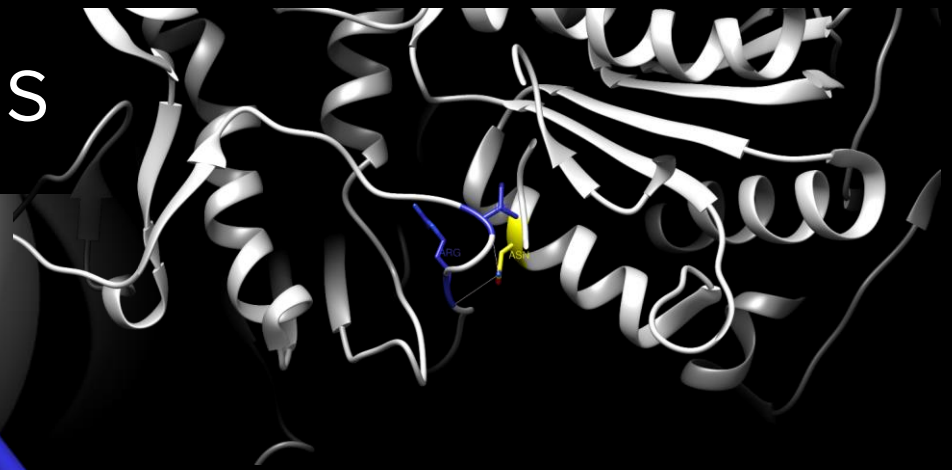
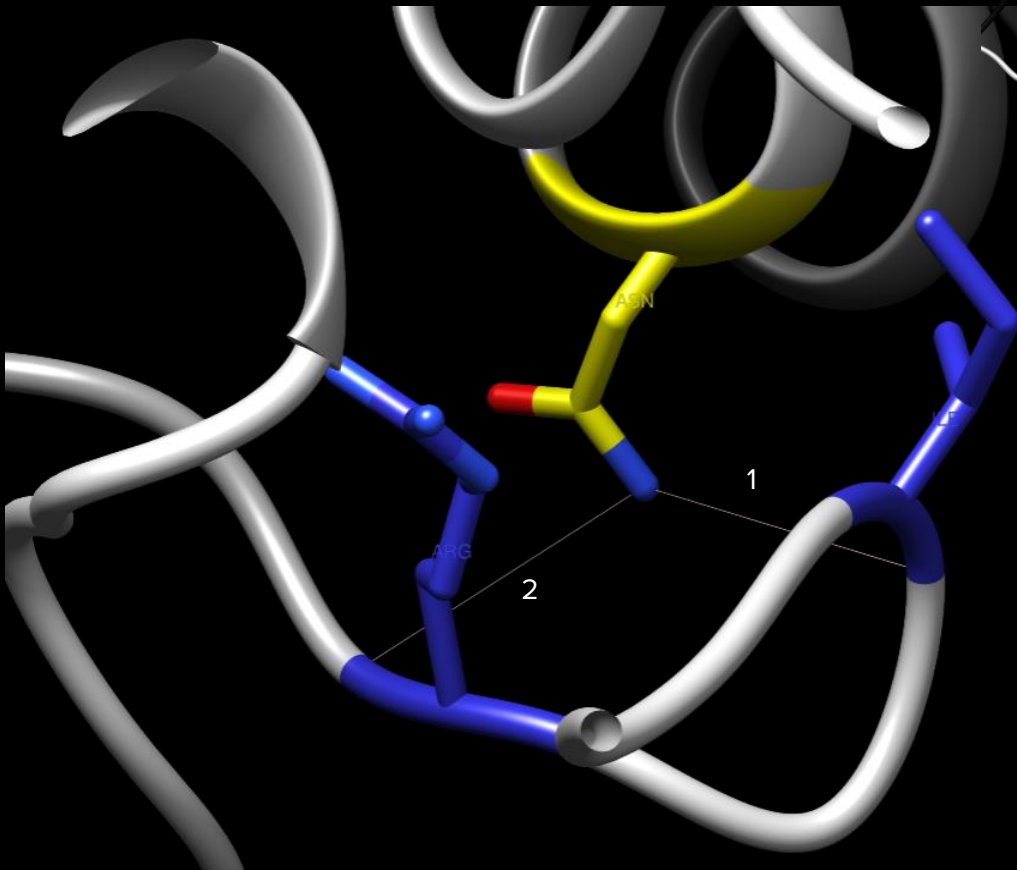
LYS 134.A NZ ASP 65.E OD1 2.761Å

LYS 134.A NZ ASP 65.E OD2 3.033Å

HOH 809.A O LYS 134.A O 2.754Å



ALPHA-BETA INTERACTIONS

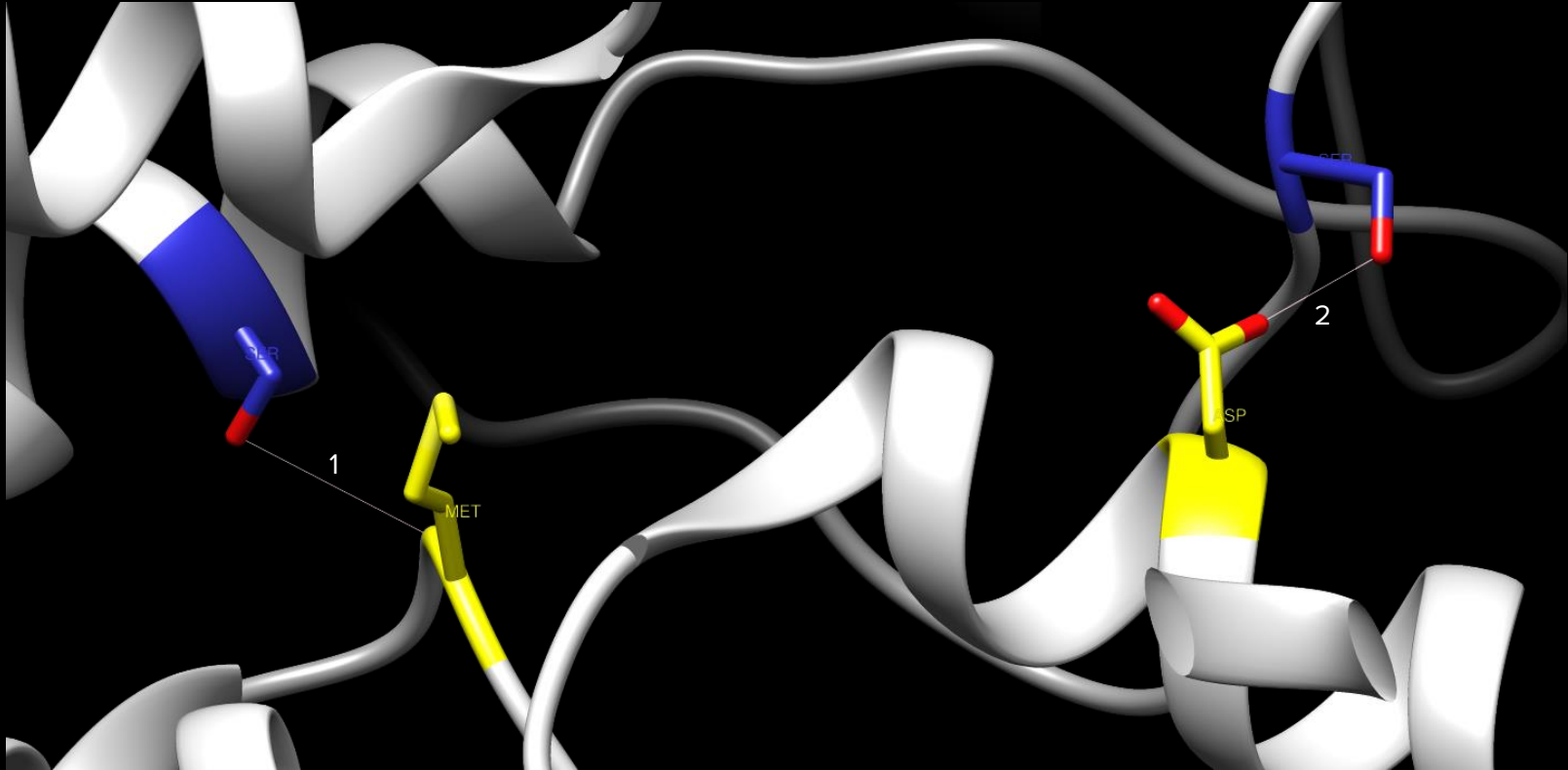


1. ASN 195.E ND2 ILE 138.A O 2.763Å
2. ASN 195.E ND2 ARG 141.A O 3.088Å

ALPHA-BETA INTERACTIONS

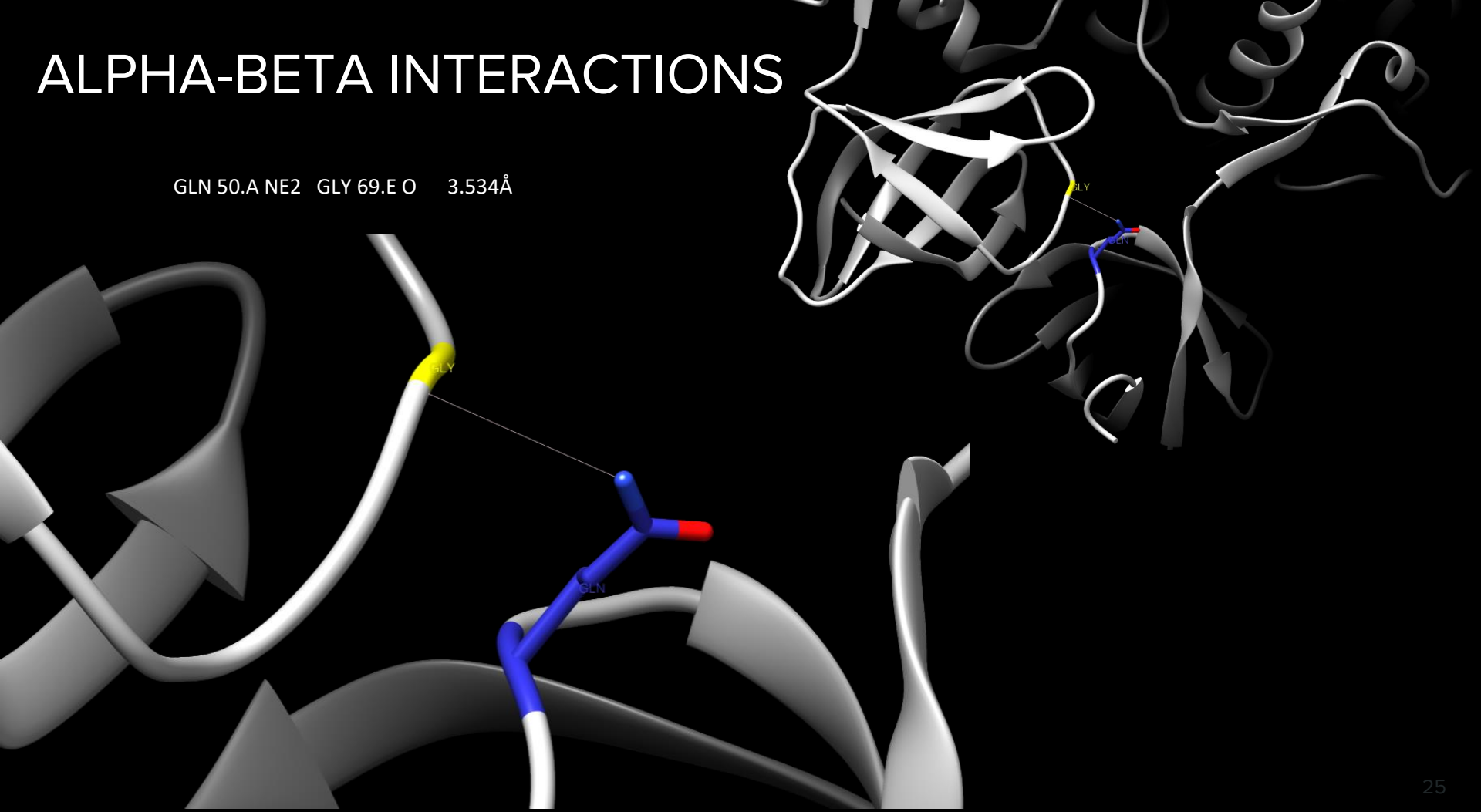
1. SER 305.A OG MET 222.E O 2.713Å

2. SER 143.A OG ASP 196.E OD1 2.703Å



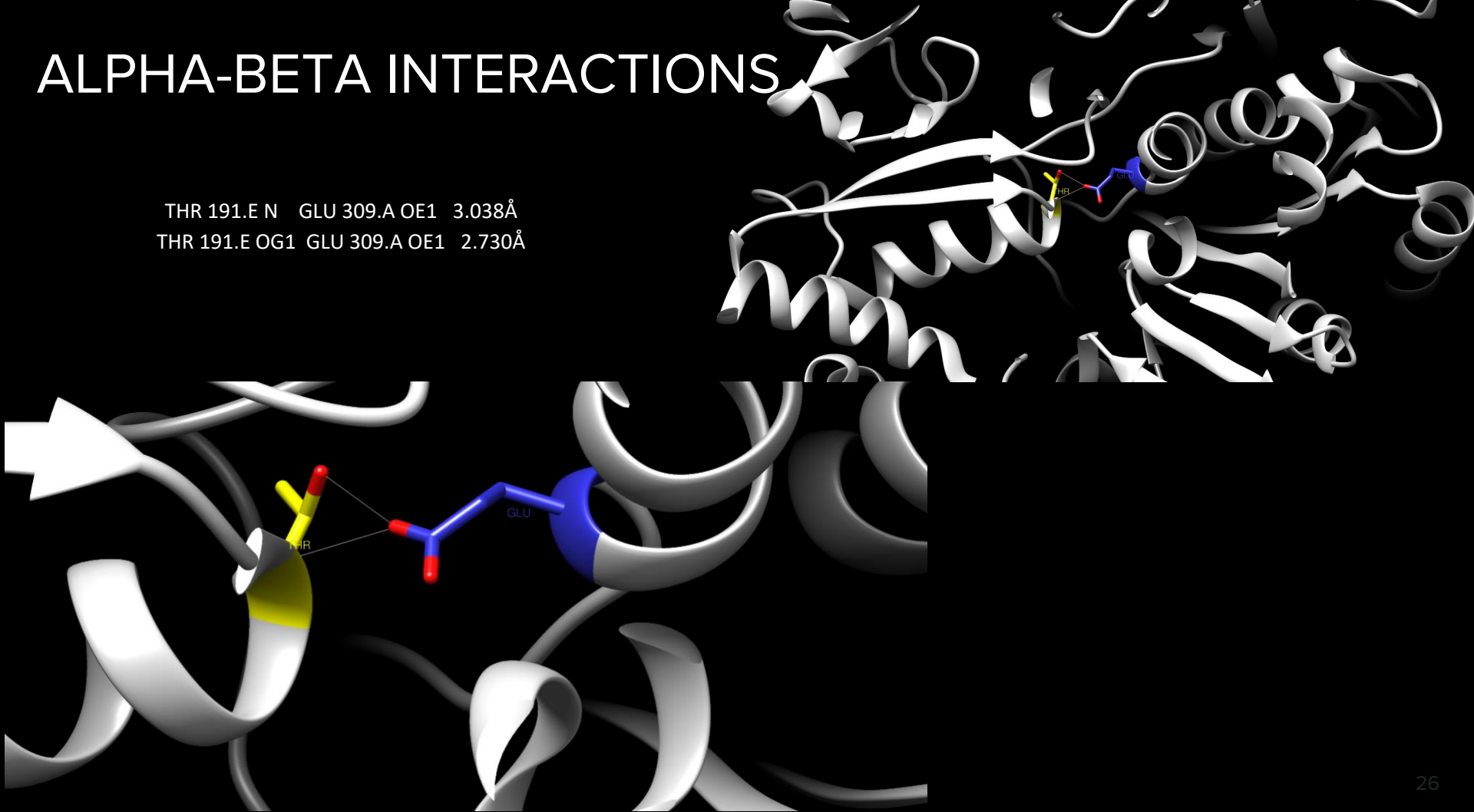
ALPHA-BETA INTERACTIONS

GLN 50.A NE2 GLY 69.E O 3.534Å



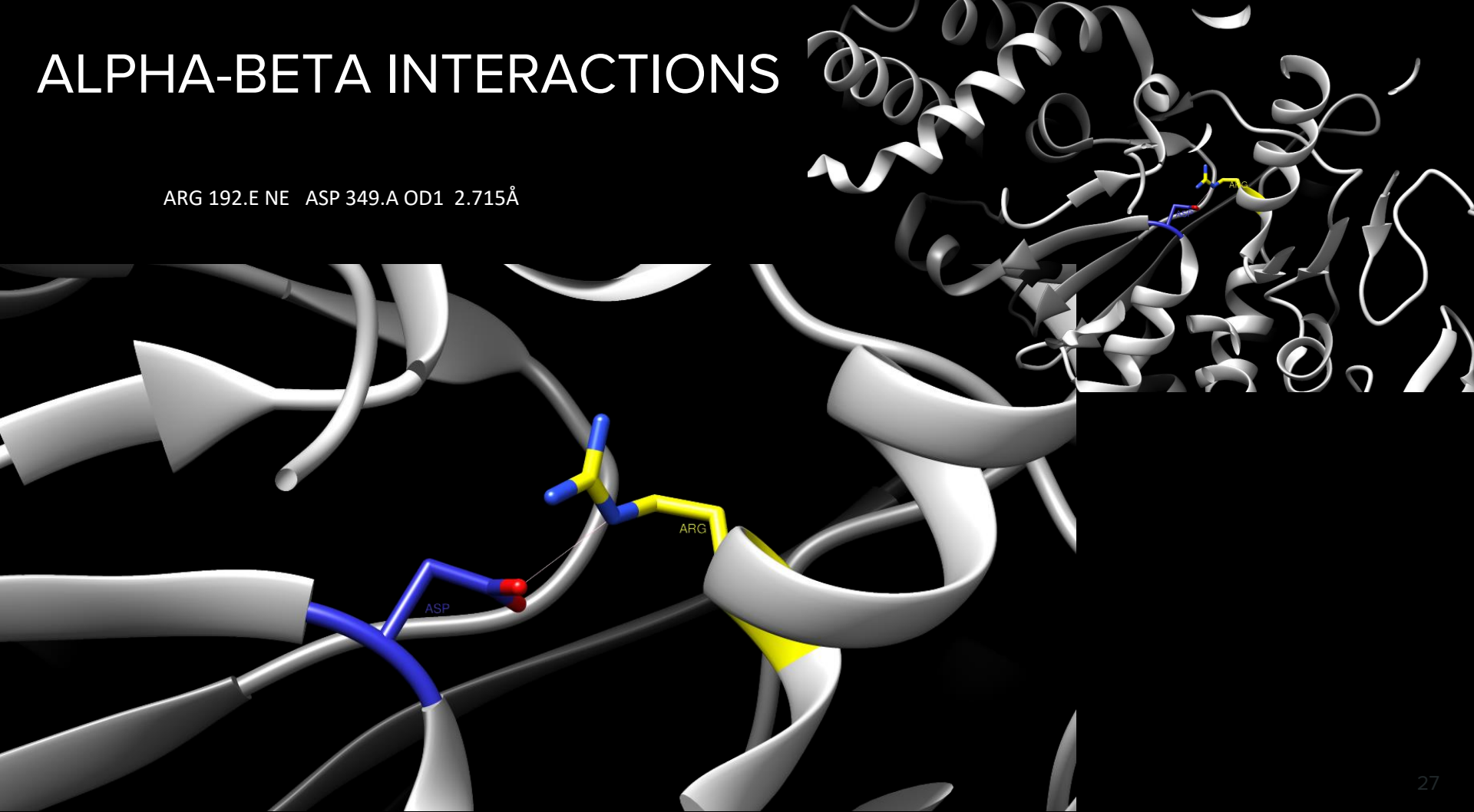
ALPHA-BETA INTERACTIONS

THR 191.E N GLU 309.A OE1 3.038Å
THR 191.E OG1 GLU 309.A OE1 2.730Å



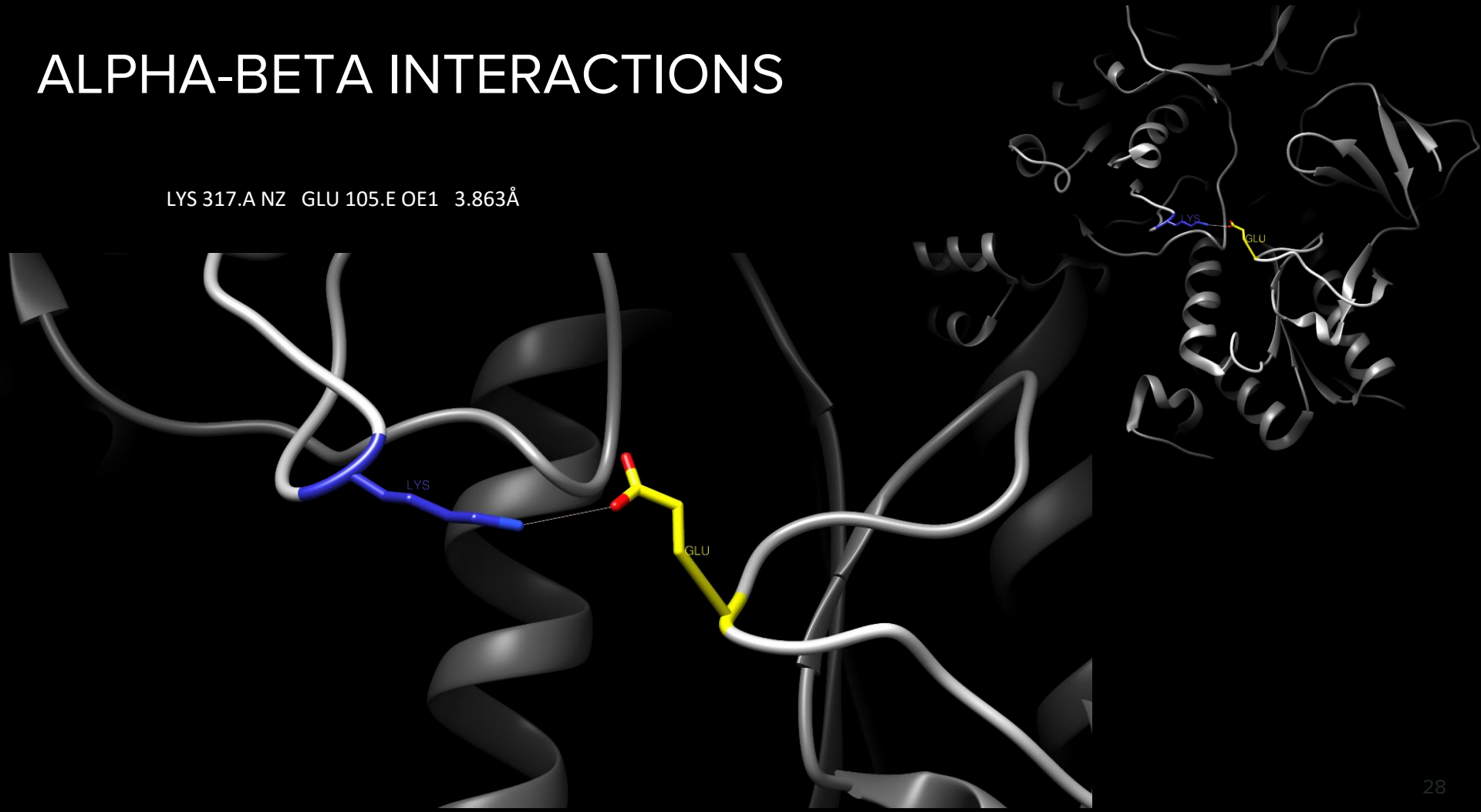
ALPHA-BETA INTERACTIONS

ARG 192.E NE ASP 349.A OD1 2.715Å



ALPHA-BETA INTERACTIONS

LYS 317.A NZ GLU 105.E OE1 3.863Å



LIGAND INTERACTIONS

ALPHA

- Arg375
- Thr178

BETA

- Lys163
 - Arg190
 - Gly162
 - Thr164
 - Glu189
 - Gly160
 - Arg260
 - Asn257
- } Only TP
- } Only E

Types of interactions

1. Hydrogen bonds
2. Salt bridges
3. Ionic/electrostatic interactions

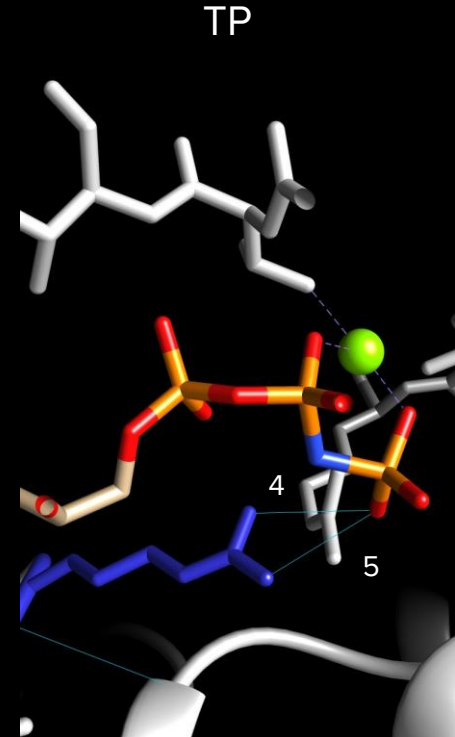
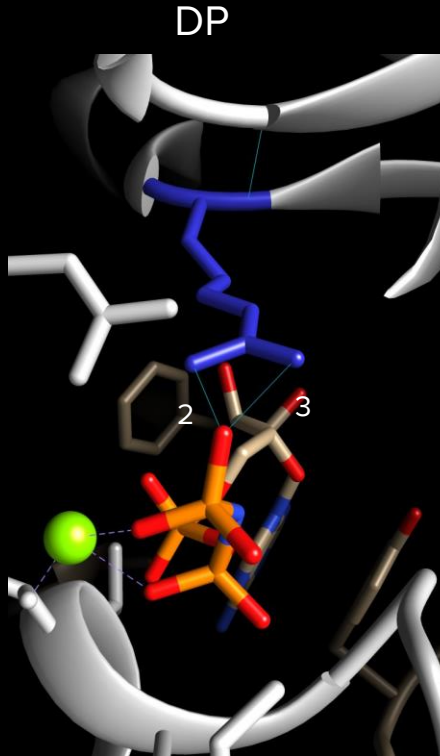
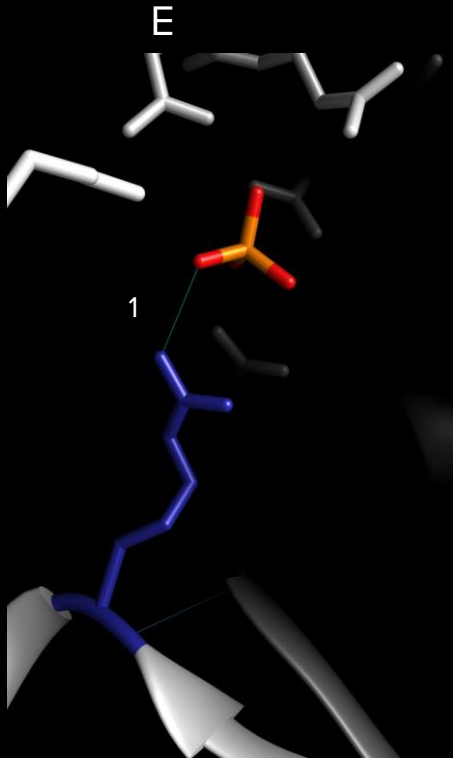
Nucleotide Phosphate interaction

N. phosphate + Magnesium

LIGAND INTERACTIONS

α Arg375

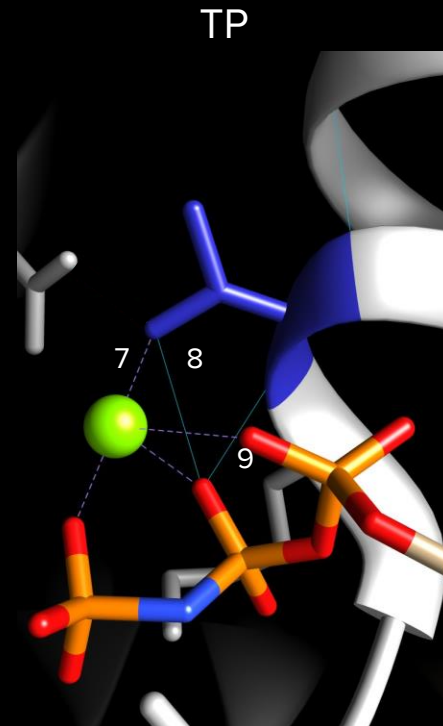
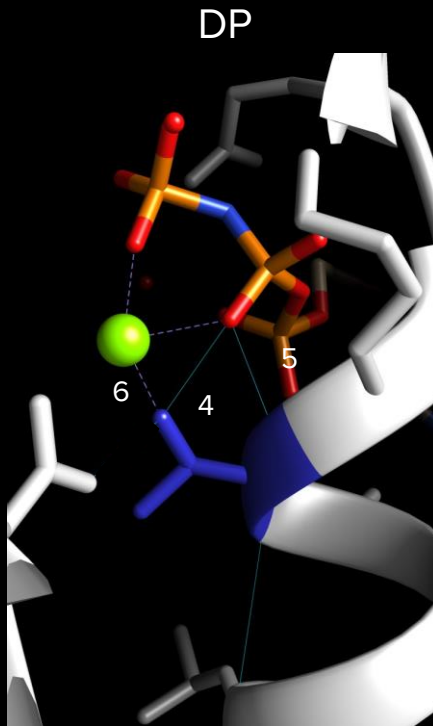
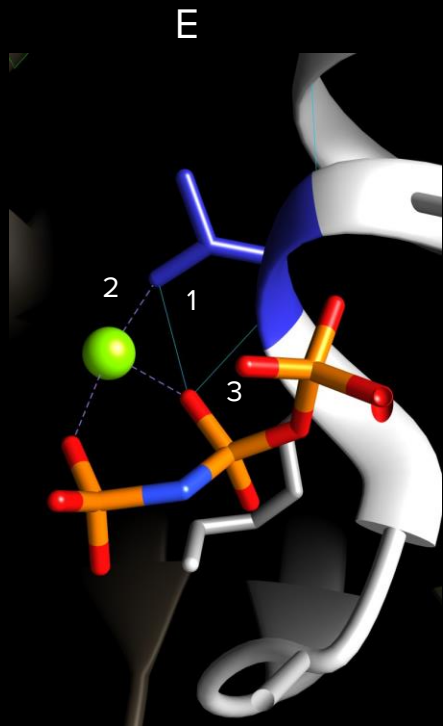
1. NH₂(Arg)-PO₄ 2,998Å
2. NH₂(Arg)-O3G (ANP) 2,668Å
3. NH₂(Arg)-O3G (ANP) 2,857Å
4. NH₂(Arg)-O3G (ANP) 3,348Å
5. NH₂(Arg)-O3G (ANP) 3,241Å



LIGAND INTERACTIONS

α Thr178

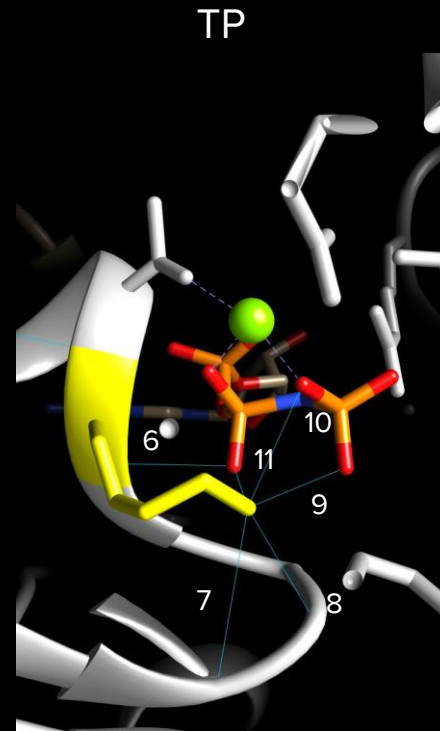
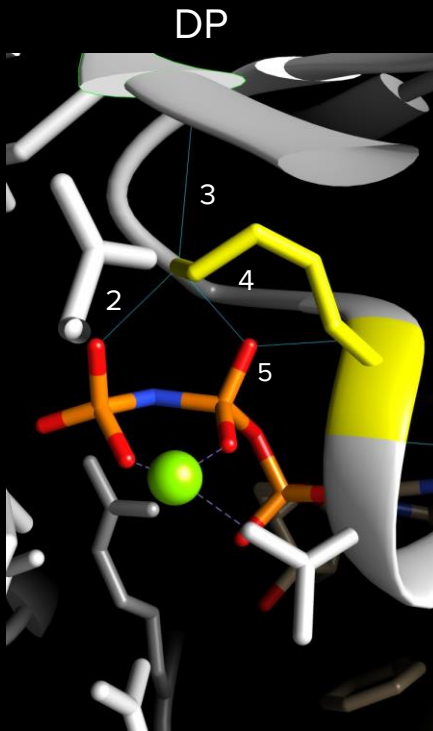
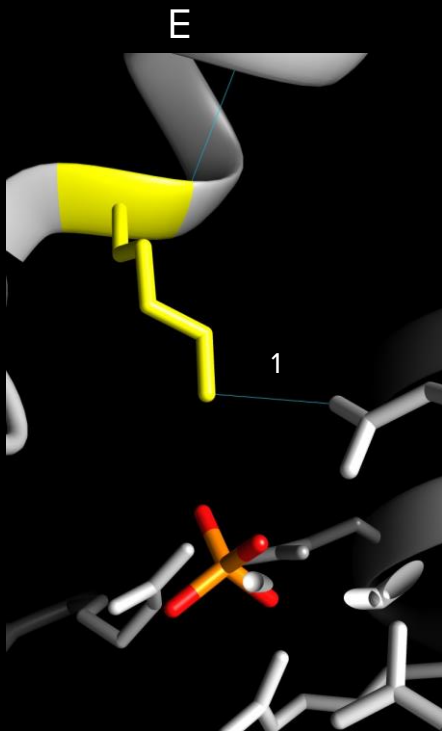
- | | | | |
|----|---------------------------|----|---------------------------|
| 1. | OG1(Thr)-O2B(ANP) 2,975Å | 6. | OG1(Thr)-Mg 1,875Å |
| 2. | OG1(Thr)-Mg 2,081Å | 7. | OG1(Thr)-Mg 2,186Å |
| 3. | N(Thr)-O2B(ANP) 3,260Å | 8. | OG1(Thr)-O2B (ANP) 3,141Å |
| 4. | OG1(Thr)-O2B (ANP) 2,669Å | 9. | N(Thr)-O2B (ANP) 3,220Å |
| 5. | N(Thr)-O2B (ANP) 3,024Å | | |



LIGAND INTERACTIONS

β Lys163

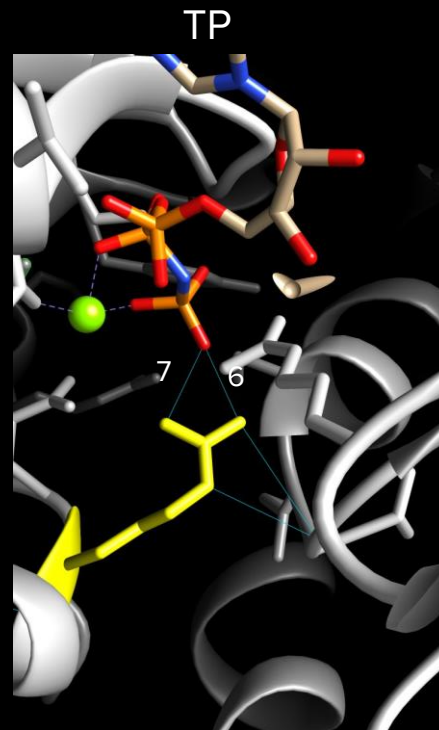
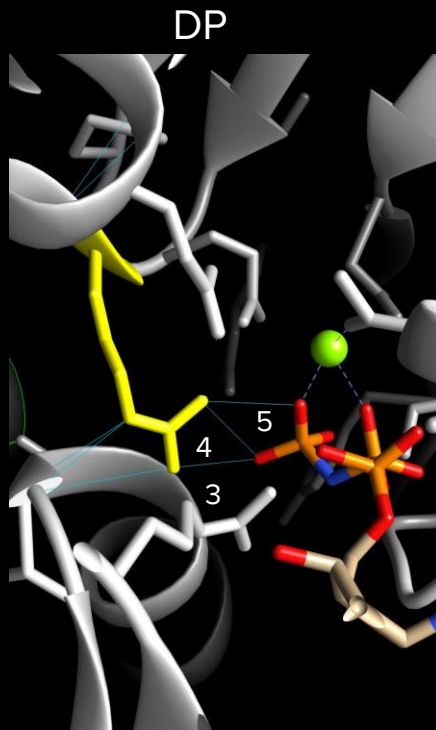
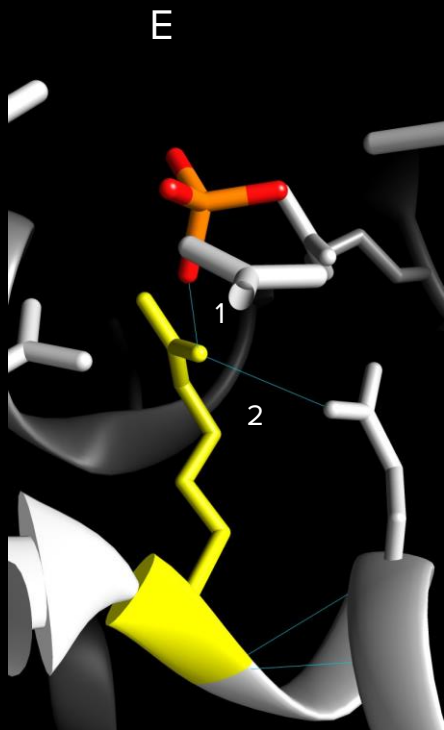
- | | | | |
|----|-------------------------|-----|-------------------------|
| 1. | NZ(Lys)-OD2(Asp) 2,989Å | 7. | NZ(Lys)-O(Gly) 2,934Å |
| 2. | NZ(Lys)-O1G(ANP) 2,573Å | 8. | NZ(Lys)-O(Gly) 3,237Å |
| 3. | NZ(Lys)-O(Gly) 2,877Å | 9. | NZ(Lys)-O1G(ANP) 2,842Å |
| 4. | NZ(Lys)-O1B(ANP) 2,715Å | 10. | NZ(Lys)-O2G(ANP) 3,271Å |
| 5. | N(Lys)-O1B(ANP) 2,869Å | 11. | NZ(Lys)-O1B(ANP) 2,650Å |
| 6. | N(Lys)-O1B(ANP) 3,206Å | | |



LIGAND INTERACTIONS

β Arg190

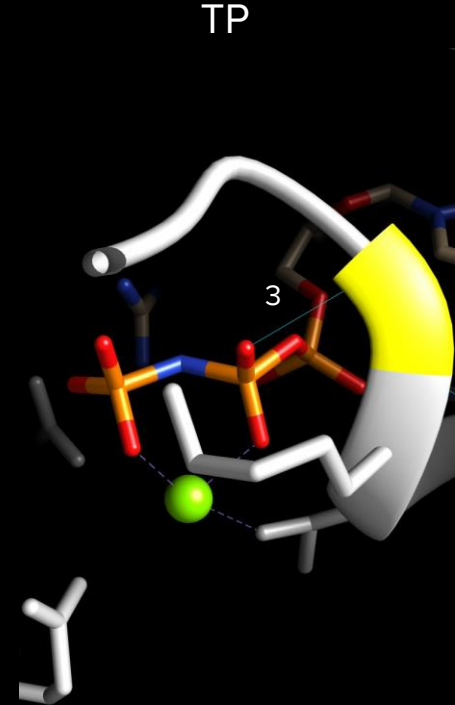
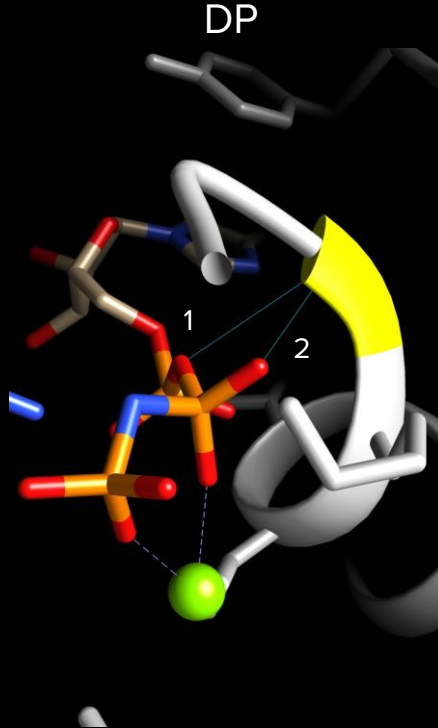
1. NH1(Arg)-O1(PO4) 2,826Å
2. NH1(Arg)-O(Thr) 2,892Å
3. NH2(Arg)-O3G(ANP) 2,971Å
4. NH1(Arg)-O3G(ANP) 3,093Å
5. NH1(Arg)-O2G(ANP) 3,059Å
6. NH2(Arg)-O3G(ANP) 2,833Å
7. NH1(Arg)-O3G(ANP) 3,030Å



LIGAND INTERACTIONS

β Gly162

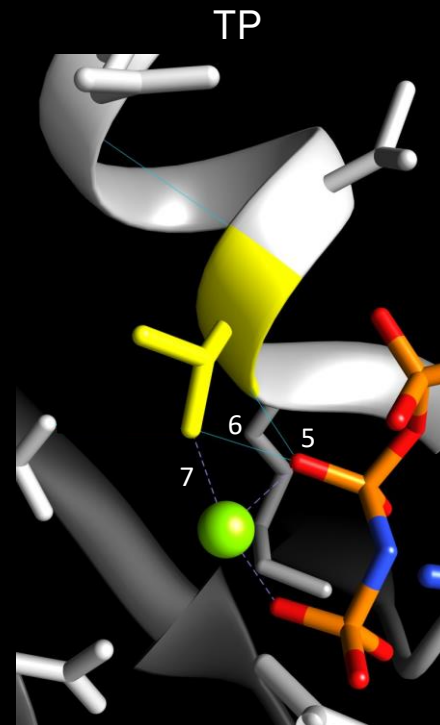
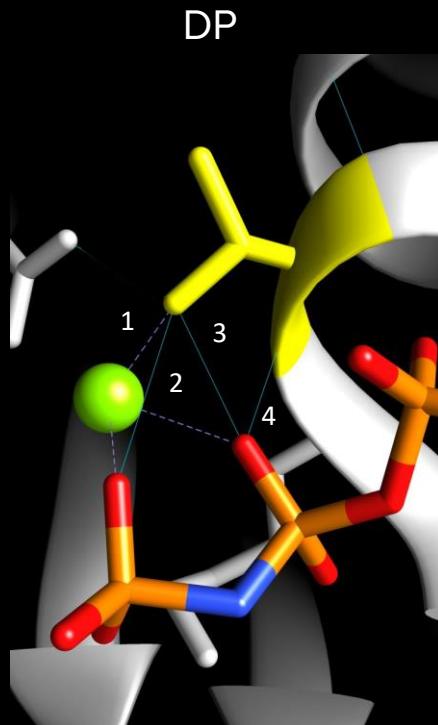
1. N(Gly)-O3A(ANP) 2,832Å
2. N(Gly)-O1B(ANP) 2,920Å
3. N(Gly)-O1B(ANP) 3,165Å



LIGAND INTERACTIONS

β Thr164

1. OG1(Thr)-Mg 1,906Å
2. OG1(Thr)-O2G (ANP) 3,418Å
3. OG1(Thr)-O2B (ANP) 2,640Å
4. N(Thr)-O2B (ANP) 3,143Å
5. N(Thr)-O2B (ANP) 2,692Å
6. OG1(Thr)-O2B (ANP) 2,581Å
7. OG1(Thr)-Mg 2,137Å

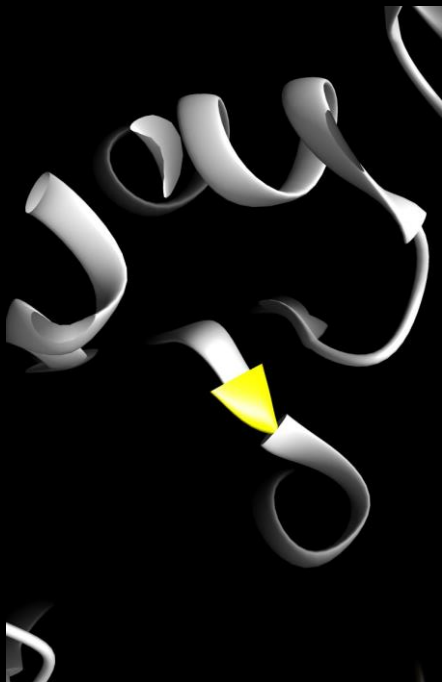


LIGAND INTERACTIONS

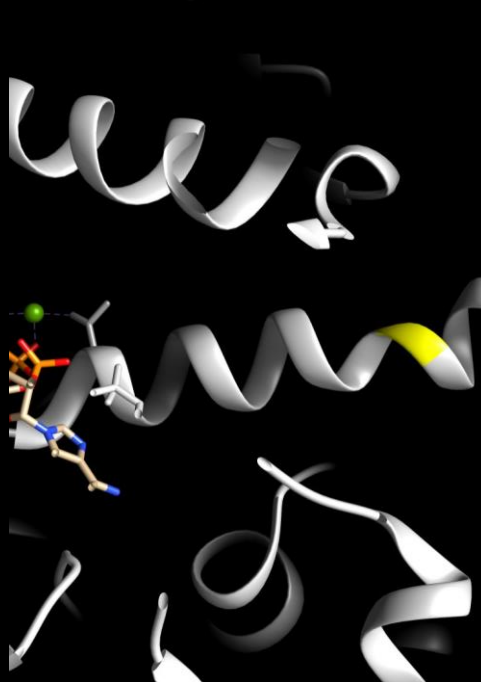
β Glu189

1. OE1(Glu)-Mg 2,709Å

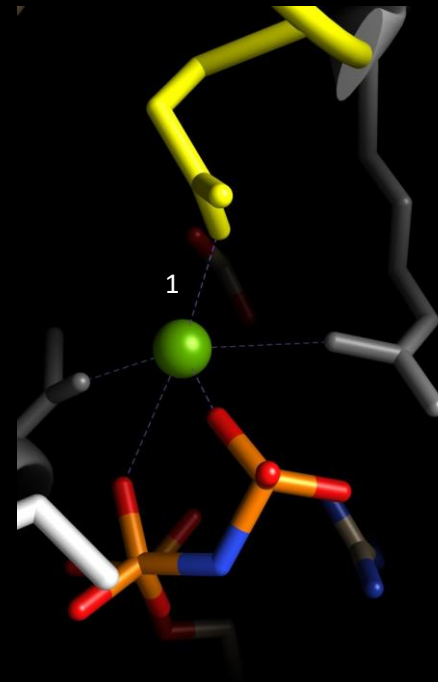
E



DP



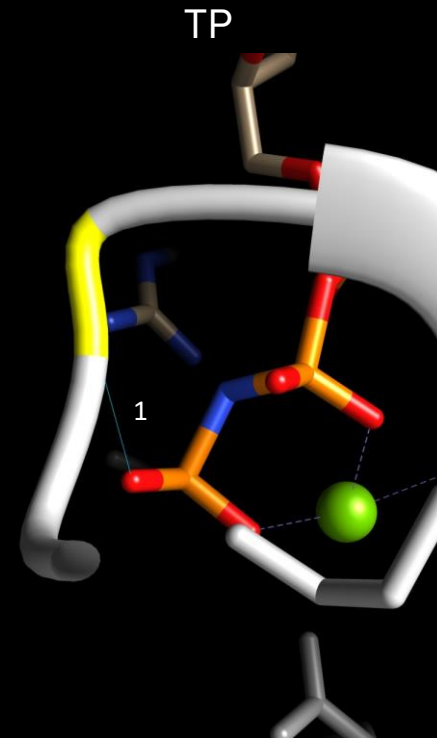
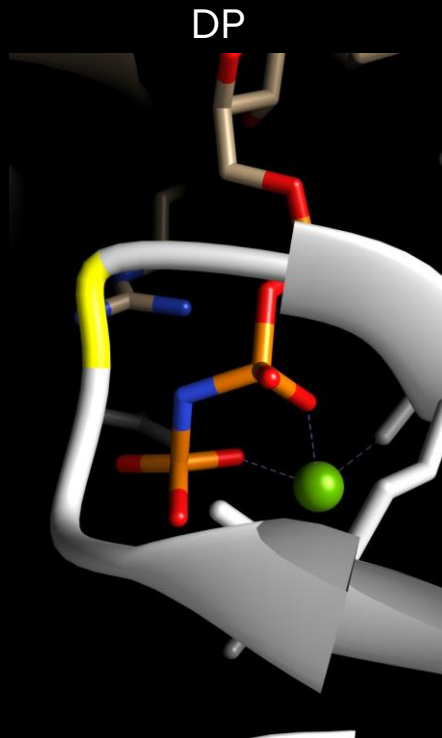
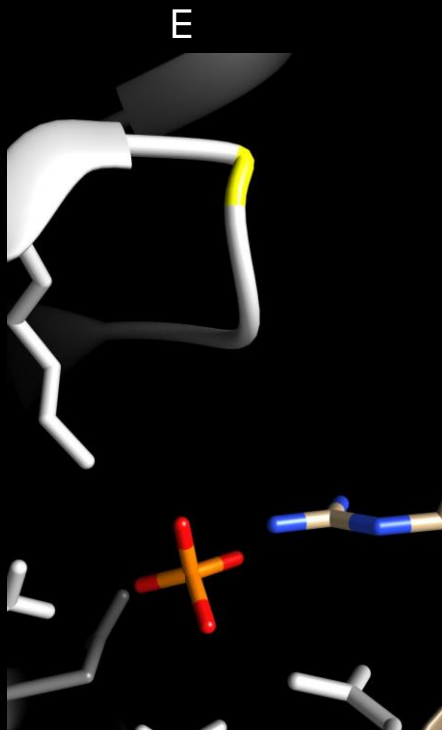
TP



LIGAND INTERACTIONS

β Gly160

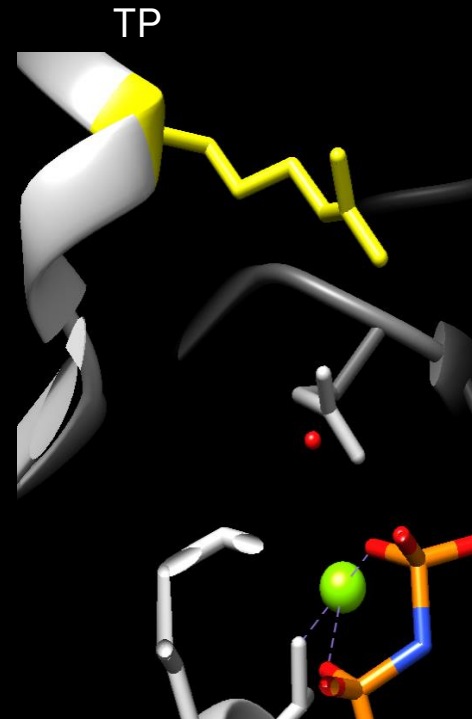
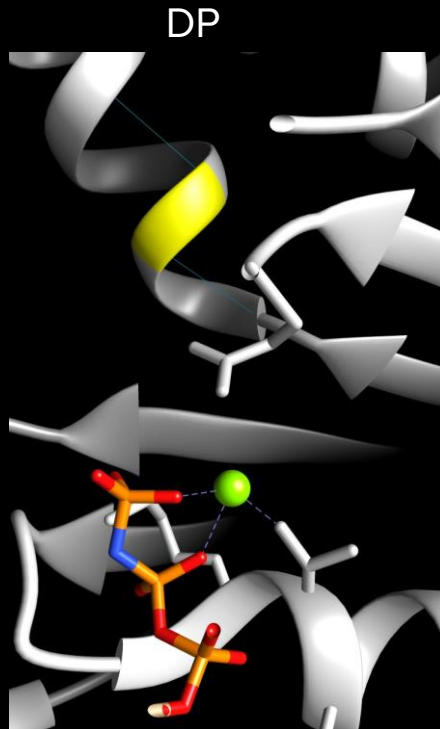
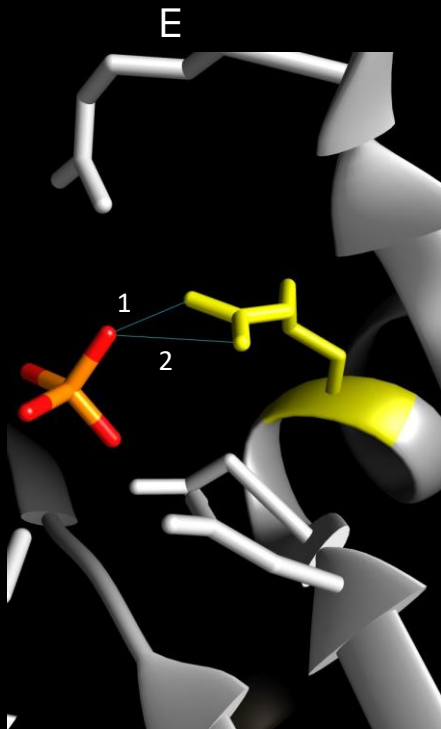
1. N(Gly)-O1G (ANP) 2,683Å



LIGAND INTERACTIONS

β Arg260

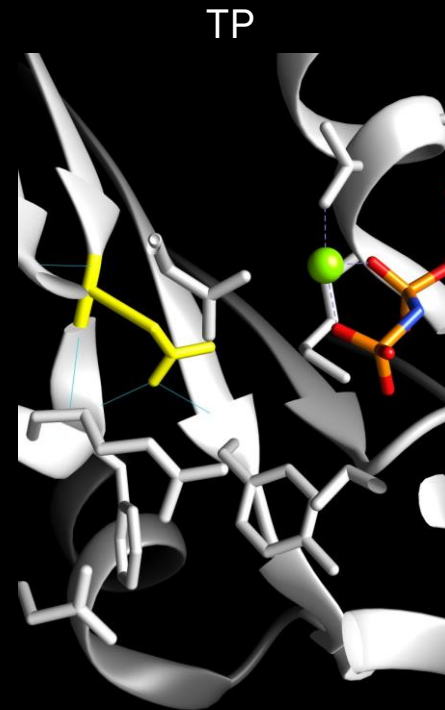
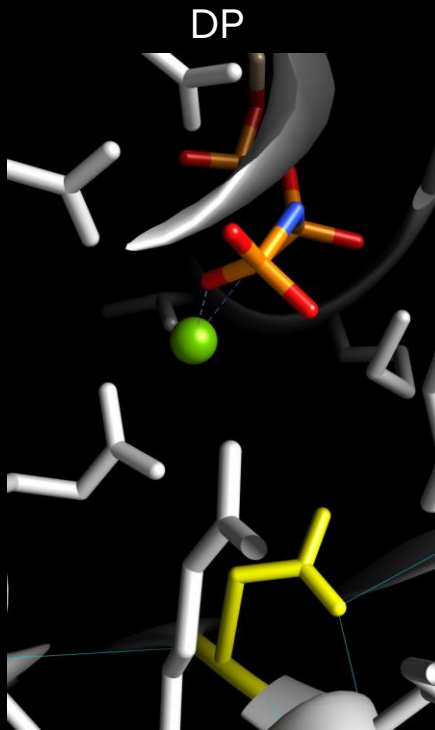
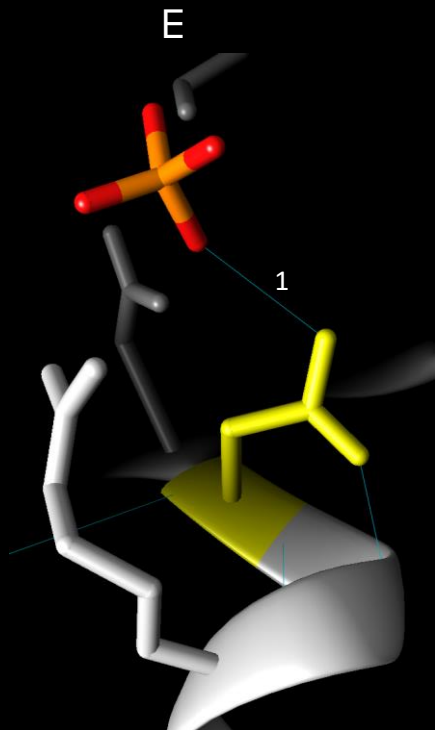
1. NH1Arg-O1(PO4) 3,262Å
2. NH2(Arg)-O1(PO4) 3,092Å



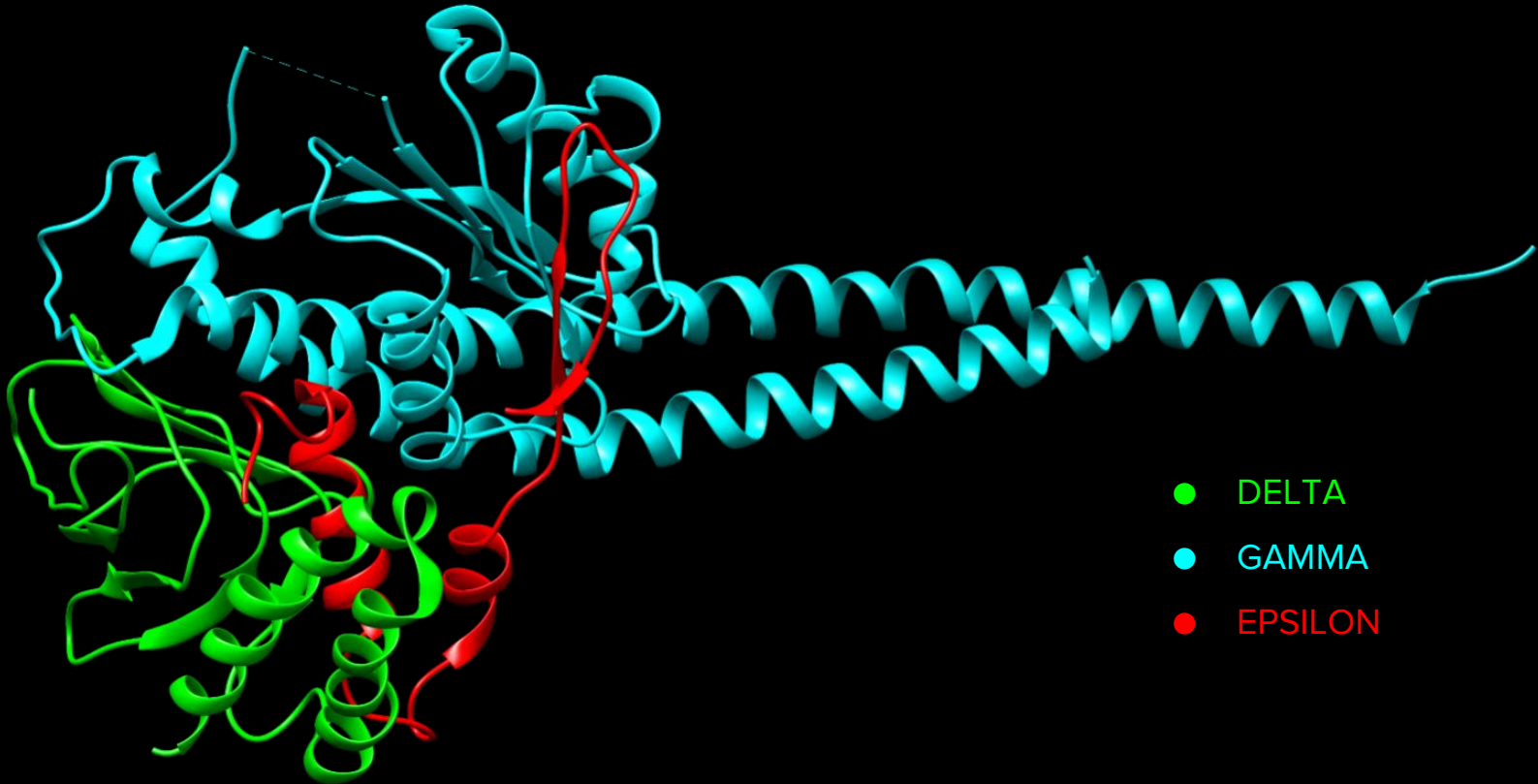
LIGAND INTERACTIONS

β Asn257

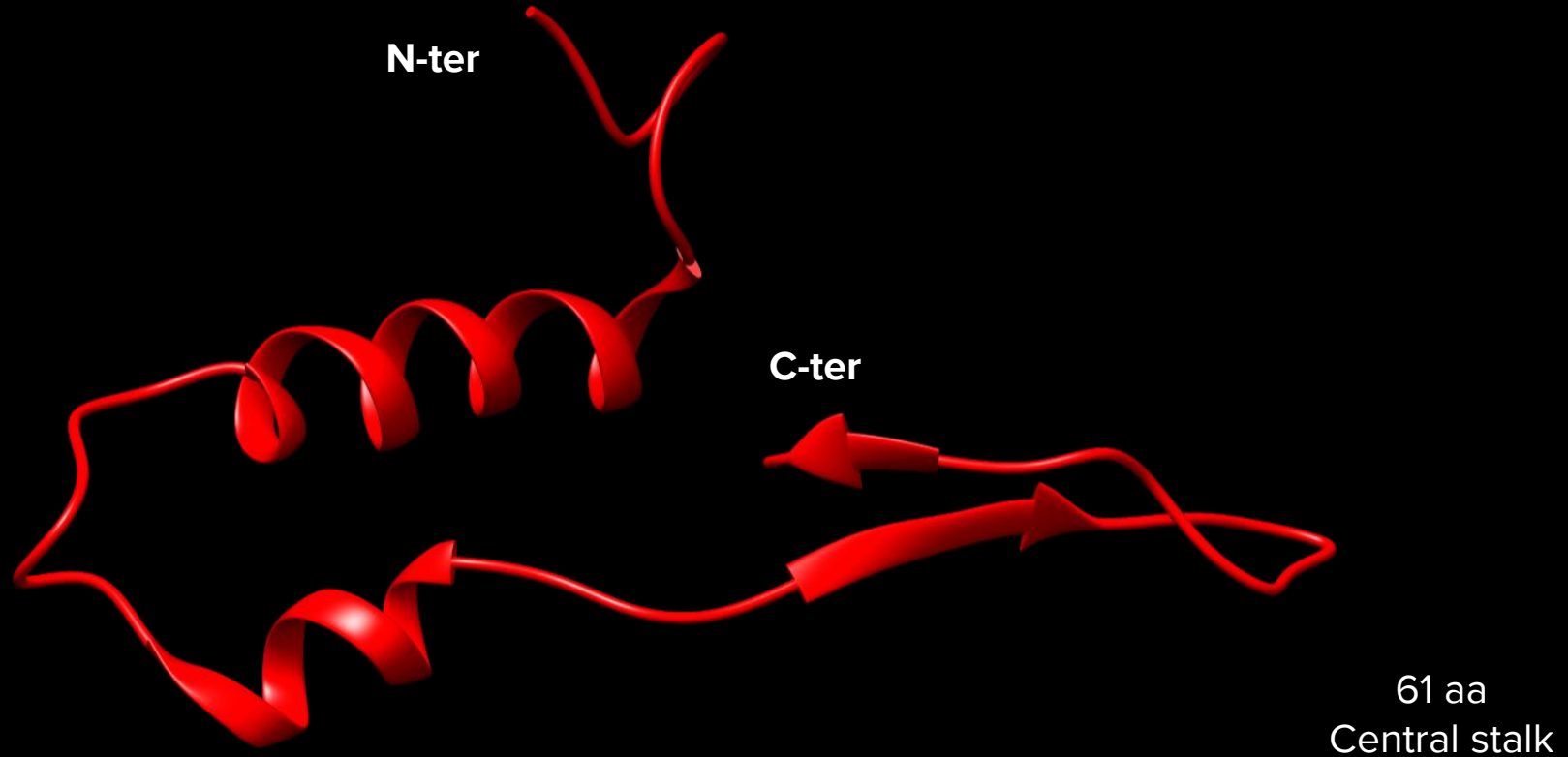
1. ND2(Asn)-O4(PO4) 2,978Å



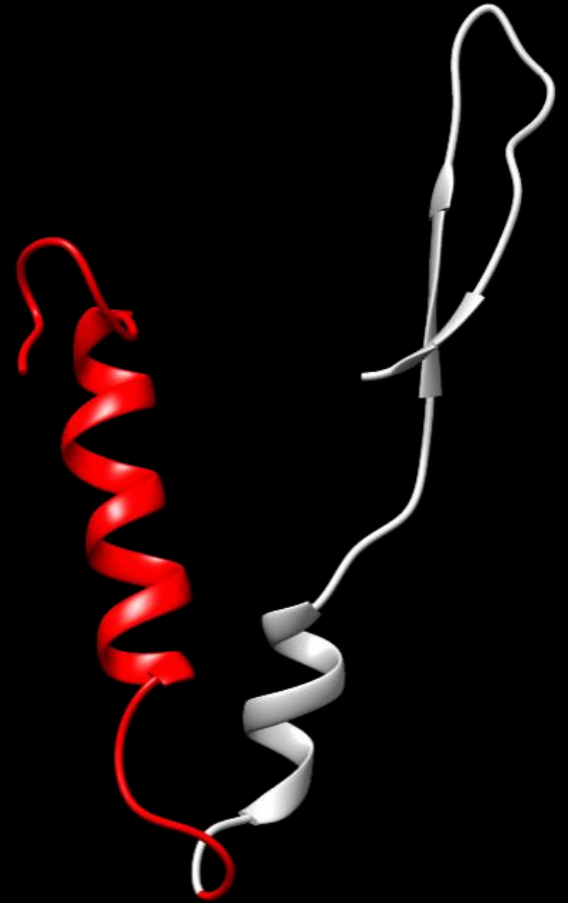
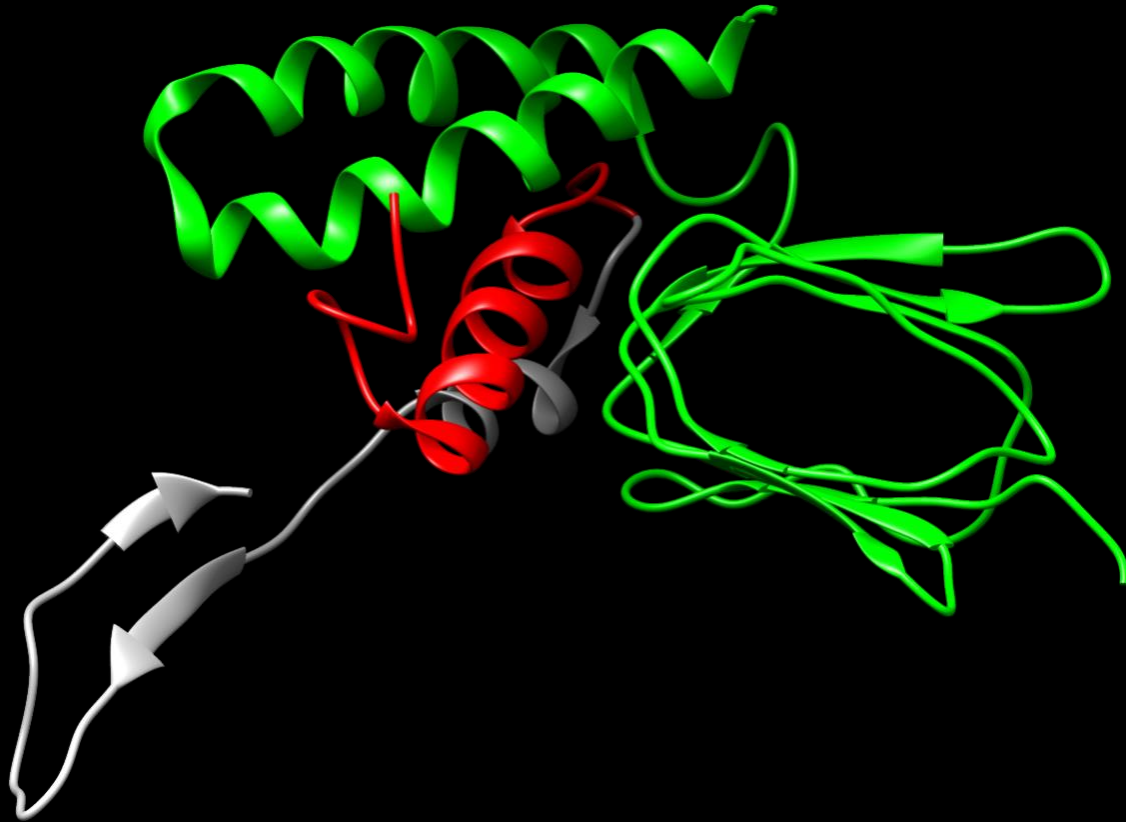
CENTRAL STALK: γ , δ and ϵ subunits



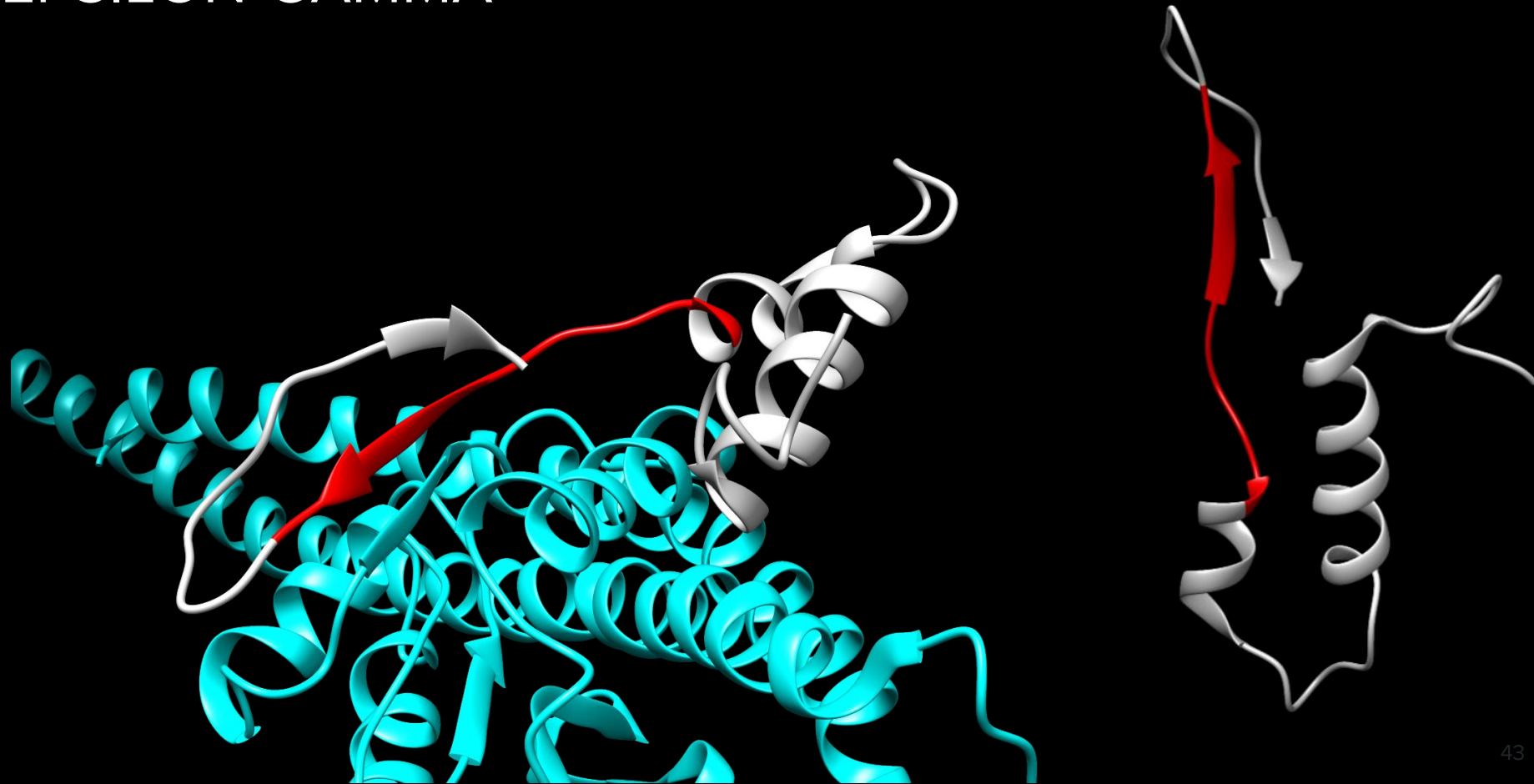
EPSILON



EPSILON-DELTA



EPSILON-GAMMA



EPSILON

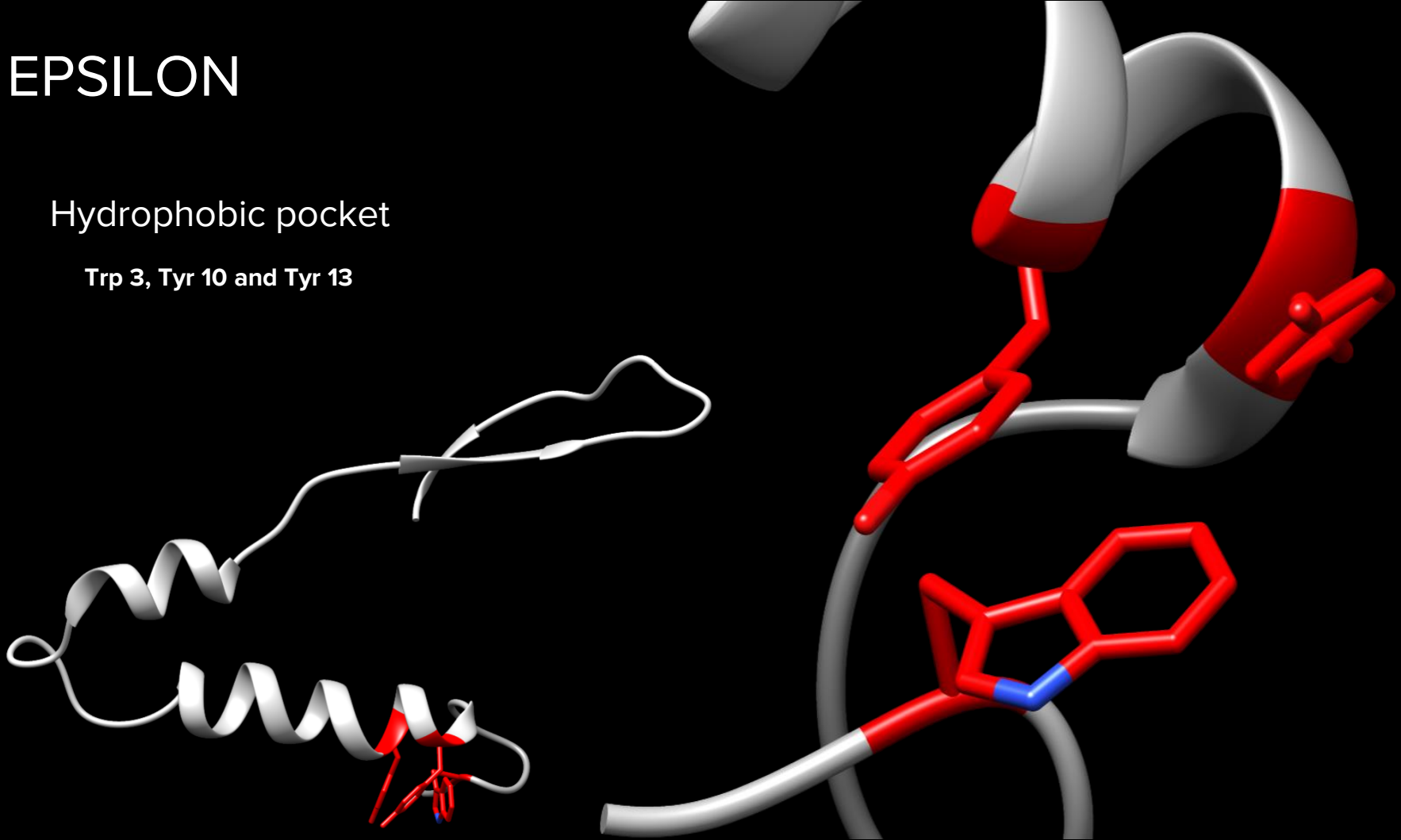
- Total residues = 61
- **Polar residues = 33 - Percentage: 54.1**
- Nonpolar residues = 28 - Percentage: 45.9
- Acidic residues = 3 - Percentage: 4.9
- Basic residues = 7 - Percentage: 11.5
- Basic residues with His = 7 - Percentage: 11.5



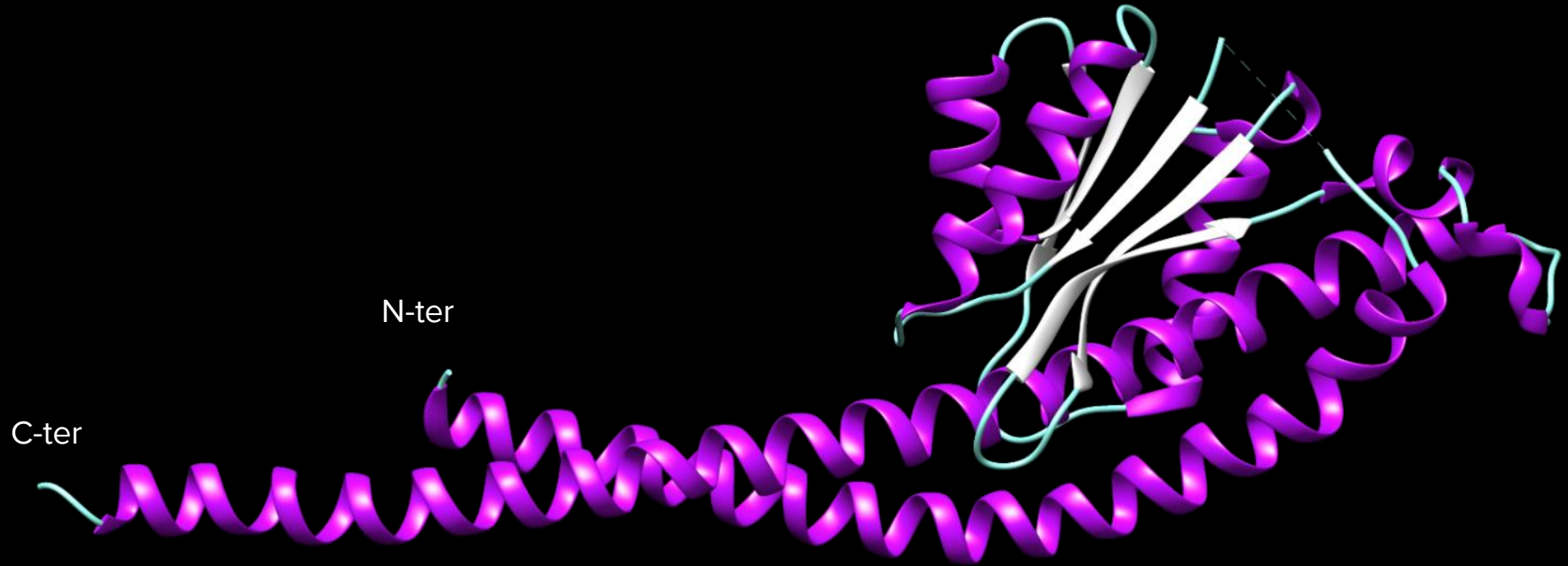
EPSILON

Hydrophobic pocket

Trp 3, Tyr 10 and Tyr 13



GAMMA



N-ter

C-ter

278 aa
Central stalk

GAMMA

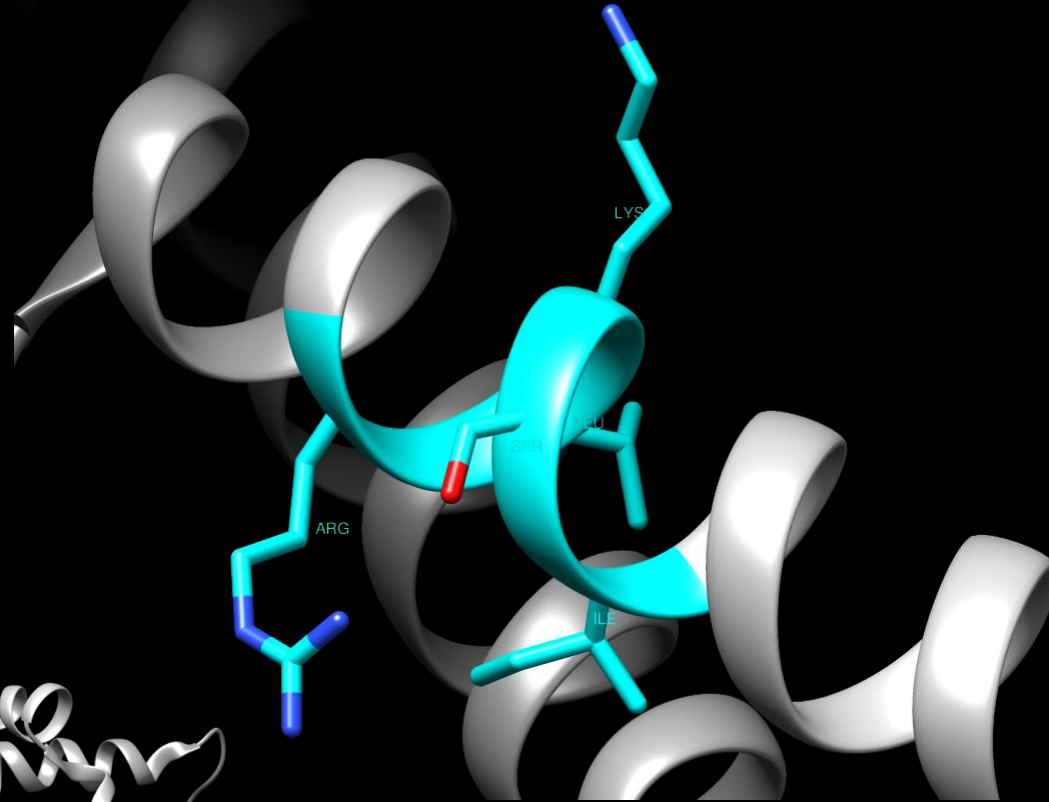
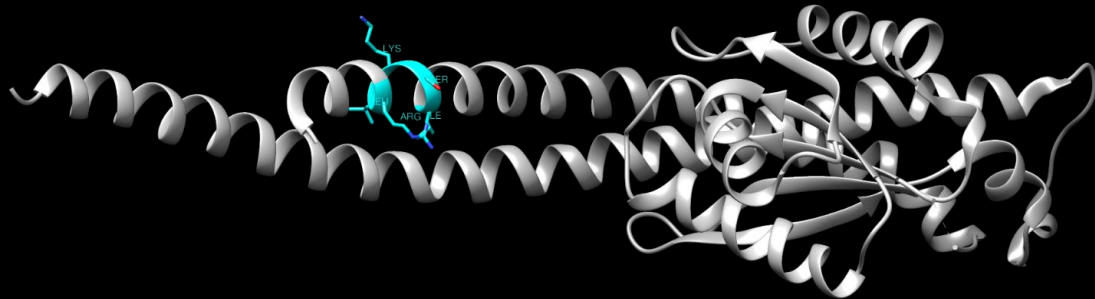
- Total residues = 278
- **Polar residues = 155 - Percentage: 55.8**
- Nonpolar residues = 123 - Percentage: 44.2
- Acidic residues = 33 - Percentage: 11.9
- Basic residues = 38 - Percentage: 13.7
- Basic residues with His = 41 - Percentage: 14.7



GAMMA

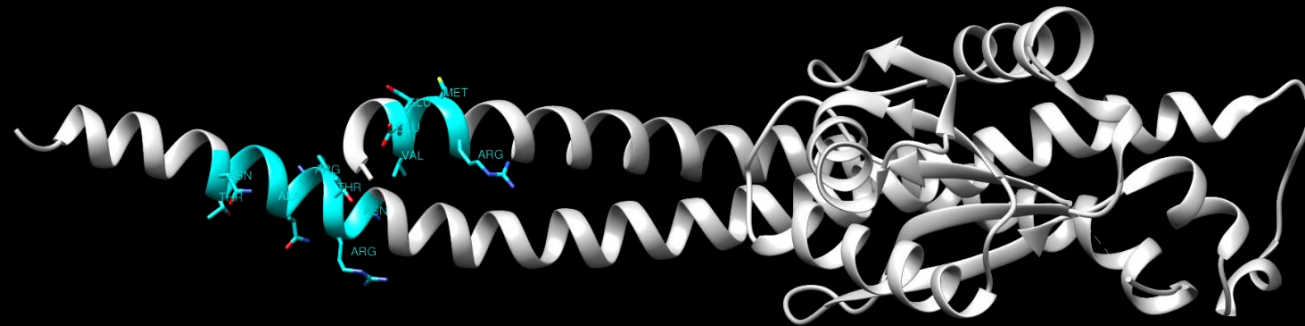
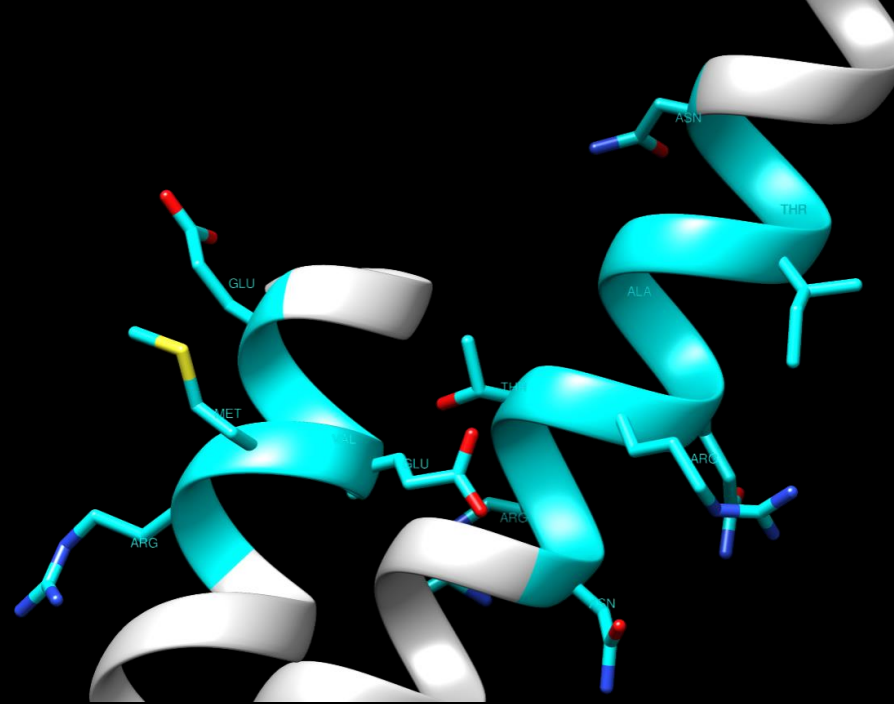
Residues 9-13

The rotation angle of these residues determinate the affinity of the catalytic sites.



GAMMA

Affinity determining segments

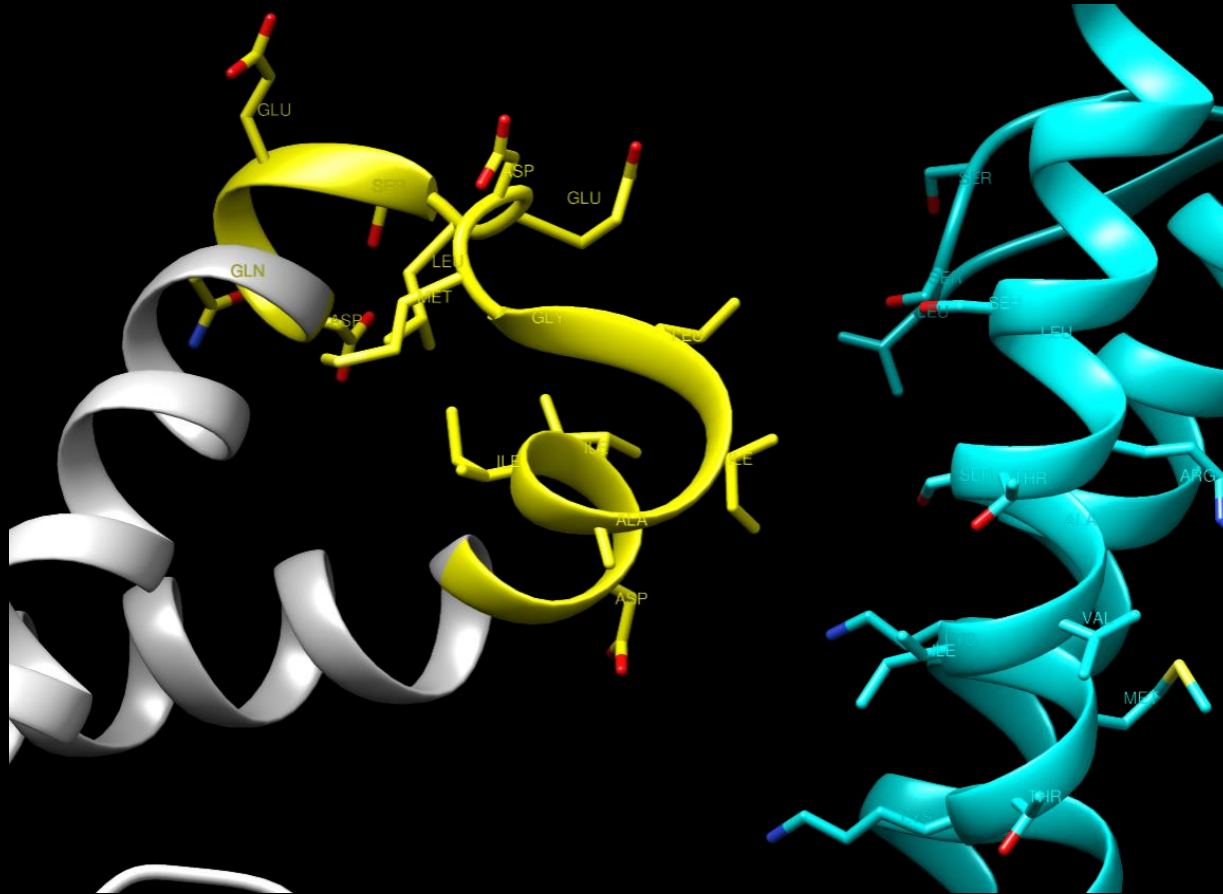


**Residues 5-9
(N-ter) and
256-265 (C-ter)**

GAMMA-BETA INTERACTIONS

Catch 2
(β E386-400)

Conserved acidic
region

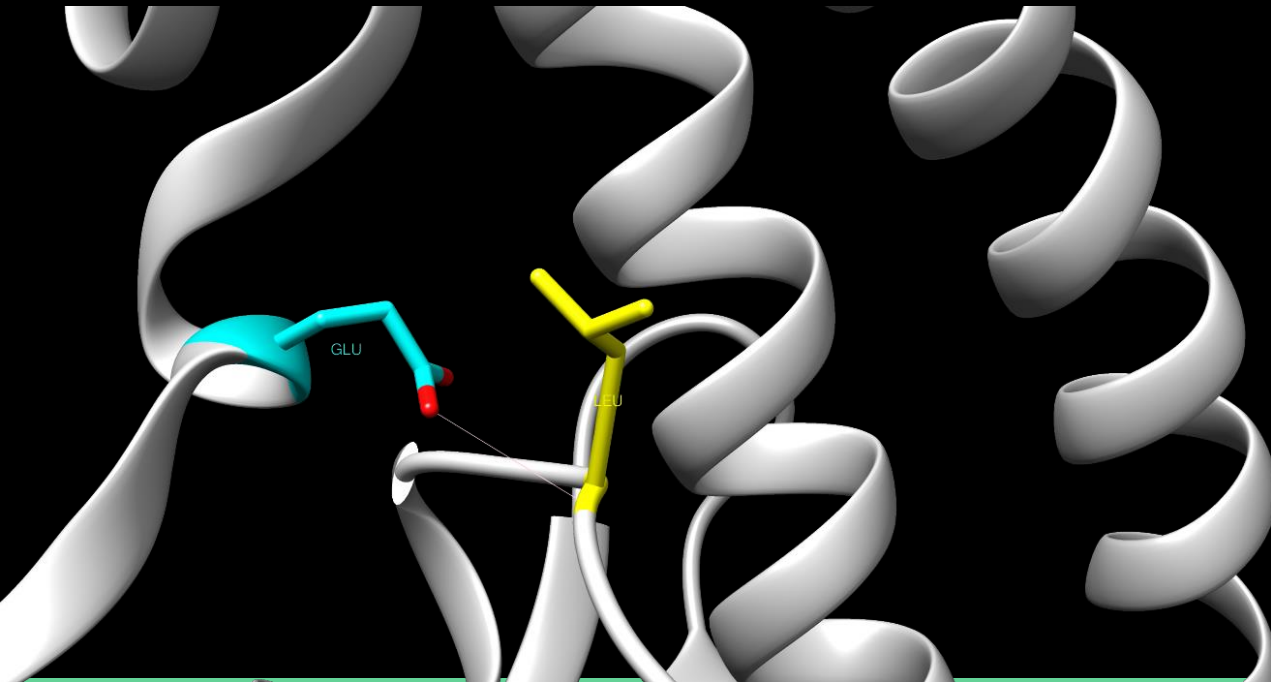


γ -subunit

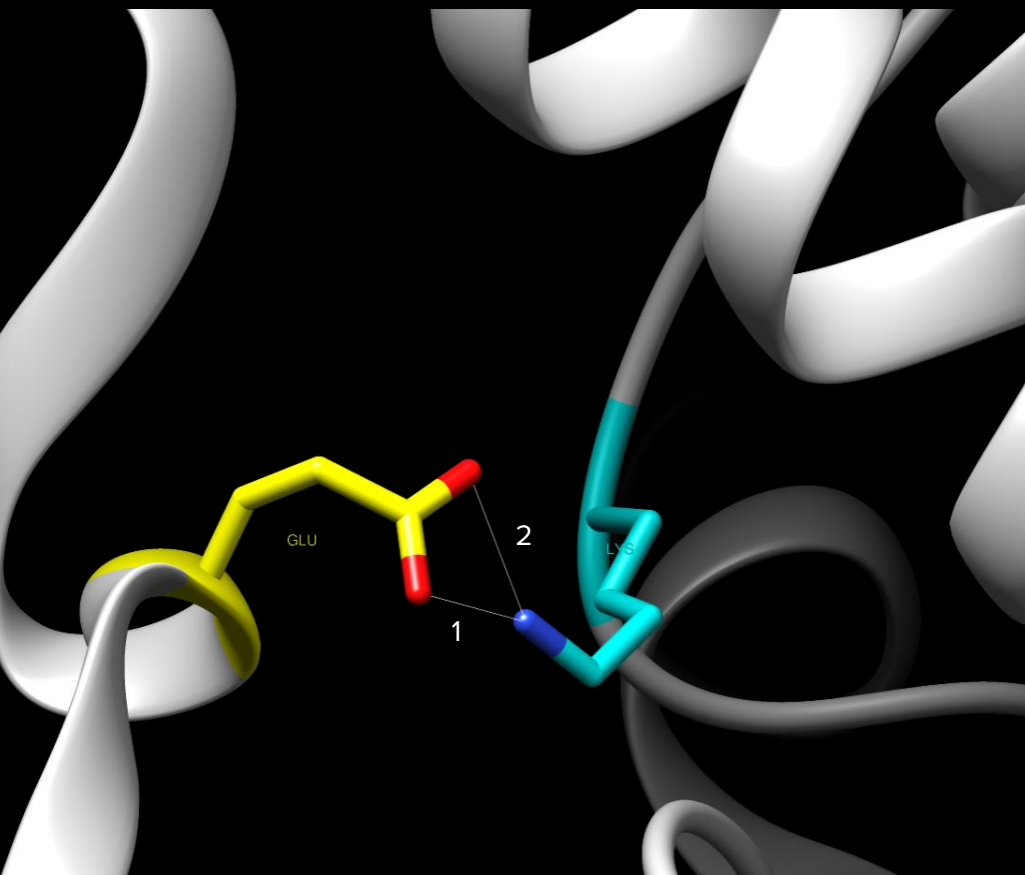
GAMMA-BETA INTERACTIONS

Beta TP

LEU 83.G N GLU 395.F OE1 3.005 Å



GAMMA-BETA INTERACTIONS



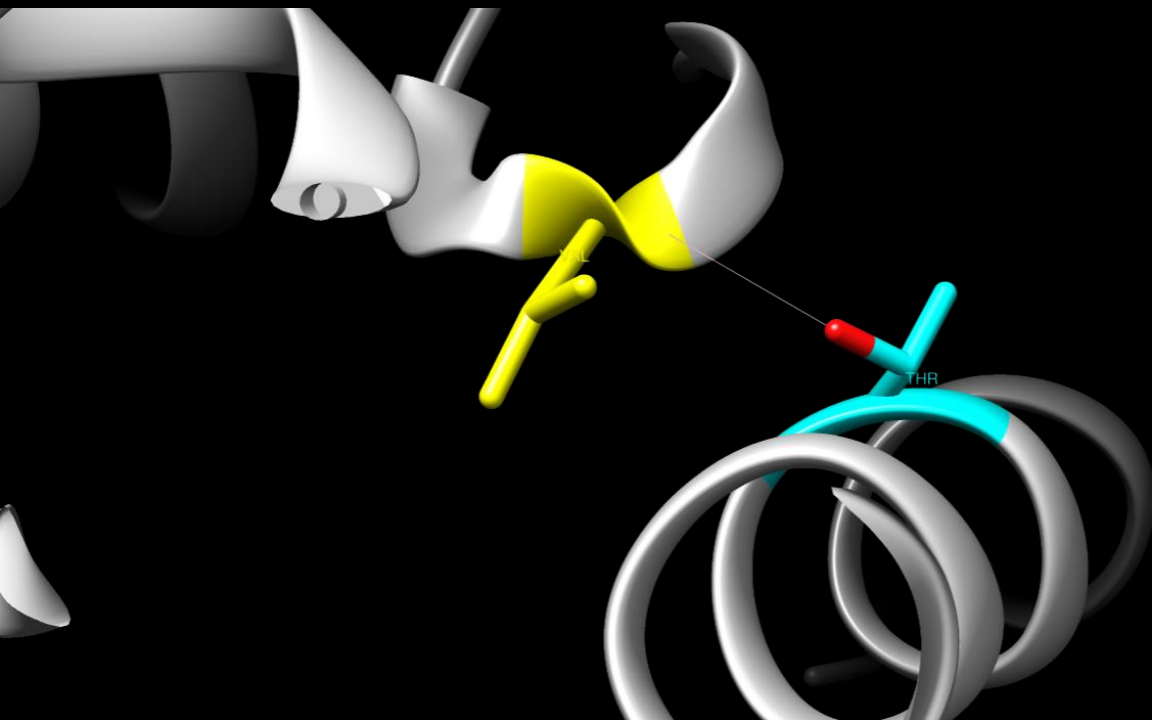
Beta DP

1. LYS 81.G NZ GLU 395.D OE1 4.170Å
2. LYS 81.G NZ GLU 395.D OE2 3.759Å

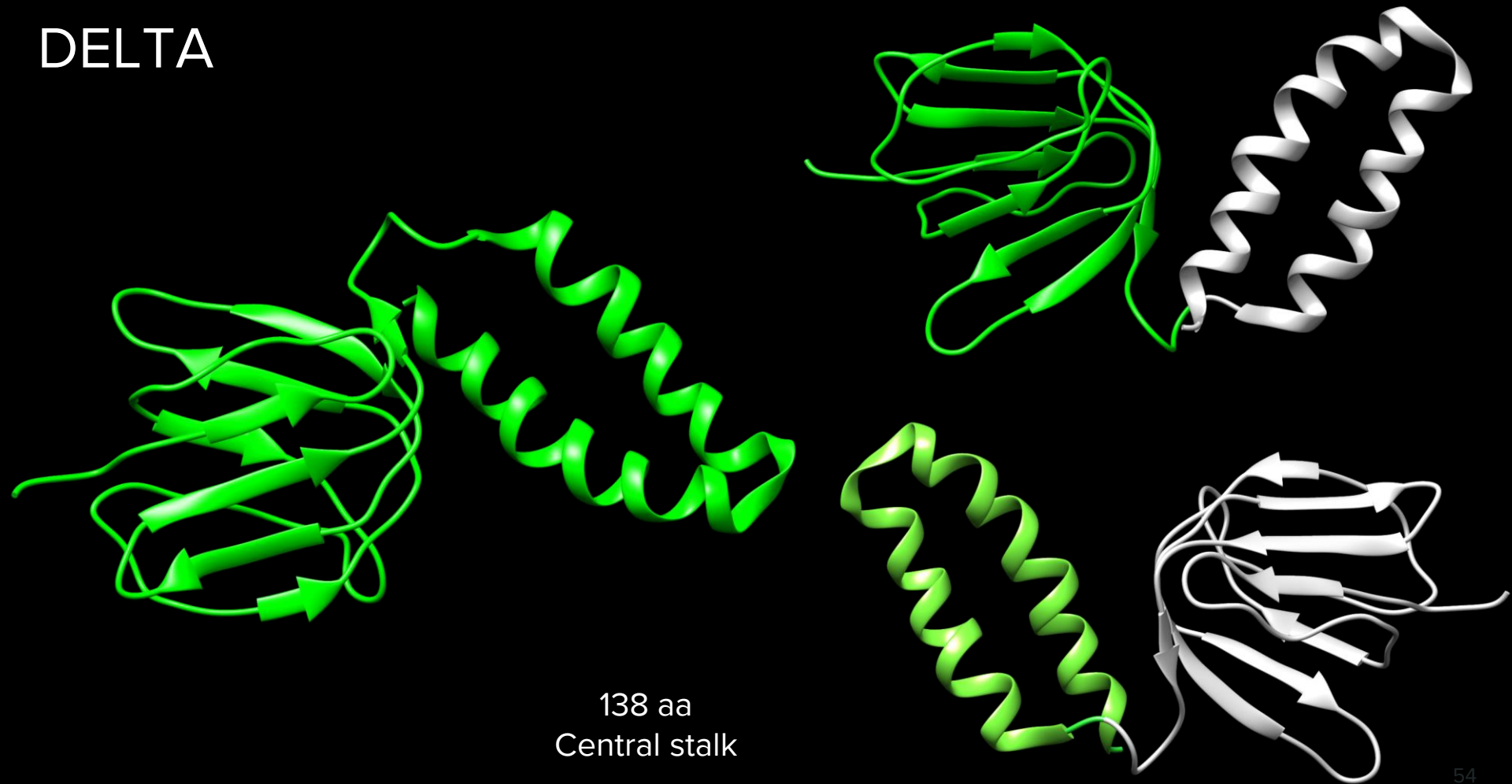
Catch 2 (386-400)

GAMMA-BETA INTERACTIONS

VAL 279.E N THR 264.G OG1 3.086Å

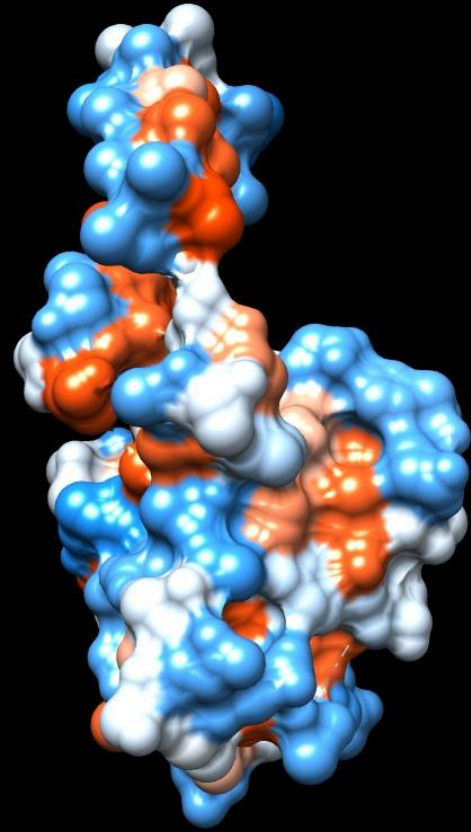


DELTA



DELTA

- Total residues = 138
- **Polar residues = 72 - Percentage: 52.2**
- Nonpolar residues = 66 - Percentage: 47.8
- Acidic residues = 16 - Percentage: 11.6
- Basic residues = 10 - Percentage: 7.2
- Basic residues with His = 12 - Percentage: 8.7



F₀ ATP SYNTHASE

● SUBUNIT OSCP

● SUBUNIT d

● SUBUNIT b

● SUBUNIT h

● SUBUNIT f

● SUBUNIT e

● SUBUNIT g

● SUBUNIT k

● SUBUNIT i/j

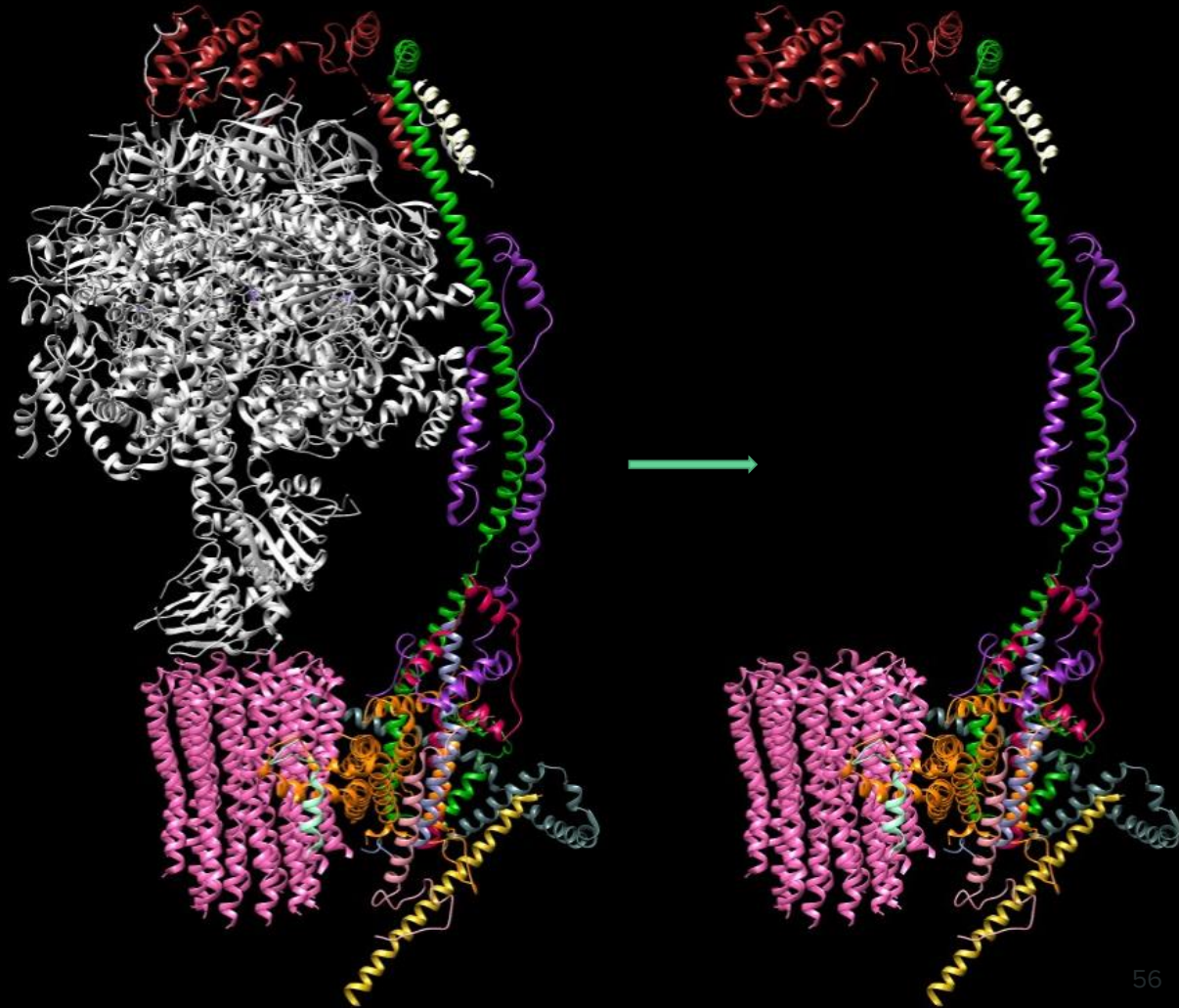
● SUBUNIT c

● SUBUNIT a

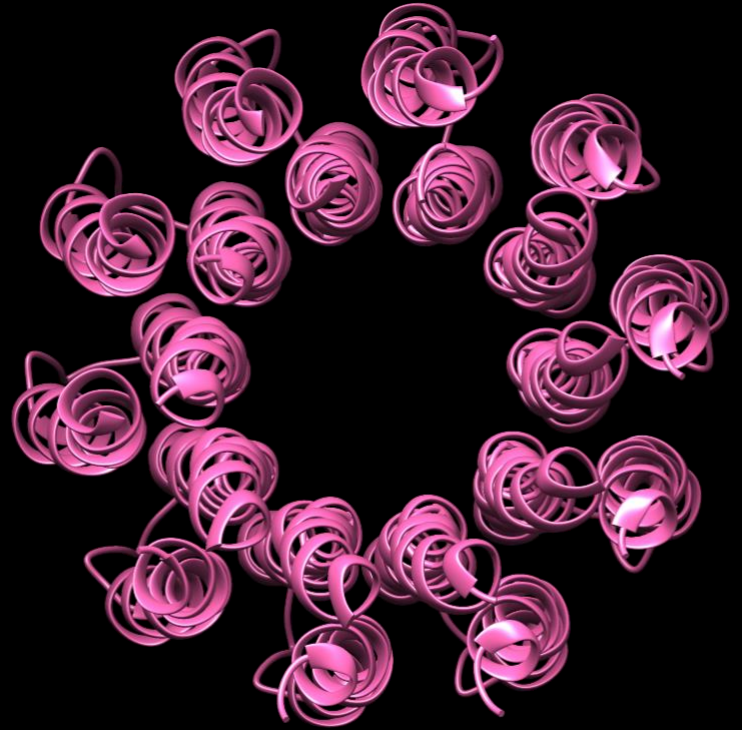
● SUBUNIT 8

Peripheral
stalk

Rotor

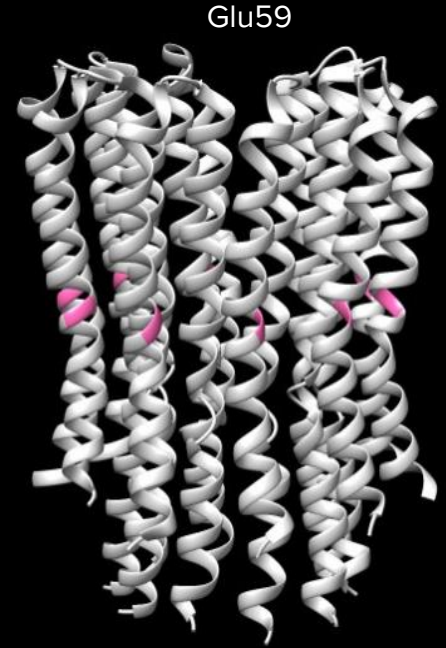
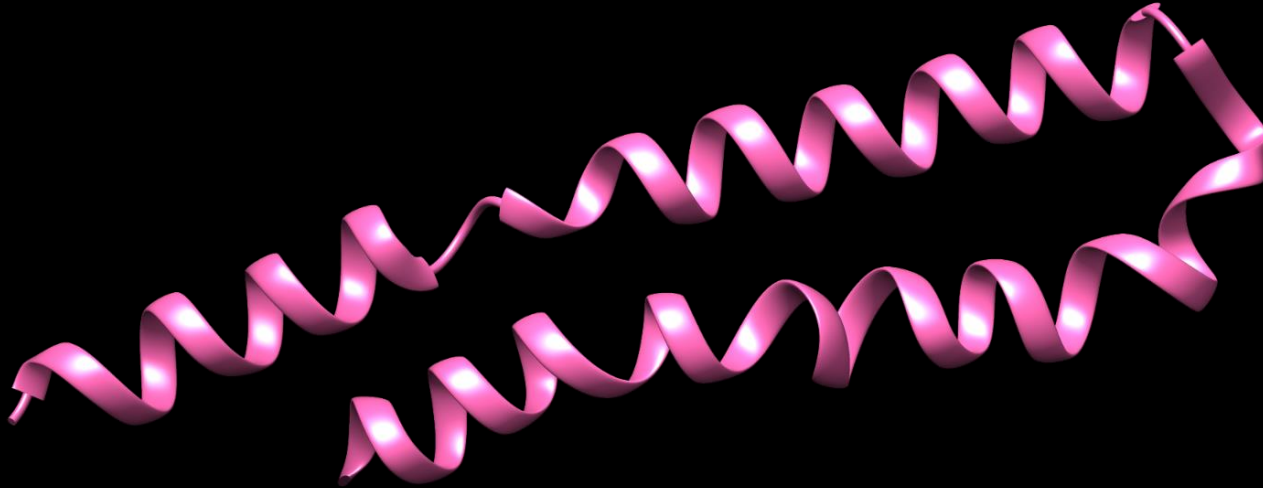


SUBUNIT c: OLIGOMER



c-ring (10 monomers)

SUBUNIT c: MONOMER

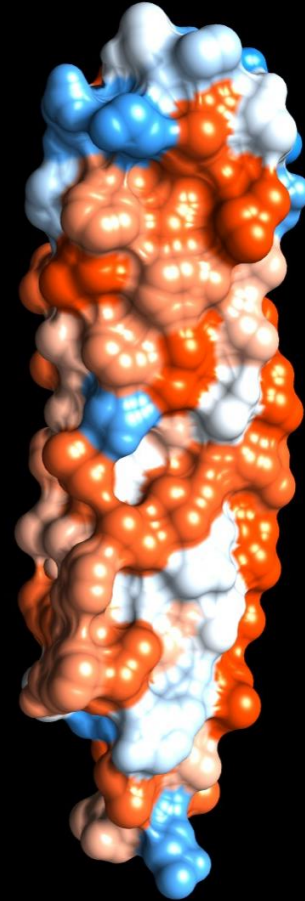


74 aa

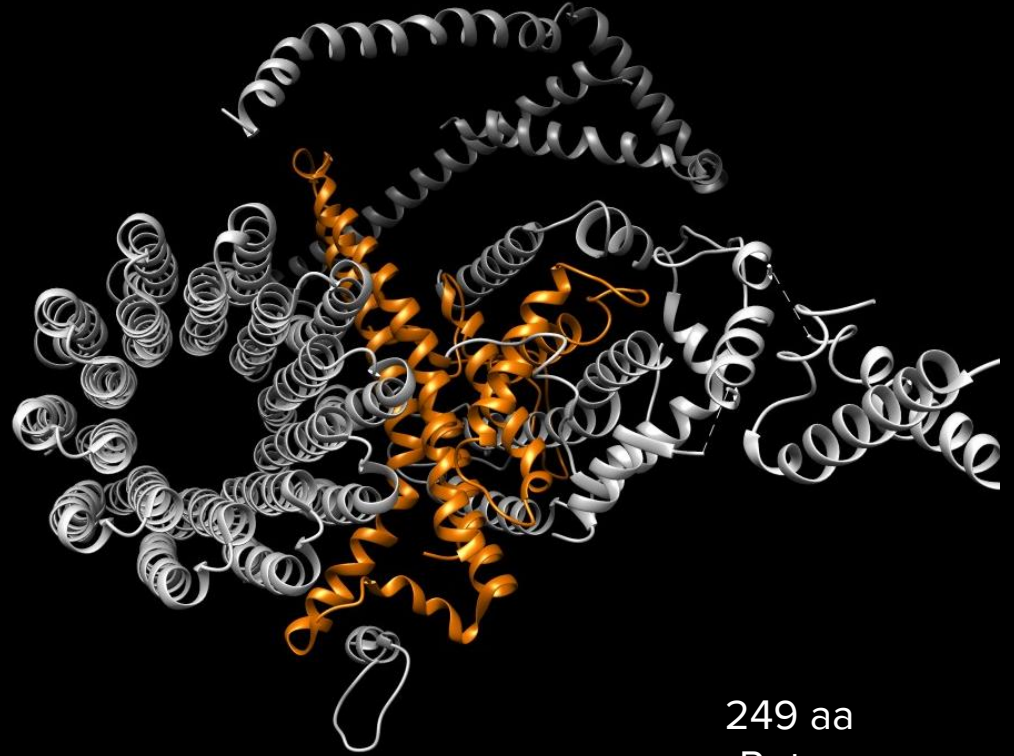
Rotor, H⁺ transport
2 transmembrane helices
Highly polar Arg loop

SUBUNIT c

- Total residues = 76
- Polar residues = 27 - Percentage: 35.5
- **Nonpolar residues = 49 - Percentage: 64.5**
- Acidic residues = 2 - Percentage: 2.6
- Basic residues = 3 - Percentage: 3.9
- Basic residues with His = 3 - Percentage: 3.9



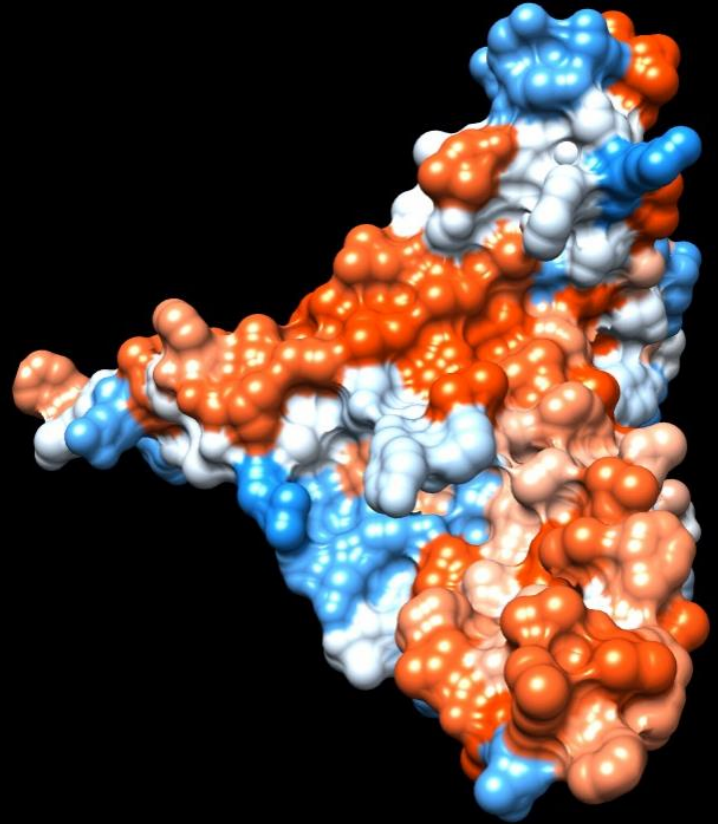
SUBUNIT a



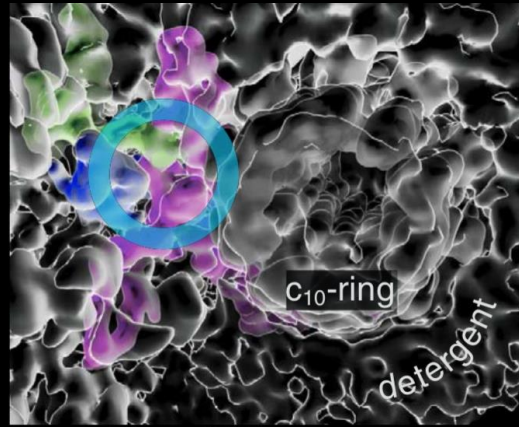
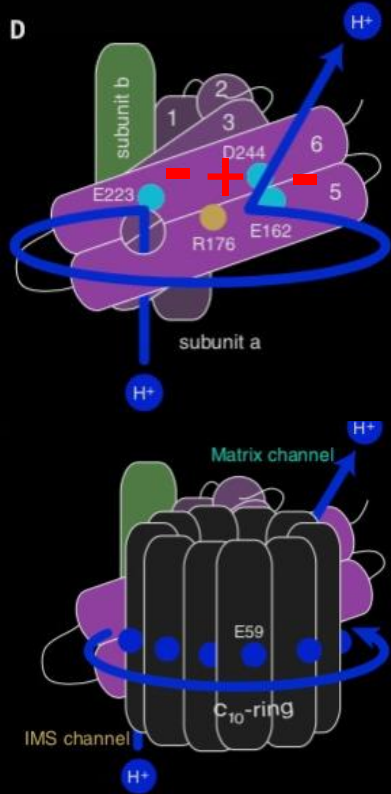
249 aa
Rotor
6 helices

SUBUNIT a

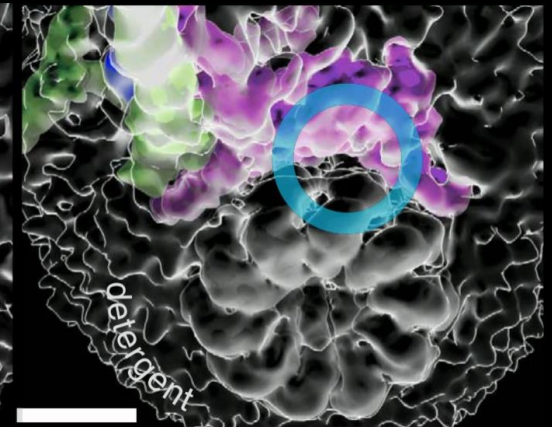
- Total residues = 249
- Polar residues = 90 - Percentage: 36.1
- **Nonpolar residues = 159 - Percentage: 63.9**
- Acidic residues = 8 - Percentage: 3.2
- Basic residues = 9 - Percentage: 3.6
- Basic residues with His = 13 - Percentage: 5.2



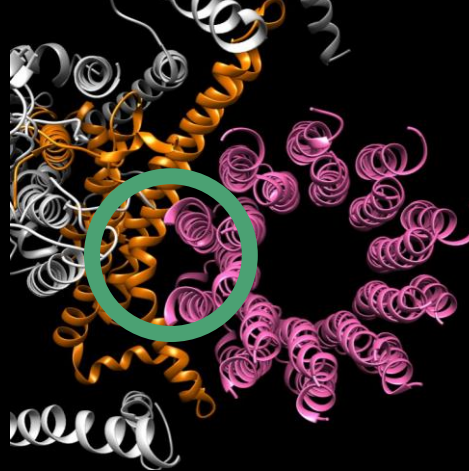
PROTON FLUX



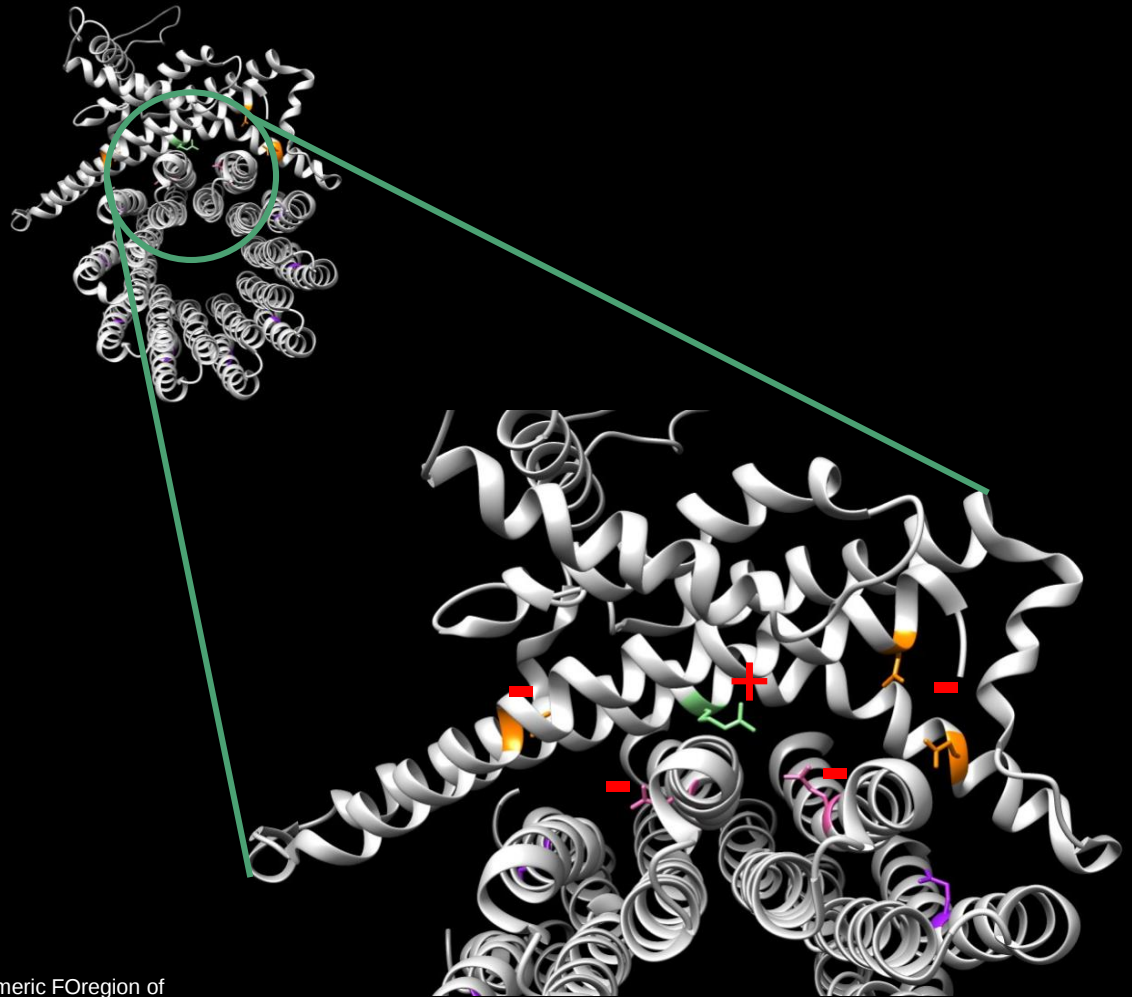
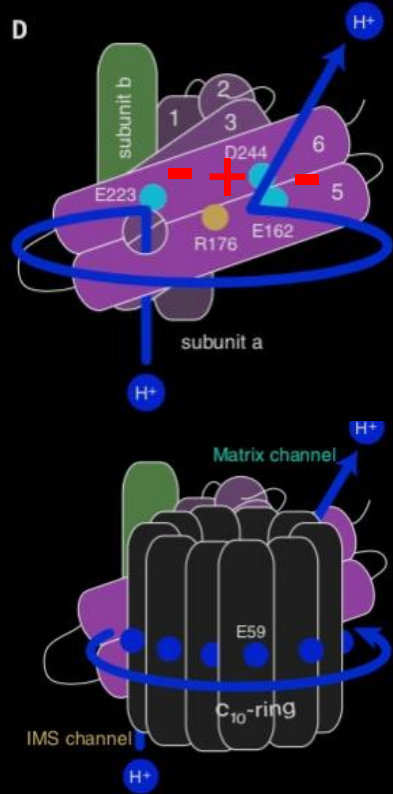
viewed from IMS



viewed from matrix

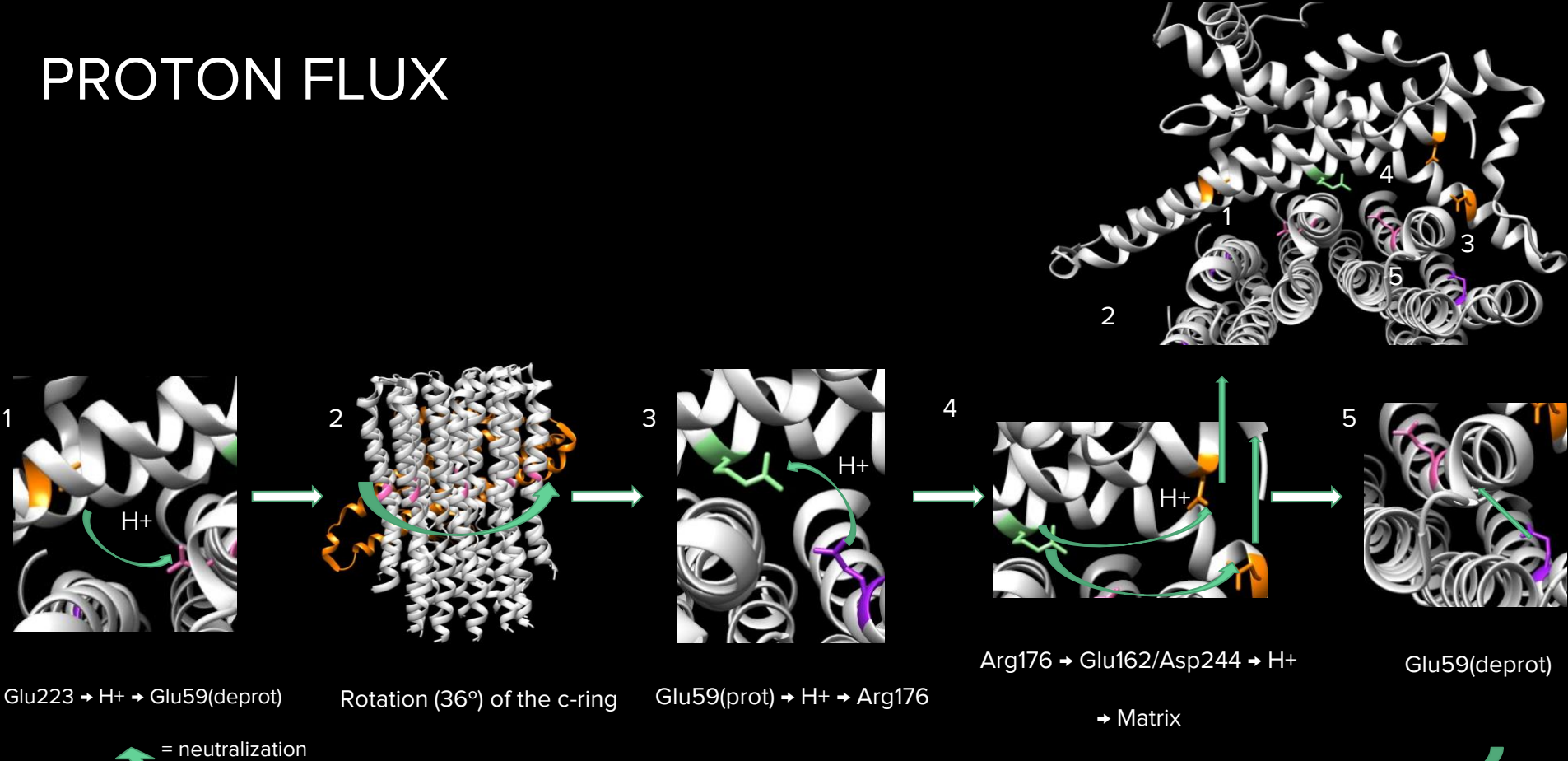


PROTON FLUX



Guo, H., Bueler, S. and Rubinstein, J. (2017). Atomic model for the dimeric FOregion of mitochondrial ATP synthase. *Science*, 358(6365), pp.936-940

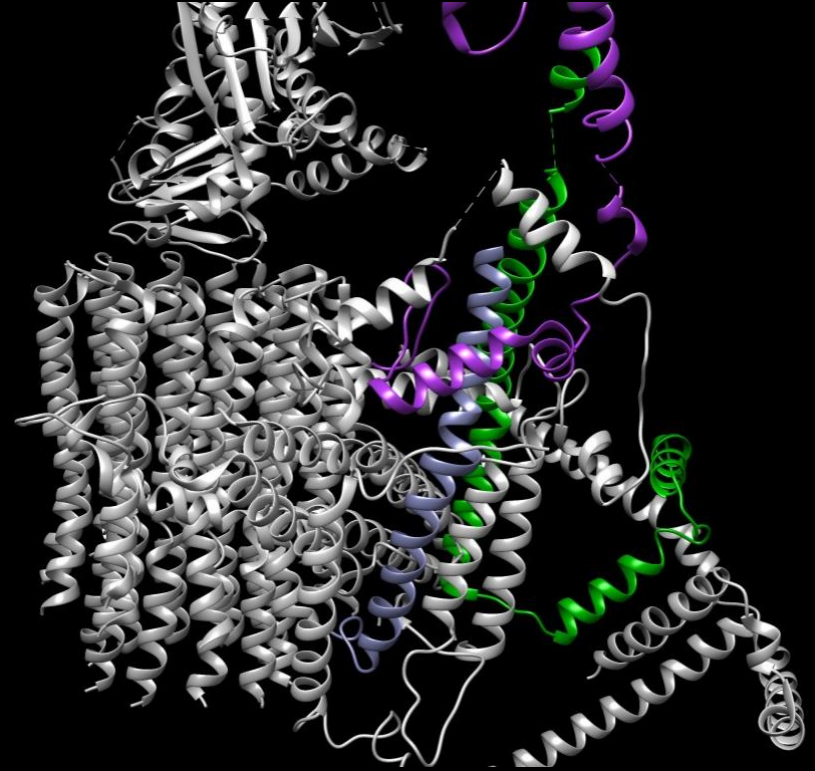
PROTON FLUX



SUBUNIT d

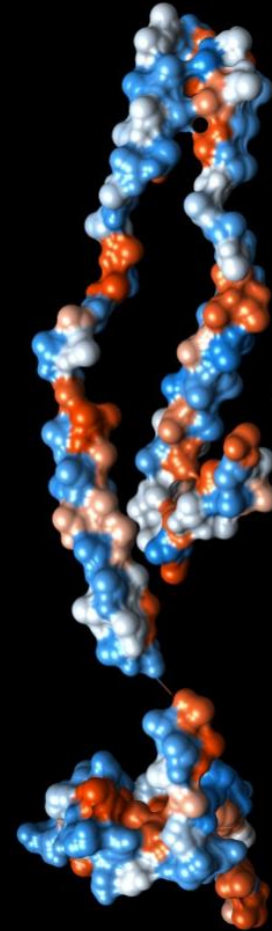


173 aa
4 helices
Peripheral stalk

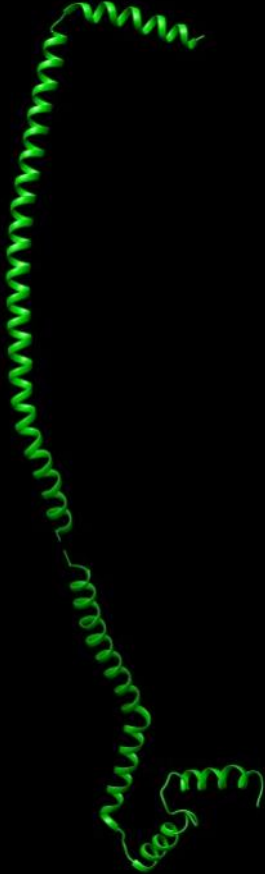


SUBUNIT d

- Total residues = 173
- **Polar residues = 105 - Percentage: 60.7**
- Nonpolar residues = 68 - Percentage: 39.3
- Acidic residues = 26 - Percentage: 15
- Basic residues = 29 - Percentage: 16.8
- Basic residues with His = 31 - Percentage: 17.9



SUBUNIT b

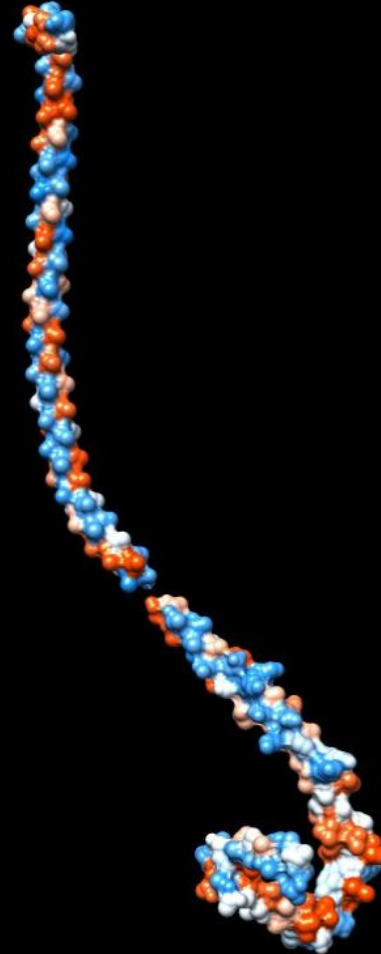


209 aa
Peripheral stalk
5 helices



SUBUNIT b

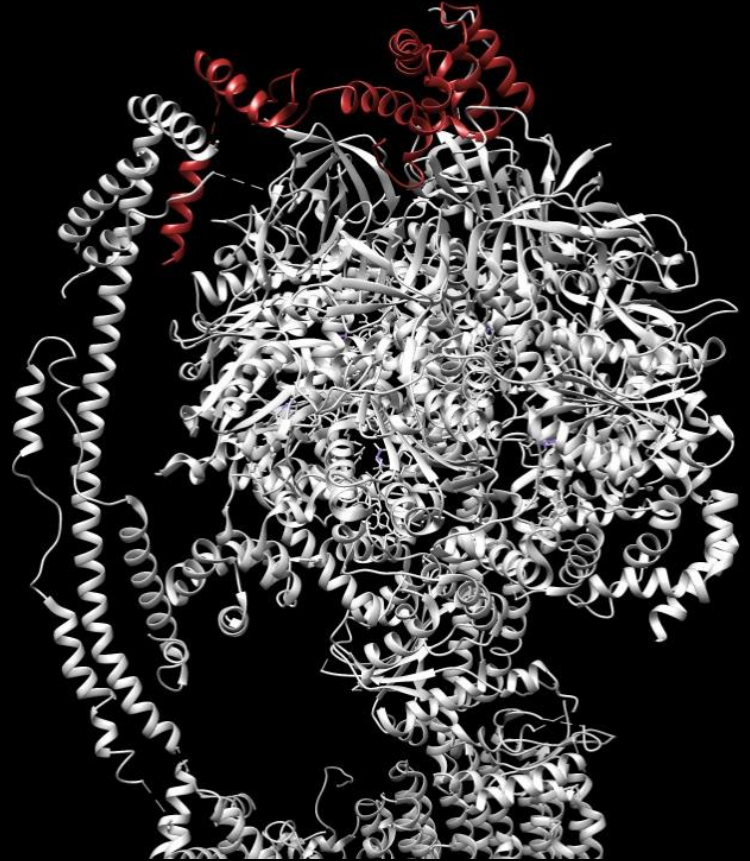
- Total residues = 209
- **Polar residues = 114 - Percentage: 54.5**
- **Nonpolar residues = 95 - Percentage: 45.5**
- Acidic residues = 27 - Percentage: 12.9
- Basic residues = 27 - Percentage: 12.9
- Basic residues with His = 29 - Percentage: 13.9



SUBUNIT OSCP

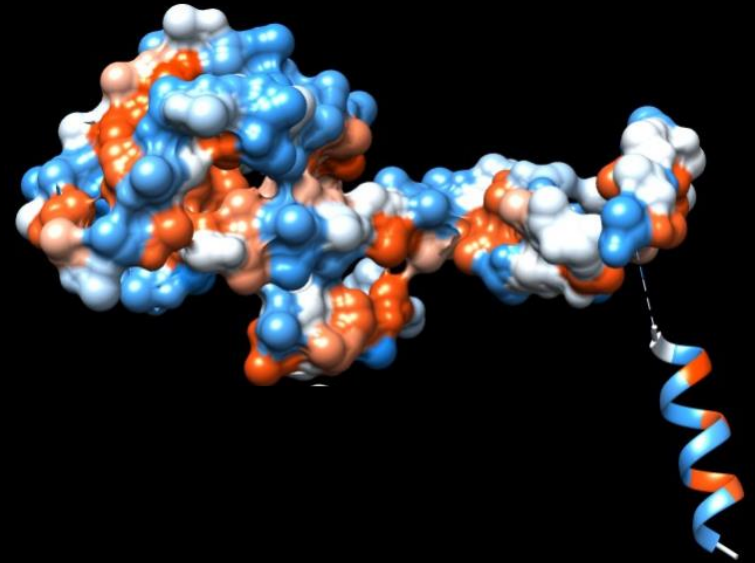


195 aa
Peripheral stalk
8 helices



SUBUNIT OSCP

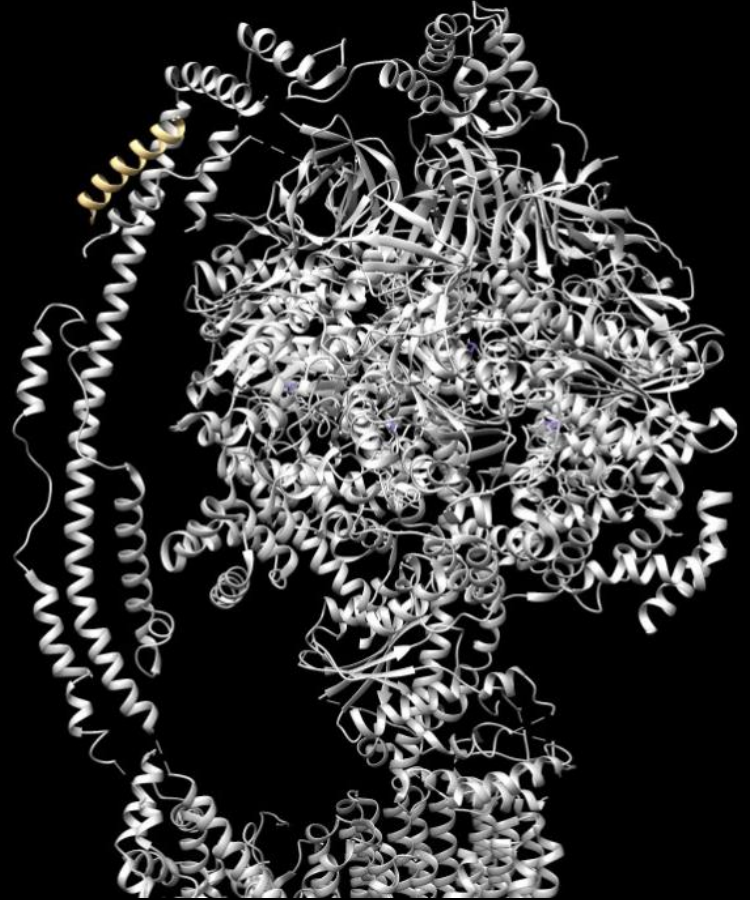
- Total residues = 195
- **Polar residues = 107 - Percentage: 54.9**
- Nonpolar residues = 88 - Percentage: 45.1
- Acidic residues = 21 - Percentage: 10.8
- Basic residues = 27 - Percentage: 13.8
- Basic residues with His = 30 - Percentage: 15.4



SUBUNIT h



20 aa
Peripheral stalk
1 helix



SUBUNIT f

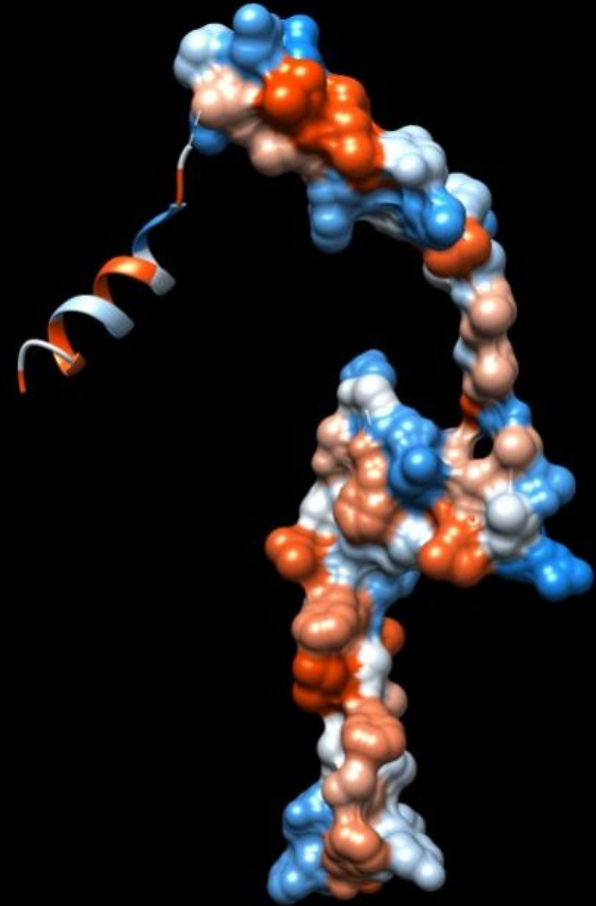


95 aa
Supernumerary subunit
4 helices

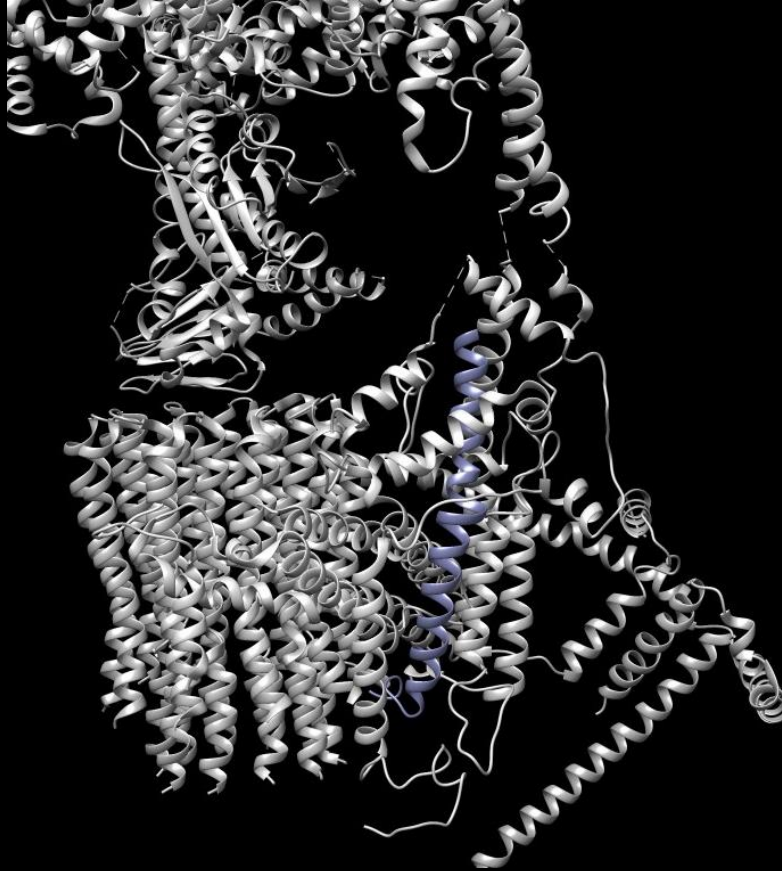


SUBUNIT f

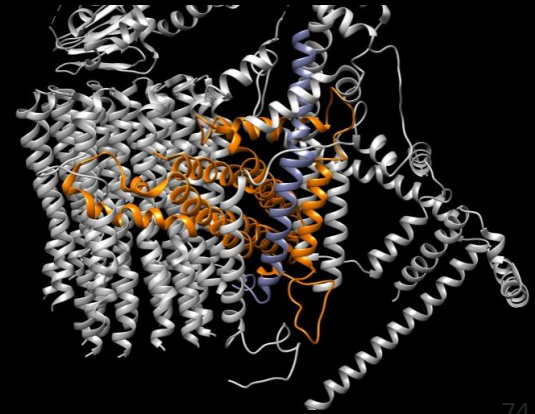
- Total residues = 95
- **Polar residues = 46 - Percentage: 48.4**
- **Nonpolar residues = 49 - Percentage: 51.6**
- Acidic residues = 5 - Percentage: 5.3
- Basic residues = 13 - Percentage: 13.7
- Basic residues with His = 19 - Percentage: 20



SUBUNIT 8

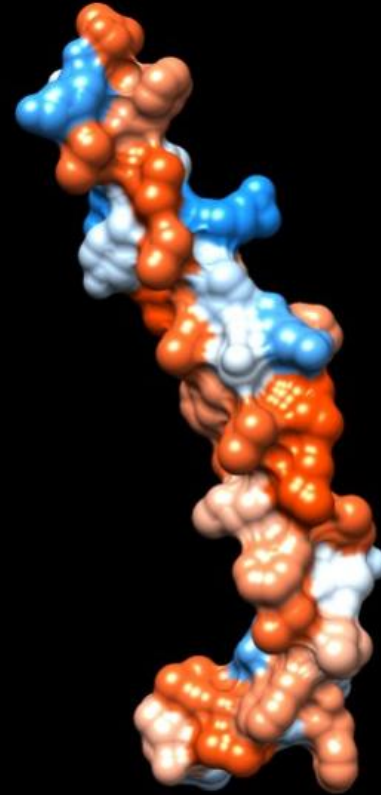


48 aa
Rotor
1 transmembrane helix

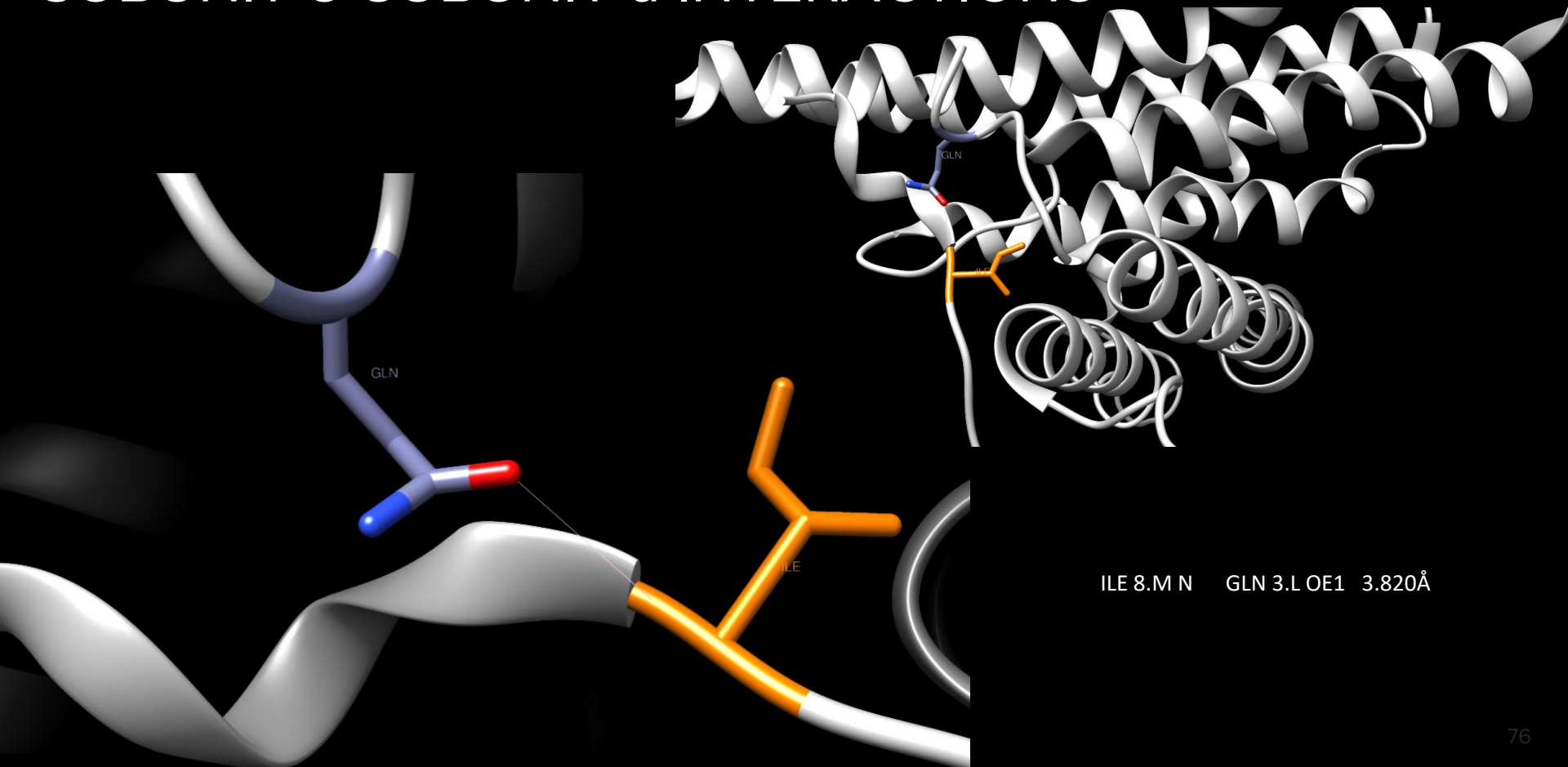


SUBUNIT 8

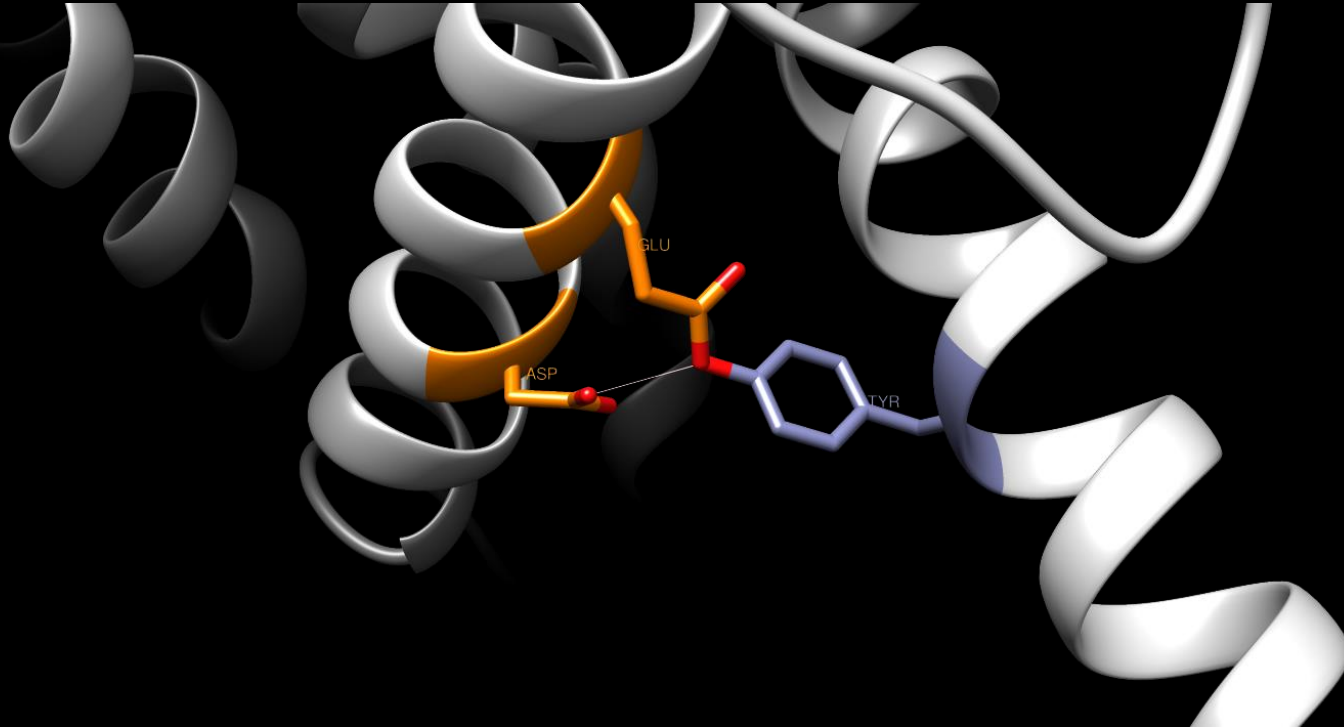
- Total residues = 48
- Polar residues = 13 - Percentage: 27.1
- **Nonpolar residues = 35 - Percentage: 72.9**
- Acidic residues = 0 - Percentage: 0.0
- Basic residues = 3 - Percentage: 6.25
- Basic residues with His = 3 - Percentage: 6.25



SUBUNIT 8-SUBUNIT α INTERACTIONS



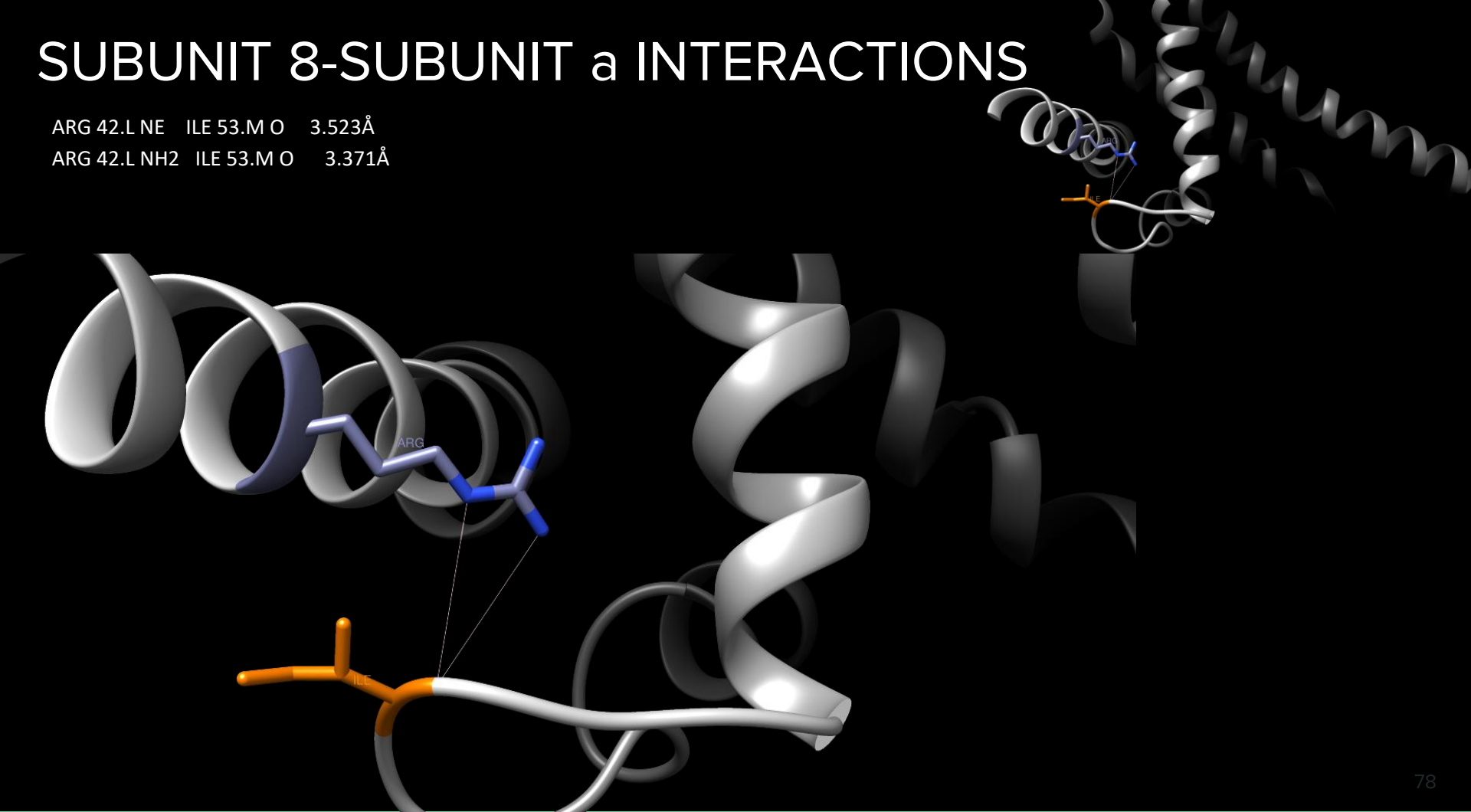
SUBUNIT 8-SUBUNIT α INTERACTIONS



TYR 39.L OH GLU 63.M OE2 2.417Å
TYR 39.L OH ASP 67.M OD2 2.986Å

SUBUNIT 8-SUBUNIT α INTERACTIONS

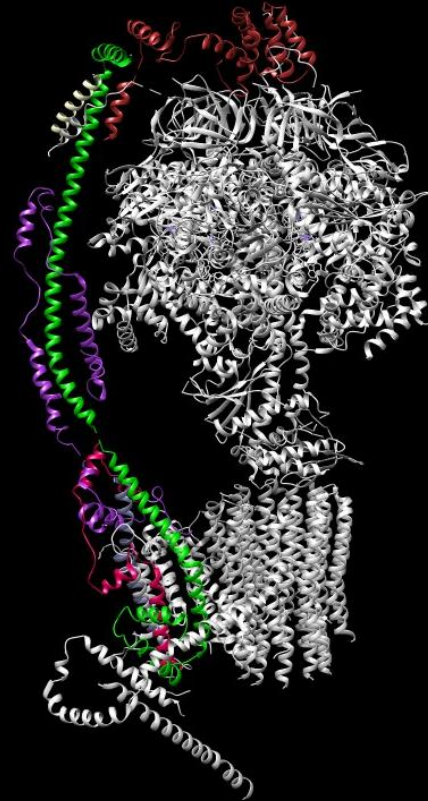
ARG 42.L NE ILE 53.M O 3.523Å
ARG 42.L NH2 ILE 53.M O 3.371Å



PERIPHERAL STALK

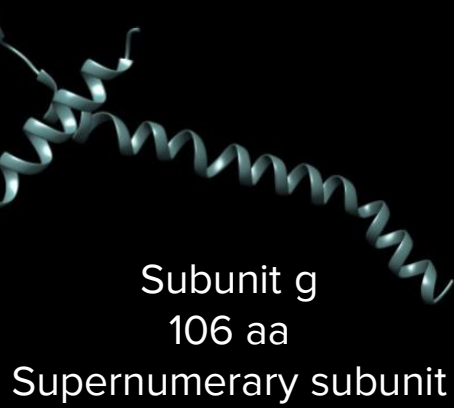


- SUBUNIT b
- SUBUNIT d
- SUBUNIT OSCP
- SUBUNIT h

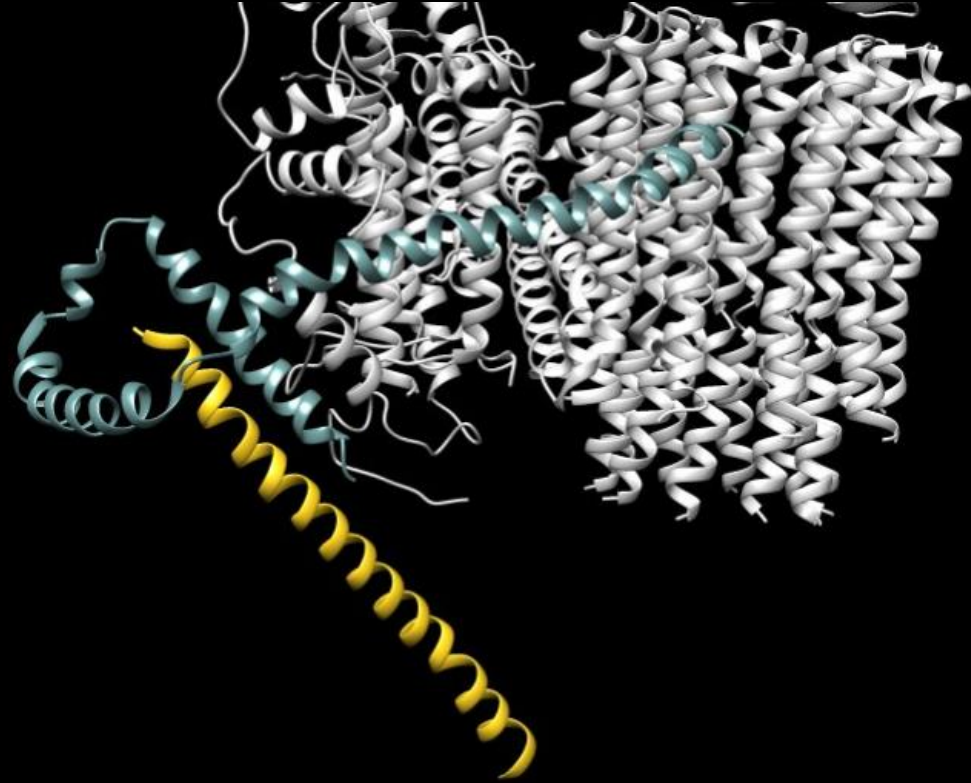


- SUBUNIT b
- SUBUNIT d
- SUBUNIT OSCP
- SUBUNIT h
- SUBUNIT f
- SUBUNIT 8

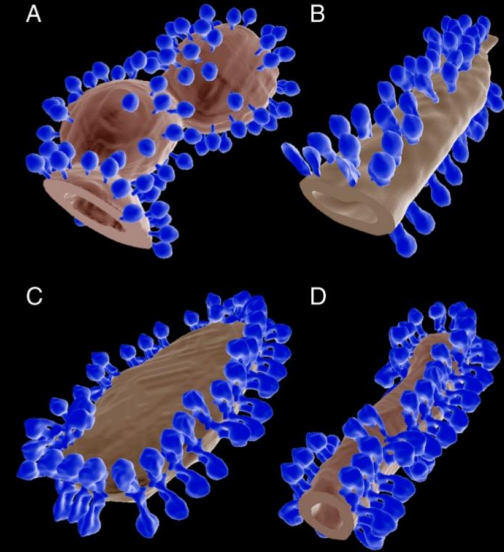
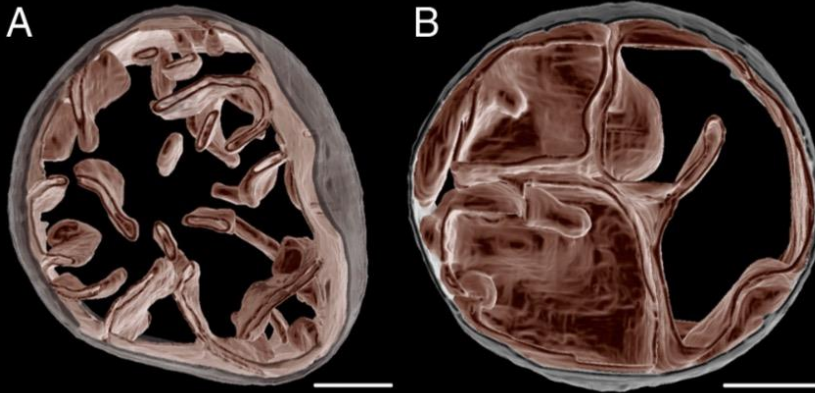
SUBUNITs e and g



Subunit e
49 aa
Supernumerary subunit
1 helix

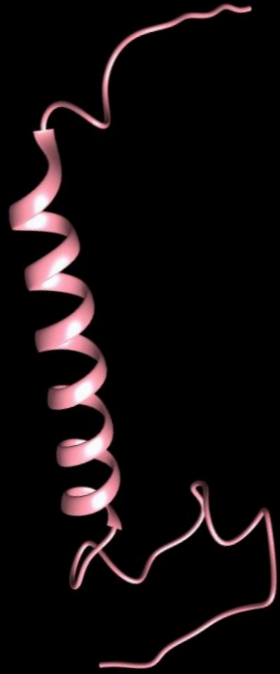


SUBUNIT e



Davies, K., Anselmi, C., Wittig, I., Faraldo-Gomez, J. and Kuhlbrandt, W. (2012). Structure of the yeast F1Fo-ATP synthase dimer and its role in shaping the mitochondrial cristae. *Proceedings of the National Academy of Sciences*, 109(34), pp.13602-13607.

SUBUNIT i/j



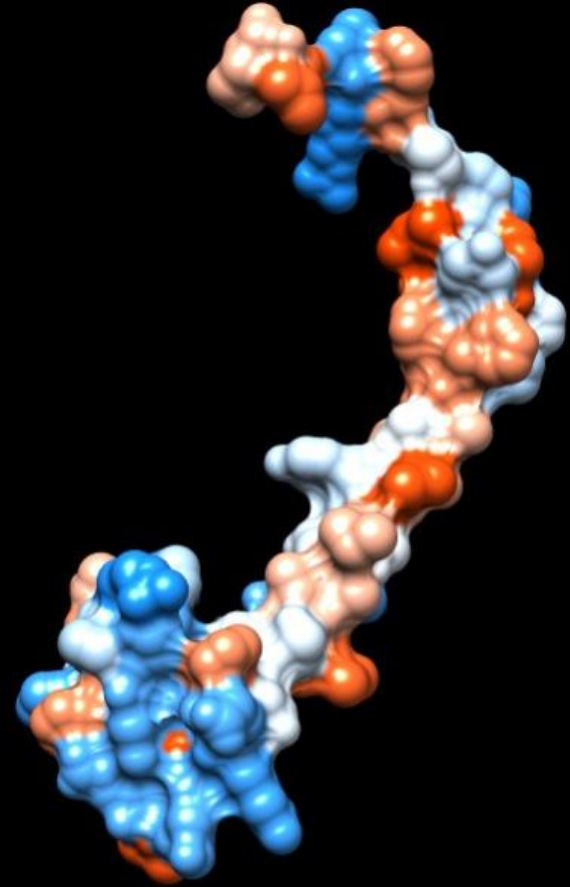
59 aa

Supernumerary subunit
1 transmembrane helix



SUBUNIT i/j

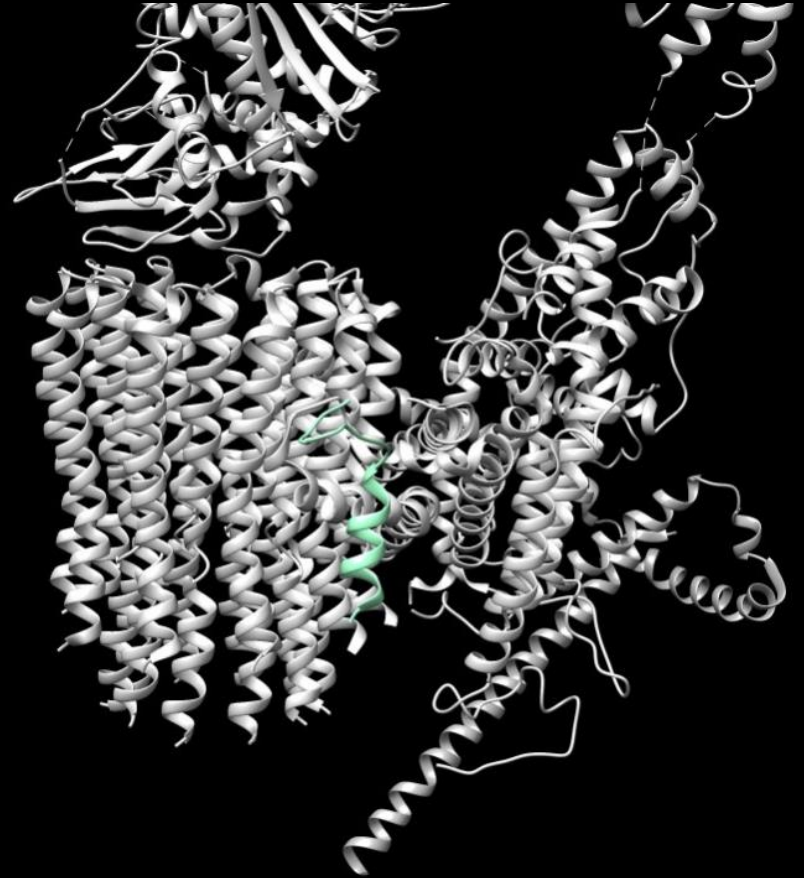
- Total residues = 59
- Polar residues = 26 - Percentage: 44.1
- **Nonpolar residues = 33 - Percentage: 55.9**
- Acidic residues = 5 - Percentage: 8.5
- Basic residues = 9 - Percentage: 15.3
- Basic residues with His = 9 - Percentage: 15.3



SUBUNIT k

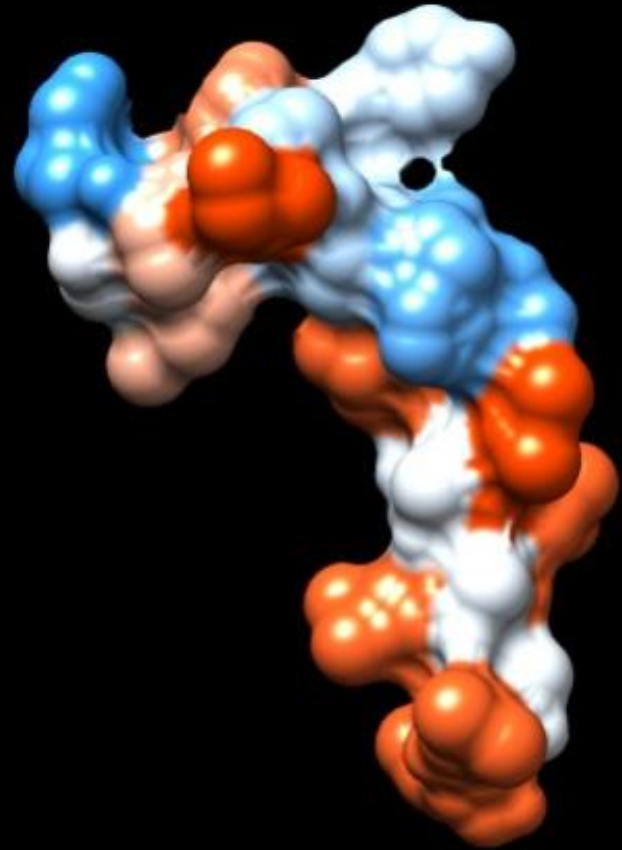


28 aa
Supernumerary subunit
1 transmembrane helix

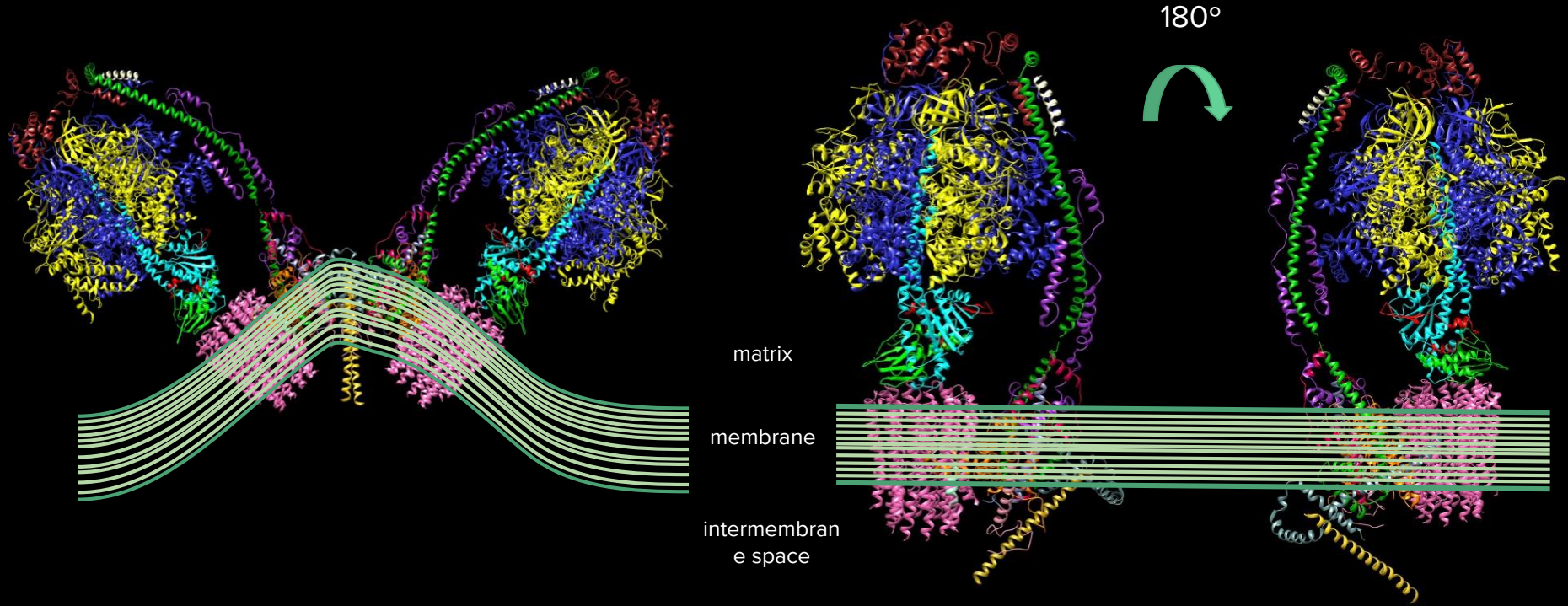


SUBUNIT k

- Total residues = 68
- Polar residues = 36 - Percentage: 52.9
- **Nonpolar residues = 32 - Percentage: 47.1**
- Acidic residues = 8 - Percentage: 11.8
- Basic residues = 10 - Percentage: 14.7
- Basic residues with His = 13 - Percentage: 19.1

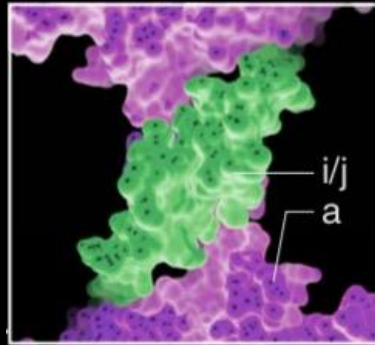
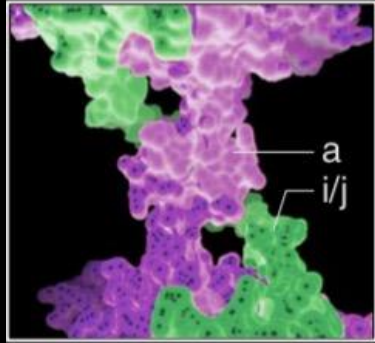


ATP SYNTHASE dimer



F₀ ATP SYNTHASE DIMER

viewed from matrix

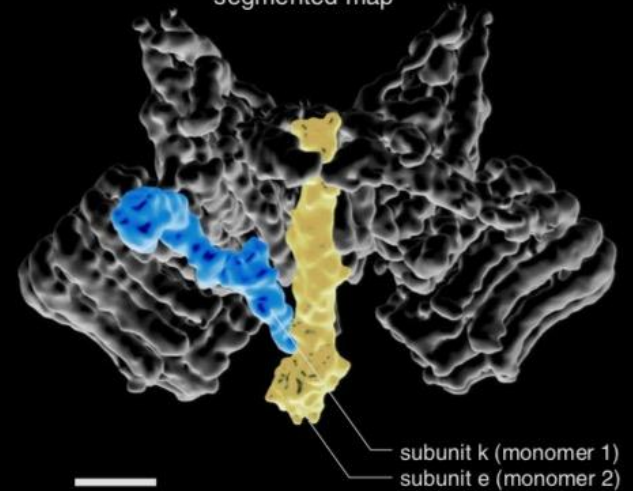


viewed from IMS



c

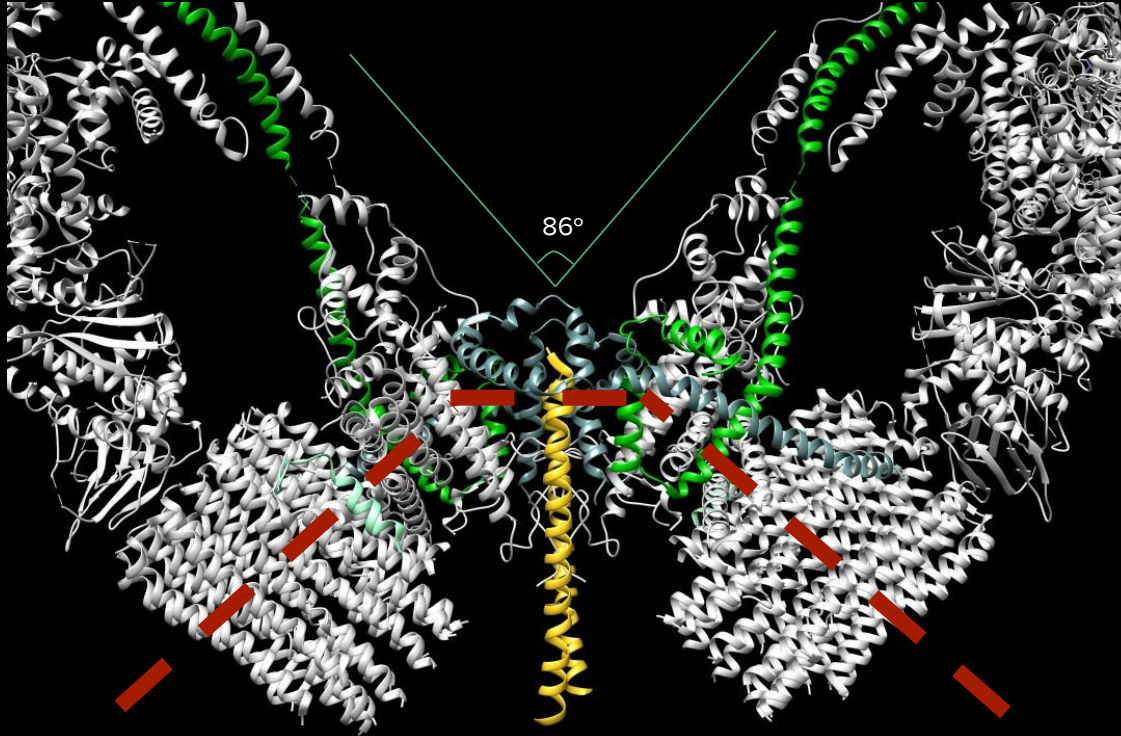
unsharpened
segmented map



- SUBUNIT a
- SUBUNIT i/j
- SUBUNIT e
- SUBUNIT k

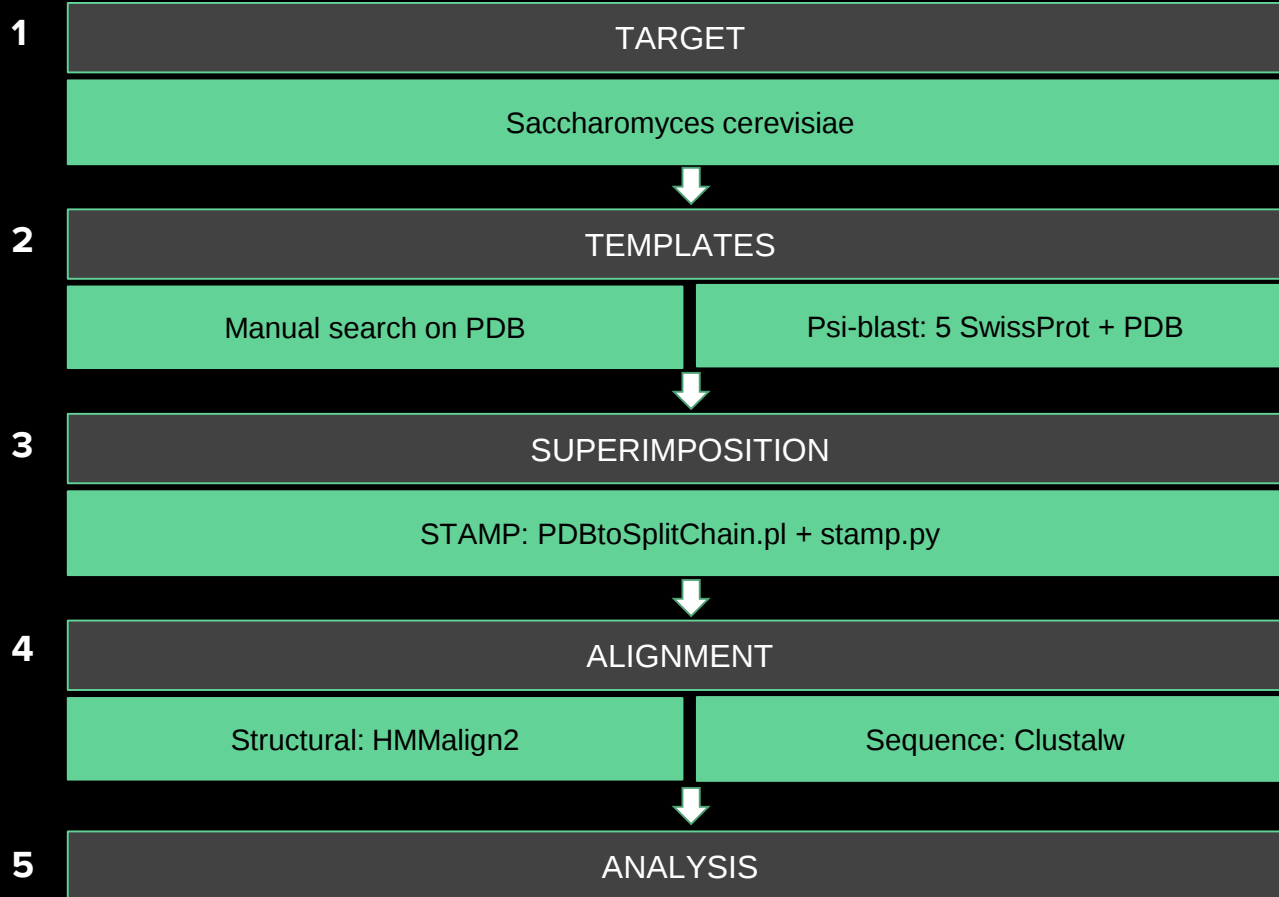
subunit k (monomer 1)
subunit e (monomer 2)

F₀ ATP SYNTHASE DIMER

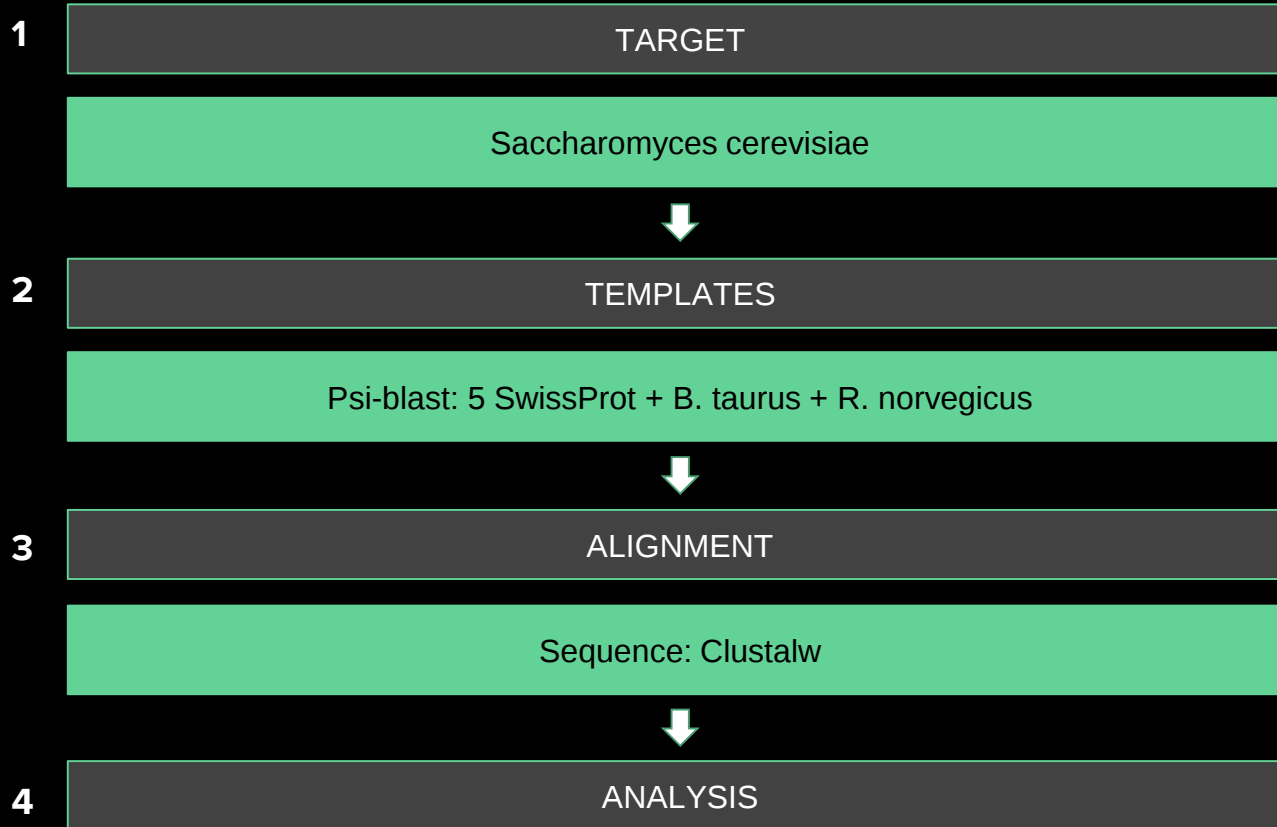


- SUBUNIT b
- SUBUNIT e
- SUBUNIT g
- SUBUNIT k

STRUCTURE ALIGNMENT



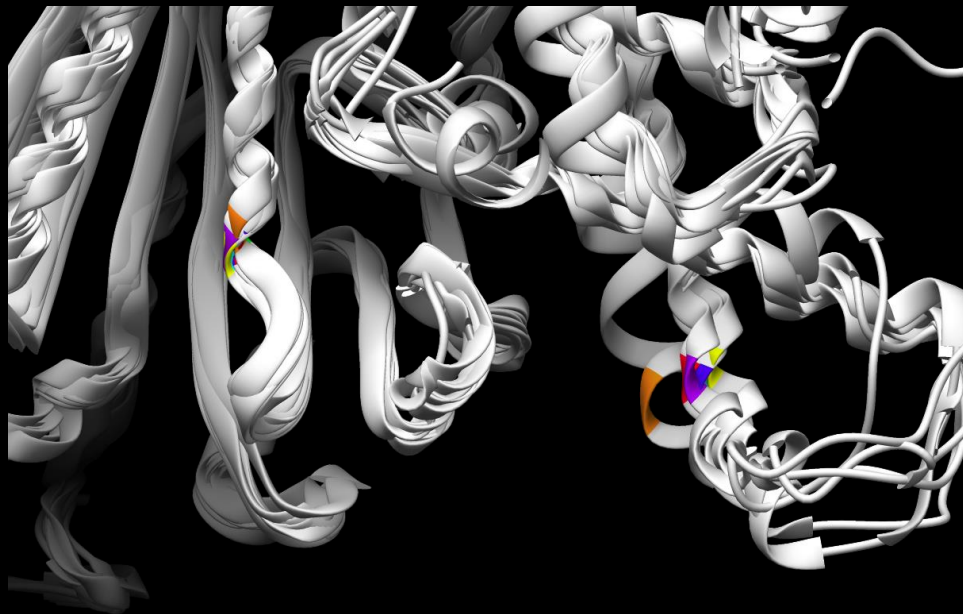
SEQUENCE ALIGNMENT



F1: Alpha structural alignment



Sc: 7.91 RMS: 1.09



F1: Alpha structural alignment

```

Saccharomyces_cerevisiae  -----nlnE-TGRVLAVGGDIARVGL--N-NIDAEELVEF-SS----GVK
Bos_taurus                -----dleE-TGRVLISIGDGIARVHGL--R-NVDAEEMVEF-SS----GLK
Trypanosoma_brucei        -----sffkttEMIGYVHSIDGTIATLIPAGNPGVRYNTIIQI-QVspptfAA
Mycobacterium_smegmatis   -----IGTVIDAGDGIHVEGL--PSVHTQELLEFP-GG--GVL
Rattus_norvegicus         ssileerigadtsvdleE-TGRVLISIGDGIARVHGL--R-NVDAEEMVEF-SS----GLK
Bacillus_sp               -----E-VGTVIQVGGDIARVHGL--E-KVMAGELLEF-EN----GVM
Thermotoga_maritima       -----ksfeekldleD-TGKVIQVGGDIARVHGL--N-KVLSSELVEFVET---GVK

                                G45 L46   Q50 A51
                                [ ] [ ] [ ] [ ]

Saccharomyces_cerevisiae  GMLNLNPG-QVGIVLFGSDRLVKEGELVKRTGNIVDVPVPGLLGRVVDALGNPID--G
Bos_taurus                GMSLNLNPD-NVGVVVFGNDKLIKEGDIVKRTGAIVDVPVGEELLGRVVDALGNAID--G
Trypanosoma_brucei        GLVFNLEKdGRIGIIMDNITEVGSQKVMATGQLLHIPPVAGVLGKVVNPLGHEVPVS-
Mycobacterium_smegmatis   GVALNLDEH-SVGAIVLGEFEKIEEGQVKRTGEVLSVPVGDALFLGRVNVNPLQPID--G
Rattus_norvegicus         GMSLNLNPD-NVGVVVFGNDKLIKEGDIVKRTGAIVDVPVGEELLGRVVDALGNAID--G
Bacillus_sp               GMAQNLEED-NVGVVILPGPYTEIREGTQVKRTGRIMEVPGVGEALLGRVNVNPLQPLD--G
Thermotoga_maritima       GVAFNLEED-NVGIIILGEYKDIKEGHTVRRLLRIEVPVGEELLGRVNVNPLGLEPD--G

                                K134 I138 R141 S143   T178
                                [ ] [ ] [ ] [ ] [ ]

Saccharomyces_cerevisiae  KGPIDAAGRSRAQVAPDILFRFVHEPVQTLKAVDALVPIGRQRELIIGDRQTGKTA
Bos_taurus                KGPIGSKARRRVGLKAPCIIPRIIVREPMQTGIKAVDLSLVPPIGRQRELIIGDRQTGKTS
Trypanosoma_brucei        -----TLGKVDTCAPNIVSRSPVNNYLLTGFKAVDTMIPIGRQRELIIGDRQTGKTS
Mycobacterium_smegmatis   QGDIAAETRRALELQAPSVMGRCSVSEPLQTGIKAIDAMTPIGRQRLQIIGDRKTGKTA
Rattus_norvegicus         KGPVGSKIRRRVGLKAPCIIPRIIVREPMQTGIKAVDLSLVPPIGRQRELIIGDRQTGKTS
Bacillus_sp               RGPETAEYRPIESAPCVMDKSVHEPLQGTGIKAIDSMIPIGRQRELIIGDRQTGKTT
Thermotoga_maritima       KGPINAKNFRPIEIKAPCIIVKEDVDTPLQTGIKAIDS-IPIGRQRELIIGDRQTGKTA

                                K134 I138 R141 S143   T178
                                [ ] [ ] [ ] [ ] [ ]

Saccharomyces_cerevisiae  VALDTILNQKRWNNGSDESKLYCVYVAVGQKRSTVAQLVQTLQEHQDAMKYSIIVAATAS
Bos_taurus                IAIDTIINQKRFNDGTDEKKLYCIYVAIGQKRSTVAQLVKRLTDADAMKYTIIVVSATAS
Trypanosoma_brucei        IAVSTIINQVRINQQLTSKNAVSIYVYSIGQRCSNVARIHRLQSYGALRYTTVMAATAS
Mycobacterium_smegmatis   VCDVDTILNQ-R-----VRCVYVAGIKGQGTIIASVKRALEEGGAEYTTIIVAAPAS
Rattus_norvegicus         IAIDTIINQKRFNDGTDEKKLYCIYVAIGQKRSTVAQLVKRLTDADAMKYTIIVVSATAS
Bacillus_sp               IAIDTIINQKQG-----DVICIIYVAGIKQKRSTVAGVETLRQHDALDYTIIVVSATAS
Thermotoga_maritima       IAIDTIINQKQG-----GVYCIYVAGIKQKSAIARIIDKLQRYGA-EYTTVVVASAS

                                K134 I138 R141 S143   T178
                                [ ] [ ] [ ] [ ] [ ]

Saccharomyces_cerevisiae  EAAPLQYLAPFTAASIGEWFRDNGKHALIVYDDLSKQAVAYRQLSLLRRPPGREAYPGD
Bos_taurus                DAAPLQYLAPYSGCSMGGEYFRDNGKHALIYDDLSKQAVAYRQMSLLRRPPGREAYPGD
Trypanosoma_brucei        EPAGLQYLAPYAGVTMGGEYFMNRGRHCLVYDDLSKQAVAYRQISLLRRPPGREAYPGD
Mycobacterium_smegmatis   DAAGFKWLPAYTGSATGQHMYNGKHWLVIFVDDLSKQADAYRAISLLRRPPGREAYPGD
Rattus_norvegicus         DAAPLQYLAPYSGCSMGGEYFRDNGKHALIYDDLSKQAVAYRQMSLLRRPPGREAYPGD
Bacillus_sp               EPAPLLYLAPYAGCAGEYFMYKKGKHALVYDDLSKQAAAYREL SLLRRPPGREAYPGD
Thermotoga_maritima       DPASLQYIAPYAGCA-GEYFAYSGRDALVYDDLSKHAVAYRQLSLL-RRPPGREAYPGD

```

```

Saccharomyces_cerevisiae  VFYLHRLRLRAAKLSEKGGSGSLTALPVIEQTGGDVSAYIPTNVISITDQGIFLEAEFL
Bos_taurus                VFYLHRLRLRAAKMNDLGGGSLTALPVIEQTAGDVSAYIPTNVISITDQGIFLETFL
Trypanosoma_brucei        VFYLHRLRLRAAMLSPKGGGSLTALPVIEQLSNDVTAYIVTNVISITDQGIYLDTKLF
Mycobacterium_smegmatis   VFYLHRLRLRAAKLSEKGGGSLTALPVIEQTAGDVSAYIPTNVISITDQCFLESDLF
Rattus_norvegicus         VFYLHRLRLRAAKMNDLGGGSLTALPVIEQTAGDVSAYIPTNVISITDQGILETFL
Bacillus_sp               VFYLHRLRLRAAKLSEKGGGSLTALPVIEQTAGDVSAYIPTNVISITDQGILETFL
Thermotoga_maritima       IFYLHRLRLRAVRLNLDLGGGSLTALPVIEQTANDISAYIPTNVISITDQGIYLEPLGF

                                S305 E309   K317   T348 D349
                                [ ] [ ] [ ] [ ] [ ]

Saccharomyces_cerevisiae  YKGIKIRPAINVGLSVSRVGSAAQVKALKQVAGSLKFLAQYREVAA-FA-Q-S-DLDASTK
Bos_taurus                YKGIKIRPAINVGLSVSRVGSAAQTRAMKQVAGTMKLELAQYREVAA-FA-QFGSOLDAAQT
Trypanosoma_brucei        TGGQRPAINVGLSVSRVGSAAQNAAMKQVAGLKGILAEYRKLAAD-D-----VQ--T
Mycobacterium_smegmatis   NQGVIRPAINVGLSVSRVGSAAQIKAMKEVAGSLRLDLQYRELEA-FAaFAS-DLDAASK
Rattus_norvegicus         YKGIKIRPAINVGLSVSRVGSAAQTRAMKQVAGTMKLELAQYR--EA-----TQ
Bacillus_sp               YSGVRPAINVGLSVSRVGSAAQIKAMKVAGTLRLDLAQYRELQA-FA-QFGSOLDKATQ
Thermotoga_maritima       YAGQIRPAINVGLSVSRVGSAAQIKAKVAGLQVAG-LRIDLAQYRELET-FA-QFATELDPAIR

                                R375
                                [ ]

Saccharomyces_cerevisiae  QTLVRGERLTQLLKQNYSPPLATEEQVPLIYAGVNGHLDGIELSRIGFEFFSFLSY----
Bos_taurus                QLLSRGVRLTQLLKQNYSPMAIEEQVAVIYAGVRGYLDKLEPSKITKFENAFSLH---
Trypanosoma_brucei        IPMIRGARFVALFNQ-KQ-PSYFMNAIVSLYACLNGYLDVQVQVYKFEYLLVHRDLGI
Mycobacterium_smegmatis   AQLDORGARLVELLKQNPQYSPPLAVEEQVVAIFLGTQGHLDSPVEDVQRFESSELH---
Rattus_norvegicus         QLLSRGVRLTQLLKQNYSPMAIEEQVAVIYAGVRGYLDKLEPSKITKFENAFSLH---
Bacillus_sp               AKLNRGERTVEILKQDEHKMPVEEQVSIYAVNTGFMDDIPVEDVRRFEELLFSF----
Thermotoga_maritima       AQIIRGQRL-ELLKQNPQYSP-PVEEQVVLFAVGRVLDLDPVEEVRRFEKEFLRF----

                                -----LKSNNHELLTEIREKGEL-SKELLASLKSATESFVAT-----
Saccharomyces_cerevisiae  -----VISQHQALLGKIRTGDKI-SEESDAKLKEIVTNFLAG----FEA-----
Bos_taurus                MYGTAKNKKFFMY-VQELNLYIRFF-TLNSPILHGEELMKQHTLFLQHYQSKmaik
Trypanosoma_brucei        -----VKASHSDIFDGIRETAKL-SEEAEEKLVSVINEFFKKG----FXXxxxxxx
Mycobacterium_smegmatis   -----VVSQHQSLDGNIRDTGDKI-SEQSDAKLKEIVTNFLAG----FEP-----
Rattus_norvegicus         -----MRANKDSLLDHIRTGEL-P-D-TKELDAAIEEFKKG----FTP-----
Bacillus_sp               -----HEKHQDILDDIKTKKEL-TSETEEKLKAIEEFKTT----FRV-----
Thermotoga_maritima       -----HEKHQDILDDIKTKKEL-TSETEEKLKAIEEFKTT----FRV-----

                                -----LKSNNHELLTEIREKGEL-SKELLASLKSATESFVAT-----
Saccharomyces_cerevisiae  -----LKSNNHELLTEIREKGEL-SKELLASLKSATESFVAT-----
Bos_taurus                -----VISQHQALLGKIRTGDKI-SEESDAKLKEIVTNFLAG----FEA-----
Trypanosoma_brucei        MYGTAKNKKFFMY-VQELNLYIRFF-TLNSPILHGEELMKQHTLFLQHYQSKmaik
Mycobacterium_smegmatis   -----VKASHSDIFDGIRETAKL-SEEAEEKLVSVINEFFKKG----FXXxxxxxx
Rattus_norvegicus         -----VVSQHQSLDGNIRDTGDKI-SEQSDAKLKEIVTNFLAG----FEP-----
Bacillus_sp               -----MRANKDSLLDHIRTGEL-P-D-TKELDAAIEEFKKG----FTP-----
Thermotoga_maritima       -----HEKHQDILDDIKTKKEL-TSETEEKLKAIEEFKTT----FRV-----

```

F1: Alpha

Trypanosoma brucei_subunit_alpha
Saccharomyces cerevisiae_subunit_alpha
Bos taurus_subunit_alpha
Rattus norvegicus_subunit_alpha
Mycobacterium smegmatis_subunit_alpha
Bacillus_sp_subunit_alpha
Thermotoga_maritima_subunit_alpha

G45 L46

```

-----AATAPAGASTTSST--SSAQKSFKK--TTEMIGYVHSIDGTIATLIPAGNP 48
-----ASTKAQPTVESSSILEERIKGVSDKANLNETGRVLAVGDIARV---FSLN 47
-----QKTGTAEVSSSILEERILGADTSVDLEETGRVLSIGDGIARV---HGLR 45
-----QKTGTAEVSSSILEERILGADTSVDLEETGRVLSIGDGIARV---HGLR 45
-----MAELTISAADLEGAEIDYVSSFSADTEREEIGTVIDAGDIAHV---ESLP 48
-----MSIRPEEISALIKKQIENYADLEVVEVGTVIQVGDGIARV---HGLE 45
MGSDKIHMHHLRINPGETTKVLEEKIKSFEEKIDLEDTGKVIQVGDGIARA---YGLN 57

```

Trypanosoma brucei_subunit_alpha
Saccharomyces cerevisiae_subunit_alpha
Bos taurus_subunit_alpha
Rattus norvegicus_subunit_alpha
Mycobacterium smegmatis_subunit_alpha
Bacillus_sp_subunit_alpha
Thermotoga_maritima_subunit_alpha

Q50 A51 L68 E69

```

GVNNTIIQIQVSPPTTFAAGLVFNLEKDRIGIILMDNITEVQSGQKVMATGQLLHIPVG 108
NIQAEELEVEF---SSGVKGMALNLEP-GQVGIVLFGSDRLVKEGELVKRTGNIVDPVPG 102
NVQAEEVVEF---SSGLKGMALNLEP-DNVGVVVFQNDKLIKEGDIVKRTGAIVDPVPG 100
NVQAEEVVEF---SSGLKGMALNLEP-DNVGVVVFQNDKLIKEGDIVKRTGAIVDPVPG 100
SVMTQELLEF---PGGVLGVALNLEP-HSVGAVILGEFEKIEEGQVQKRTGEVLVSPVG 103
KVMAGELLEF---ENGVMGMAONLEP-DNVGVVILGPYTEIREGTQVKTGRIMEVPGV 100
KVMSELVEF---VETGVKGVAFNLEP-DNVGIILGEYKDIKEGHTVRRLLKRIIEVPVG 113

```

Trypanosoma brucei_subunit_alpha
Saccharomyces cerevisiae_subunit_alpha
Bos taurus_subunit_alpha
Rattus norvegicus_subunit_alpha
Mycobacterium smegmatis_subunit_alpha
Bacillus_sp_subunit_alpha
Thermotoga_maritima_subunit_alpha

K134 I138 R141 S143

```

AGVLGKVVNPLGHEVPVGLVTRSRRLDSTLGKVDTPAPNLSVSPVNNLLTGFAKVD 168
PGLLGRVVDALGNPIDGK----GPIDAAGRSRAQVHAPGLPNSVHEPVQTGLKAVD 157
EELLGRVVDALGNAIDGK----GPISKARRRVGLHAPGLIPNISVREPMQTGIKAVD 155
DELLGRVVDALGNAIDGK----GPVGSKIRRRVGLHAPGLIPNISVREPMQTGIKAVD 155
DAFLGRVVNPLGQPIDGQ----GDIAAETRRALDAPSIVVQVSVSEPLQTGIKAIDA 158
EALLGRVVNPLGQPLDGR----GPIETAERYPIESAPGMDRKSVHEPLQTGIKAIDS 155
EELLGRVVNPLGQPLDGR----GPIAKNFRPIETHAPGLIYKPEVDTPLQTGIKAIDS 168

```

Trypanosoma brucei_subunit_alpha
Saccharomyces cerevisiae_subunit_alpha
Bos taurus_subunit_alpha
Rattus norvegicus_subunit_alpha
Mycobacterium smegmatis_subunit_alpha
Bacillus_sp_subunit_alpha
Thermotoga_maritima_subunit_alpha

T178

```

MIPIGRGORELIVGDRQTGHTIAVSTIINQVRINQOILSKNAVISIYYSIGQRCSNVAR 228
LVPIGRGORELIGDRQTGHTIAVALDTILNOKRWNGSDESKKLYCVYAVGQKRSTVAQ 217
LVPIGRGORELIGDRQTGHTIAIDTIINQKRFNDGTDEKKKLYCIYVAIGQKRSTVAQ 215
LVPIGRGORELIGDRQTGHTIAIDTIINQKRFNDGTDEKKKLYCIYVAIGQKRSTVAQ 215
MTPIGRGORELIGDRQTGHTIAVDTILNQREAWLTGDPKQOVRCVYVAIGQKTIIAS 218
MIPIGRGORELIGDRQTGHTIAIDTIINQK-----GQDVICIYVAIGQKQSTVAG 207
MIPIGRGORELIGDRQTGHTIAIDTIINQK-----GQGVYCIYVAIGQKKSIAIR 220

```

Trypanosoma brucei_subunit_alpha
Saccharomyces cerevisiae_subunit_alpha
Bos taurus_subunit_alpha
Rattus norvegicus_subunit_alpha
Mycobacterium smegmatis_subunit_alpha
Bacillus_sp_subunit_alpha
Thermotoga_maritima_subunit_alpha

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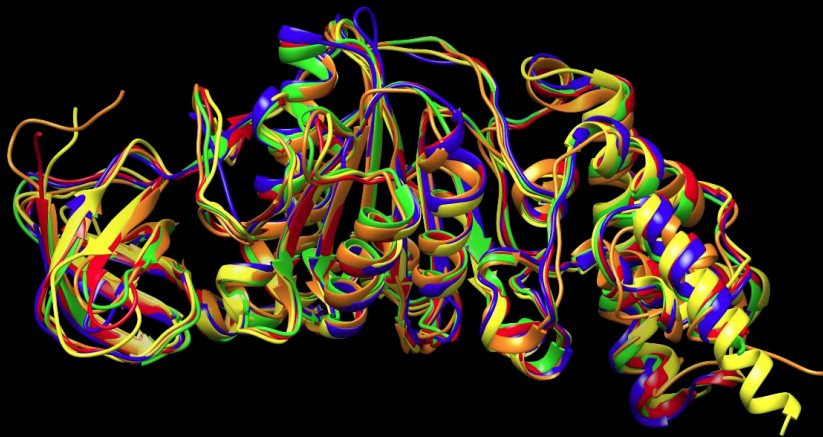
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LVKRLTDADAMKYTIIVSATASDAAPLQYLAPYSGCSMGVEYFRDNGKHALIYDDLKQA 275
LVKRLTDADAMKYTIIVSATASDAAPLQYLAPYSGCSMGVEYFRDNGKHALIYDDLKQA 275
VKRALEEGGMEYTTTIVAAPASDAAGFKWLAPYTGSAIGQHMVYNGKHVLIYVDLQKQA 278
VVETLRQHDALDYTIIVTASASEPAPLLYAPYAGCAMEGYFMYKGHKHALVYDDLKQA 267
IIDKLRYQGAMEYTTVVVASADPASLQYIAPYAGCAMEGYFAYSGRDLVYDDLKQA 280

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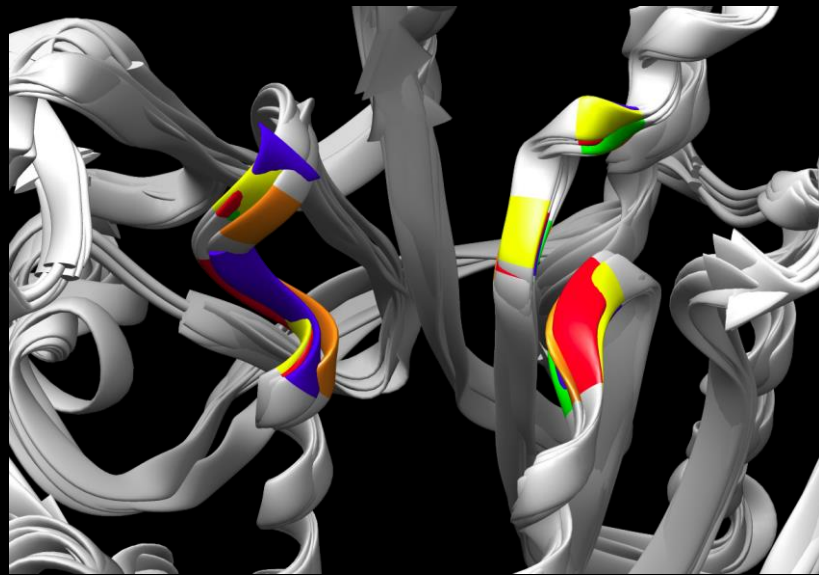
F1: Alpha

[illegible]

F1: Beta structural alignment



Sc: 8.88 RMS: 1.18



F1: Beta structural alignment

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

-----stpitGK^{V16}ITAVIGAIVDVHFEQSELPAILNALEIK-T--PQGLKLVLEVAQHLGEN
-----tGTRIAVAVIGAVVDVQFDE-GLPPILNALEVQ-G--RETRLVLEVAQHLGES
-----dhkgrVGHMSQVIGAVVDVHFAD-GVPPVLTAIDVVDKIGRDEPLTLEIVQHLDHAH
-----AGRWIRITGPVVDVVEFPRGSPVELFNALHAE-I--TK-TLTLEVAQHLGDS
saapkgatGTGTVAVIGAVVDVQFDE-GLPPILNALEVQ-G--RESRLVLEVAQHLGES
-----nKGRRIQVGMGPVVDIQFESGQLPDIYNATIERP--QGGLTLEAAVHVLGDN

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

TVRTIAM^{D65 G69 L70 R72}GGTEGLVGEKVLDTGGPISVPVRETGRINNVIGEPIDERGP-IKSKLRKP
TVRTIAMGGTEGLVGGQKVLDSGAPIRIPVGPETLGRIMNVIGEPIDERGP-IKTKQFAA
TGRCIAMTTDLKLLKAKVVSTGGNISVPVRETGRIFNVLGDAIDQRGV-VEGLRMP
LVRCISAMPTDGLVGGVEVTDGTASISVPVGGQVKGHFNALGDCLD--DE----HMS
TVRTIAMGGTEGLVGGQKVLDSGAPIKVPVGPETLGRIMNVIGEPIDERGP-IKTKQFAP
VVRCAHASTDLVGLCAVDTPGASISVPVGGKATLGRFNVLTGEPIDEQGE-VNAEERHP

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

IHADPPSFAEQSTSAEILETGKIVDILLAPYARGGKIGLFGGAVGKTVIQLINNIAK
IHAEAEFEVMSVEQIILVTGIKVVDLLAPYAKGGKIGLFGGAVGKTVIIMELINNVAK
IHAVAPKLADQAADAVLTGKIVDILLPYCKGGKIGLFGGAVGKTVIIMELINNVAK
IHRKPPAFSDLEPRMETLEGLKVVDDLTPVVRGGKIALFGGAVGKTVLIQELINNVAK
IHAEAEFEIEMSVQEILVTGIKVVDLLAPYAKGGKIGLFGGAVGKTVIIMELINNVAK
IHRPAFEELSTADEILETGKIVDILLAPYAKGGKIGLFGGAVGKTVIQLINNVAQ

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

AHGGFSVFTGVGERTREGNDLYREMKETGVINLEGE-SKVALVFGQMNEPPGARARVALT
AHGGYSVFAGVGERTREGNDLYHEMIESGVINLKDATSKVALVYGMNEPPGARARVALT
GHGGFSVFAGVGERTREGNDLYLEMMQSKVIDLKGE-SKCVLVYGMNEPPGARARVALT
NFGGTSVFAGVGERTREGNDLYHEMIESGVINLKDATSKVALVYGMNEPPGARARVALS
AHGGYSVFAGVGERTREGNDLYHEMIESGVINLKDATSKVALVYGMNEPPGARARVALT
EHGGLSVFAGVGERTREGNDLYHEMKDSGVI-----SKTSMVFQGMNEPPGARLRVALT

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

GLTIAEYFRDEEGQDVLFFIDNIFRFTQAGSEVSALLGRIPSAVGYQPTLATDMGLLQER
GLTIAEYFRDQEGQDVLFFIDNIFRFTQAGSEVSALLGRIPSAVGYQPTLATDMGTMRQER
ALTMAEYFRDVEGQDVLFFIDNIFRFTQANSEVSALLGRIPAAVGYQPTLAEDLGQLQER
ALTMAEFFRDEEGQDVLFFIDNIFRFTQAGSEVSTLLGRMPSAVGYQPTLADEMGELQER
GLTIAEYFRDQEGQDVLFFIDNIFRFTQAGSEVSALLGRIPSAVGYQPTLATDMGTMRQER
GLTMAEYFRDREGQDVLFFIDNIFRFTQAGSEVSALLGRMPSAVGYQPTLATENGQLQER

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

ITTTKKGSVTSVQAVYVPADDLTDAPATTFHAHLDTATVLSRGISELGIYPAVDPLDSKS
ITTTKKGSITSVQAVYVPADDLTDAPATTFHAHLDTATVLSRAIAELGIYPAVDPLDSTS
ITSTTKGSITSVQAVYVPADDLTDAPATTFSHLDATTVLDRAVSGIYPAVNPLECAS
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ITTTKKGSITSVQAVYVPADDLTDAPATTFHAHLDTATVLSRAIAELGIYPAVDPLDSTS
ITSTKKGSITSVQAVYVPADDYTDAPATTFHAHLDTATVLSRAIAELGIYPAVDPLASTS

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

AHGGFSVFTGVGERTREGNDLYREMKETGVINLEGE-SKVALVFGQMNEPPGARARVALT
AHGGYSVFAGVGERTREGNDLYHEMIESGVINLKDATSKVALVYGMNEPPGARARVALT
GHGGFSVFAGVGERTREGNDLYLEMMQSKVIDLKGE-SKCVLVYGMNEPPGARARVAQS
NFGGTSVFAGVGERTREGNDLYHEMIESGVINLKDATSKVALVYGMNEPPGARARVALS
AHGGYSVFAGVGERTREGNDLYHEMIESGVINLKDATSKVALVYGMNEPPGARARVALT
EHGGLSVFAGVGERTREGNDLYHEMKDSGVI-----SKTSMVFQGMNEPPGARLRVALT

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

GLTIAEYFRDEEGQDVLFFIDNIFRFTQAGSEVSALLGRIPSAVGYQPTLATDMGLLQER
GLTIAEYFRDQEGQDVLFFIDNIFRFTQAGSEVSALLGRIPSAVGYQPTLATDMGTMRQER
ALTMAEYFRDVEGQDVLFFIDNIFRFTQANSEVSALLGRIPAAVGYQPTLAEDLGQLQER
ALTMAEFFRDEEGQDVLFFIDNIFRFTQAGSEVSTLLGRMPSAVGYQPTLADEMGELQER
GLTIAEYFRDQEGQDVLFFIDNIFRFTQAGSEVSALLGRIPSAVGYQPTLATDMGTMRQER
GLTMAEYFRDREGQDVLFFIDNIFRFTQAGSEVSALLGRMPSAVGYQPTLATENGQLQER

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

ITTTKKGSVTSVQAVYVPADDLTDAPATTFHAHLDTATVLSRGISELGIYPAVDPLDSKS
ITTTKKGSITSVQAVYVPADDLTDAPATTFHAHLDTATVLSRAIAELGIYPAVDPLDSTS
ITSTTKGSITSVQAVYVPADDLTDAPATTFSHLDATTVLDRAVSGIYPAVNPLECAS
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ITSTKKGSITSVQAVYVPADDYTDAPATTFHAHLDTATVLSRAIAELGIYPAVDPLASTS

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

RLLDAAVVGQEHYDVASKVQETLQT-YKSLQ^{Res 384-400}DIAILGMDELSEEDKLTVERARKIQRF
RIMDPNIVGSEHYDVARGVQKILQD-YKSLQDIAILGMDELSEEDKLTVERARKIQRF
RIMDPDVISVDHYNAQDVVQMLTK-YRELQDIAILGMDELSEEDKLTVERARKIQRF
TILDPNIVGSEHYDVARGVQKILQD-YKSLQDIAILGMDELSEEDKLTVERARKIQRF
RIMDPNIVGSEHYDVARGVQKILQD-----DKLTVERARKIQRF
RILSPAVVGEHYDVARGVQKILQD-YNDLQDIAILGMDELSEEDKLTVERARKIQRF

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

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SQPFHVAEQFTGMPGKVPVKETVIRGFKETLEKGDHNLPEEAFYVMGPIEAAVAKADLA

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Rattus_norvegicus
Bacillus_sp

A-----
E-----
Eaaeelekm

Eeh-----

F1: Beta

Mycobacterium smegmatis subunit_beta
Trypanosoma brucei subunit_beta
Bacillus_sp_subunit_beta
Saccharomyces cerevisiae subunit_beta
Bos taurus subunit_beta
Rattus norvegicus subunit_beta

```

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-----MNGKRIITQVMGPVVDIQFESGQLPDIYNAITIERPQG---GTLTVEAAV 46
-----ASAAQSTPITGKIVAVIGAIVDVHFEQSELPAILNALEIKTPQG---KLVLEVAQ 52
AAQASPSPKAGATTGRIVAVIGAVVDVQFDE-GLPPILNALEVQGRETE---RLVLEVAQ 55
----SAAPKAGTATGQIVAVIGAVVDVQFDE-GLPPILNALEVQGRES---RLVLEVAQ 51

```

Mycobacterium smegmatis subunit_beta
Trypanosoma brucei subunit_beta
Bacillus_sp_subunit_beta
Saccharomyces cerevisiae subunit_beta
Bos taurus subunit_beta
Rattus norvegicus subunit_beta

```

          V16
          D65 G69 L70 R72          E105
HLGDSLVRCISMDPTDGLVFGVEVTDTGASISVPVGDGVKGHFNALGDCLDIPGYGKDF 115
HLDAHTGRCIAMPTDGLVFGVEVTDGAPISVPVGRGRLGRIFNLGDAIDGRGPVGEK 117
HLGDNVVRCAVASTDGLVFGLEAVDTGAPISVPVGRGRLGRIFNLGDAIDGRGPVGEK 106
HLGENTVRTIAMDTGTEGLVFGKVLDSGAPIRIPVGPETLGRIMNVIGEPIDRGPIKSK 112
HLGESTVRTIAMDTGTEGLVFGKVLDSGAPIRIPVGPETLGRIMNVIGEPIDRGPIKSK 115
HLGESTVRTIAMDTGTEGLVFGKVLDSGAPIRIPVGPETLGRIMNVIGEPIDRGPIKSK 111

```

Mycobacterium smegmatis subunit_beta
Trypanosoma brucei subunit_beta
Bacillus_sp_subunit_beta
Saccharomyces cerevisiae subunit_beta
Bos taurus subunit_beta
Rattus norvegicus subunit_beta

```

          G160 G162 K163 T164
EHWSIHRKPPAFSDLEPRTEMLETGLKVVDLLTPYVRGGKIALFGGAGVGTGLVIQEMIN 175
LRMPIHAVAPKLDAQAEDAVLTGKVIDLILPYCKGGKIGLFGGAGVGTGLVIIMELIN 177
ERHPIHRPAEFEELESTADEILETGKVIDLLAPYAKGGKIGLFGGAGVGTGLVIQELIN 166
LRKPIHADPPSFAEQSTSAEILETGKVVDLLAPYARGGKIGLFGGAGVGTGLVIQELIN 172
QFAAIHAEAEFEVMSVEQIEILVTGKVVDLLAPYAKGGKIGLFGGAGVGTGLVIMELIN 175
QFAPHAHAEAEFEVMSVEQIEILVTGKVVDLLAPYAKGGKIGLFGGAGVGTGLVIMELIN 171

```

Mycobacterium smegmatis subunit_beta
Trypanosoma brucei subunit_beta
Bacillus_sp_subunit_beta
Saccharomyces cerevisiae subunit_beta
Bos taurus subunit_beta
Rattus norvegicus subunit_beta

```

          E189 R190 T191 R192          E193          N195 D196          M222
RIARNFGGTSVFAGVGERTRENDLWVELADANVL-----KDTALVFGGIDPEPGTRMR 229
NVAKGHGGFSVFAGVGERTRENDLYEMMKDSGVI-----SKTSMVFVGIDNEPPGARAR 236
NVAQEHGGLSVFAGVGERTRENDLYEMMKDSGVI-----SKTSMVFVGIDNEPPGARLR 220
NIAKAHGGFSVFTGVGERTRENDLYEMMKDSGVI-----SKTSMVFVGIDNEPPGARAR 231
NVAKAHGGFSVFAGVGERTRENDLYEMMKDSGVI-----SKTSMVFVGIDNEPPGARAR 235
NVAKAHGGFSVFAGVGERTRENDLYEMMKDSGVI-----SKTSMVFVGIDNEPPGARAR 231

```

Mycobacterium smegmatis subunit_beta
Trypanosoma brucei subunit_beta
Bacillus_sp_subunit_beta
Saccharomyces cerevisiae subunit_beta
Bos taurus subunit_beta
Rattus norvegicus subunit_beta

```

          N257 R260
VALSALTMAEYFRDEQGDVLLFIDNIFFTQAGSEVSTLLGRMPASVGYQPTLADEMG 289
VAQSALTMAEYFRDEQGDVLLFIDNIFFTQAGSEVSTLLGRMPASVGYQPTLADEMG 296
VALTGLTMAEYFRDEQGDVLLFIDNIFFTQAGSEVSTLLGRMPASVGYQPTLATDMG 280
VALTGLTMAEYFRDEQGDVLLFIDNIFFTQAGSEVSTLLGRIPASVGYQPTLATDMGL 291
VALTGLTMAEYFRDEQGDVLLFIDNIFFTQAGSEVSTLLGRIPASVGYQPTLATDMGT 295
VALTGLTMAEYFRDEQGDVLLFIDNIFFTQAGSEVSTLLGRIPASVGYQPTLATDMGT 291

```

F1: Beta

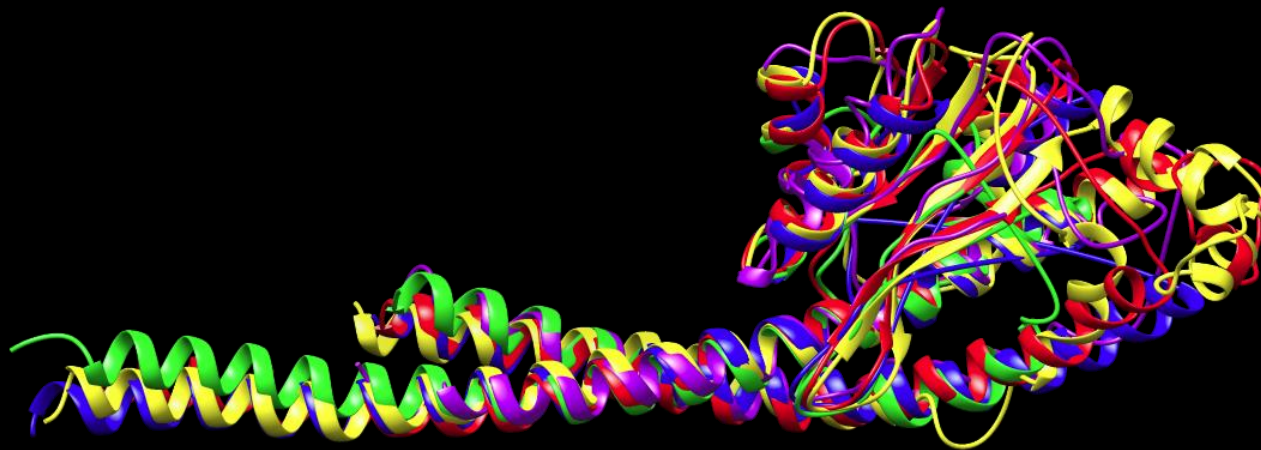
Mycobacterium_smegmatis_subunit_beta
Trypanosoma_brucei_subunit_beta
Bacillus_sp_subunit_beta
Saccharomyces_cerevisiae_subunit_beta
Bos_taurus_subunit_beta
Rattus_norvegicus_subunit_beta

RFLSQNMMAAEQFTGPGSTVPLKETIEAFDKLTKEGFHLPEQAFFLIGGLDDLAKKAE 469
KFLSQPFQVAEVFTGMTGHYVQLDDTIDSFSGLLMGTYDQVPAMAFYMVGGINSVLEKAK 476
RFLSQPFHVAEQFTGMPGKYVPVKETVRGFKIILEGKHNDLPAAFYMVGITIDEAVEKAK 460
RFLSQPFAVAEVFTGIPGKLVLRLKDTVASFKAFLGKYDNIPAHAFYMVGIEDVVAKAE 471
RFLSQPFQVAEVFTGHLGKLVLPLKETIKGFQQILAGEYDLPEQAFYMVGPIEEAVAKAD 475
RFLSQPFQVAEVFTGHMGLVLPLKETIKGFQQILAGDYDLPEQAFYMVGPIEEAVAKAD 471

* * * * *

SLGAKL-----475
KMAEEAAELEKMRRAVAQSS498
KL-----462
KLAAEAN-----478
KLAEHGS-----482
KLAEHGS-----479

F1: Gamma structural alignment



Sc: 5.86 RMS: 1.5

F1: Gamma structural alignment

	Res 5-13	K21 K24	R30	S32	
Saccharomyces_cerevisiae	AT-LKEVEMRLKSI	KNIEKIT	TKMKIVASTRL	SKAEKAKISAKKMDE-A-----EQLFY	
Bos_taurus	AT-LKDITRRLKSI	KNIQKIT	KSMKMVAAAKYARA	AERELKPARVYGV-----	
Trypanosoma_brucei	-GKLRLYKEKLEGYN	RFYSIVKTI	KMVT	LAKYRAAQGRIRTRD	FSLR-Y-----TELAF
Mycobacterium_smegmatis	-T-LRELGRIRSA	GSIKKITKAQEL	IATSRIA	KAQARVEAARPYAA-----	
Bacillus_sp	-G-MREIKRRIRSV	KNTRQITKAMKM	VAAAKLRR	AQETAENARPYAD-K	ISHPML----
Rattus_norvegicus	----RDI	TRRLKSI	KNIQKIT	KSMKMVAAAKYARA	AERELKPARVYGT-----
Saccharomyces_cerevisiae	KNAETK-N--K--EL--	IVAIT	-----DKGL	CGSIHSQL-AKAV-RRHLNDQ-P	
Bos_taurus	-----GLIIGVSS-----	DRGL	CGAIHSSV----	A-----	
Trypanosoma_brucei	---SKPqA-aKNALV--	YIPITT-----	NRGSCGALNSNI-VRCI-DSVVS---	S	
Mycobacterium_smegmatis	-----EITNMLTELS	DRGL	CGAYNANV-LRRA-EELF	SLL--	
Bacillus_sp	----EA-RpvK-KTG--	YMVITS-----	DRGL	AGPYNANI-LRLV-SKTIEERHQ	
Rattus_norvegicus	-----G-----S-----	LCGAIHSSV-AKQM-----			
Saccharomyces_cerevisiae	--N-ADIVTI--	GDKIKMQLLRTHPNNIKL-SINGIGKDAPTFQESALIADKLLSVMKA-			
Bos_taurus	-----IIGV--	GDKIRSI-----	LTFKEVGRRPPTFGDASVIALE-----		
Trypanosoma_brucei	--K-MVLMPV--	GKRGIDSFSKLYPDEFYR-GIINDMKESMHFGYATFVIENAYEVSKD-			
Mycobacterium_smegmatis	-----RVGRKALGYFS-----	FT--GF-SERPTYENAREIADT-----			
Bacillus_sp	skDeYVIFAV--	GRKGRDFFKKRGYP-VVE-EVTGI-SDTPSLTEIQDIAQSAIG--		MF	
Rattus_norvegicus	-----				

F1: Gamma structural alignment

```
Saccharomyces_cerevisiae  GT--YPKI-SIFYN-----DPVSSLSFEPSE-KPIFNAKTI---EQ-S-PSF-----
Bos_taurus                -----LSIIFN-----RFRSVISYK-----
Trypanosoma_brucei        ----ADRY-QVIFN-----RFVSAGVQRNAV-YNIPSYEKW---KedLaDAASSDNQ
Mycobacterium_smegmatis   -----LVNAFMATEFRSMLSQT-----
Bacillus_sp              ADETFDKL-TIFYN-----EFVSPIVQRPVEKQLLP----LTSL-----
Rattus_norvegicus        -----KL-----

                                D202
Saccharomyces_cerevisiae  ---GK--FEI--DTG--ANVPRDLFE--YTLANQMLTAMAQGYAAEISARRNAMDNASKNAG
Bos_taurus                -----TEYSLANIIYYSLKESTTSEQSARMTAMDNASKNAS
Trypanosoma_brucei        KNYRLFANALQNEE-EQLIRDFD--FHAALAVLNAVGENELSEQAARLVAVEGQLTNIS
Mycobacterium_smegmatis   -----AR-YIATRVYAALLEAAASESASRRRAMKSATDNAD
Bacillus_sp              -----L-P--KYAETLIYSALLDAKASEFGARMTAMGNATDNAT
Rattus_norvegicus        -----ANIIYYSLKESTTSEQSARMTAMDNASKNAS

                                Res 256-265
Saccharomyces_cerevisiae  DMINRYSILYNRTRQAVITNELVDIITGAS---s
Bos_taurus                EMIDKLTLTFNRTRQAVITKELIEIISGAAALD-
Trypanosoma_brucei        SLQORTSSLYNKTRQFGITAALIEILSAMSSLE-
Mycobacterium_smegmatis   DLIKALTLAANRERQAQITQEISEIVGGANALA-
Bacillus_sp              EMLETLTQLFNRA-----
Rattus_norvegicus        DMIDKLTLTFNRTRQAVITKELIEIISGAAALD-
```

F1: Gamma sequence alignment

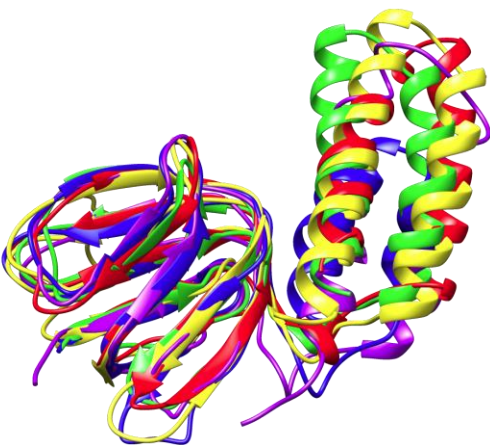
Trypanosoma brucei subunit gamma	-SGKLRLYKEKLEGYNRFYSIVKTIKMTLAKYRAAQGRIRTRD-FS---LRYTELAFS	54
Mycobacterium smegmatis subunit gamma	MAATLRRLRGRIRSAGSIKKITKAQELIATSRIAKAQARVEAARPYAAEITNMLTELA-G	59
Bacillus_sp_subunit gamma	-MQGMREIKRIRSVKNTRQITKAMMVAAAKLRRAQETAENARPYADKIKEVISSIAAG	59
Saccharomyces cerevisiae subunit gamma	--ATLKEVEMRLKSIKNIKIKTKMKIVASTRLSKAEKAKISAKKMDAEQLFYKNA--E	56
Bos taurus subunit gamma	--ATLKDITRLKSIKNIQKITKSMKMVAAAKYARAERELKPARVYGVGSLALYEKA--D	56
Rattus norvegicus subunit gamma	----PDITRLKSIKNIQKITKSMKMVAAAKYARAERELKPARVYGTGSLALYEKA--E	53
	: : : : : * : : : : : *	
Trypanosoma brucei subunit gamma	KPQASRDA--VAAAKNALVYIPITTNRGSCGALNSNIVRCIDSVVSS-----KMVLMPV	106
Mycobacterium smegmatis subunit gamma	ASALDHPLLVERKQPKRAGVLVSSDRGLCGAYNANVLRRAEELFSLRRDEGKDPVLYVV	119
Bacillus_sp_subunit gamma	TKDFSHPLM-EARPVKKTGYMVITSDRGLAGPYNANILRLVSKTIEERHQSKDEYVIFAV	118
Saccharomyces cerevisiae subunit gamma	TKNLDEVA--TETGAPKELIVAITSDKGLCGSIHSQLAKAVRRHLND---QPNADIVTI	110
Bos taurus subunit gamma	IKT-----PEDKKKHLIIGVSSDRGLCGAIHSSVAKQMKSEANLAAAGKEVKIIGV	108
Rattus norvegicus subunit gamma	IKG-----PEDKKKHLIIGVSSDRGLCGAIHSSVAKQMKNDMAALTAAGKEVMIVGI	105
	: : : : : * : : : : :	
Trypanosoma brucei subunit gamma	GKRGIDFSFKLYPDEFYRGIINDMKESMHFGYATFVIENAYEV-----S	150
Mycobacterium smegmatis subunit gamma	GRKALGYFSF-RQRTVVESWTGF-SERPTEYENAREIADTLVNAFMAGADDEGDDAGADGI	177
Bacillus_sp_subunit gamma	GRKGRDFFKK-RGYPVVEEVTGI-SDTPSLTEIQDIAQSAIGMFAD-----	162
Saccharomyces cerevisiae subunit gamma	GDKIKMQLLRTHPNNIKLSINGIGKDAPTFQESALIADKLLSVMKA-----	156
Bos taurus subunit gamma	GDKIRSILHRTHSDQFLVTFKEVGRPPPTFGDASVIALELLNS--G-----	152
Rattus norvegicus subunit gamma	GEKIKSILYRTHSDQFLVSFKDVGKRPPTFGDASVIALELLNS--G-----	149
	* : : : : *	

F1: Gamma sequence alignment

D202

Trypanosoma brucei subunit_gamma	KDADRYQVIFNRFVSAGVQRNAVYNIPSYEKWK-EDLADAASSDNQKNRYLFANALQNEE	209
Mycobacterium smegmatis subunit_gamma	LGVDLHIVFTEFRSMLSQTAVARRAAPMEVEYVGEVE-----TGPRTLY----SFEPDP	228
Bacillus sp subunit_gamma	ETFDKLTIFYNEFVSPVQRPVEKQLPLTS---EEVL-----DGPVSAY----EYEPDS	210
Saccharomyces cerevisiae subunit_gamma	GTYPKISIFYNDPVSSLSFEPSEKPIFNAKTIE---Q-----SPSFGKF---EIDTDA	203
Bos taurus subunit_gamma	YEFDEGSIIIFNRFRSVISYKTEEKPIFSLDTIS---S-----AESMSIY---D-DIDA	198
Rattus norvegicus subunit_gamma	YEFDEGSIIIFNQFKSVISYKTEEKPIFSSTVV---A-----AENMSIY---D-DIDA	195
	. :.: * : :	
Trypanosoma brucei subunit_gamma	EQLIRDFDFHAALAVLNAVGENELSEQAARLVAVEGQLTNISSLQQRRTSSLYNKTRQFG	269
Mycobacterium smegmatis subunit_gamma	ETLFDALLPRYIATRVYAALLEAAASESASRRRAMKSATDNADDLIKALTLANRERQAQ	288
Bacillus sp subunit_gamma	ESVLEVLTPKYAETLIYSALLDAKASEFGARMTAMGNATDNATEMLETLTLOFNARQAA	270
Saccharomyces cerevisiae subunit_gamma	N-VPRDLFEYTLANQMLTAMAQGYAAEISARRNAMDNASKNAGDMINRYSILYNRTRQAV	262
Bos taurus subunit_gamma	D-VLRNYQEYSLANIYYSLKESTTSEQSARMTAMDNASKNASEMIDKLTLTFRTRQAV	257
Rattus norvegicus subunit_gamma	D-VLQNYQEYNLANIYYSLKESTTSEQSARMTAMDNASKNASDMIDKLTLTFRTRQAV	254
	: : : : : * : * : : : * : : : * : *	
		Res 256-265
Trypanosoma brucei subunit_gamma	ITAALEILSAMSSLEGNAMKVRRNKFWEHAVTK	304
Mycobacterium smegmatis subunit_gamma	ITQEISEIVGGANALAGSK-----	307
Bacillus sp subunit_gamma	ITQEIAEIVAGANALR-----	286
Saccharomyces cerevisiae subunit_gamma	ITNELVDIITGASSLG-----	278
Bos taurus subunit_gamma	ITKELIEIISGAAALD-----	273
Rattus norvegicus subunit_gamma	ITKELIEIISGAAALD-----	270
	** : : * : : *	

F1: Delta structural alignment



Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Bacillus_sp

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Bacillus_sp

Saccharomyces_cerevisiae
Bos_taurus
Trypanosoma_brucei
Mycobacterium_smegmatis
Bacillus_sp

```

-----KLQFALPHETLYS-E-VTQVNLPAKSGRIGVLANHVPTVEQLLPGV
-----QMSFTFASPTQVFFNSANVRQVDVPTQTGAFGILAAHVPTLQVLRPGL
HDLPEGFEFMEHTLRLTLTRQDEFLLREEPVKCVTVTGTNGEYGIYPGHAYKIVQLNPSP
-----DLNVEIVAVERELWS-GPATFVFTRTTAGEIGILPRHIPLVAQLVDDA
-----MATVQVDIVTPERKVFQ-GEADIVIARGVEGELGVMAGHIPLVTPLKTAP
    
```

Beta-sandwich

```

VEVME-GSNSKKFFISGGFATVQPDSQLCVTAIEAPLE-SF-SENIKNLLAEAKNVSSS
VVVHAEDGTTSKYFVSSGSVTVNADSSVQLLAEAAVTLDMLDLGAAKANLEKAQSELLG
LTVEYTDGTTKKYFVSGGFAGHINNEGSCDVNTVECTLLDDLDAIAEKELAAQAALGS
MVRVEREGEDDLRIAVDGGFLSVTEETVRILVENAQFE-SEIDADAATEDAAS-----
VRIKQ-GDKETLIAVSGGFLEVR-PDKVNILADTAELP-EEIDVERAKKAKARHETILKR
    
```

Alpha-domains

```

-----REAAEAAIQVEVLENLQSV-----
A-ADEATRAEIQIRIEANEALVKAL----
A-KDDKAKSVVEIRISVIEAVIAALkhh-
-----DDERTAAWGRARLR----
LdKTDKDYLRHKRALERAQVRLQVAnks
    
```

Sc: 7.23 RMS: 1.55

F1: Delta sequence alignment

Mycobacterium smegmatis subunit_delta
Bacillus_sp_subunit_delta
Saccharomyces cerevisiae subunit_delta
Bos_taurus_subunit_delta
Trypanosoma brucei subunit_delta

```

-----MADLNVEIVAVERELWSG-PATVFVTRTTAG 30
-----MATVQVDIVTPERKVFQG-EADIVIARGVEG 30
-----AEAAAASSGLKQLQFALPHETLYSGSEVTQVNLPAKSG 37
-----AEAAAAQAPAAGPGQMSFTFASPTQVFFNSANVRQVDVPTQTG 43
QSAPHDLPEGFEFMEHKVVNKDIHAPHENLETLRLTLTRQDEFLREEPVKCVTVTGTNG 60

```

Beta-sandwich

Mycobacterium smegmatis subunit_delta
Bacillus sp subunit_delta
Saccharomyces cerevisiae subunit_delta
Bos taurus subunit_delta
Trypanosoma brucei subunit_delta

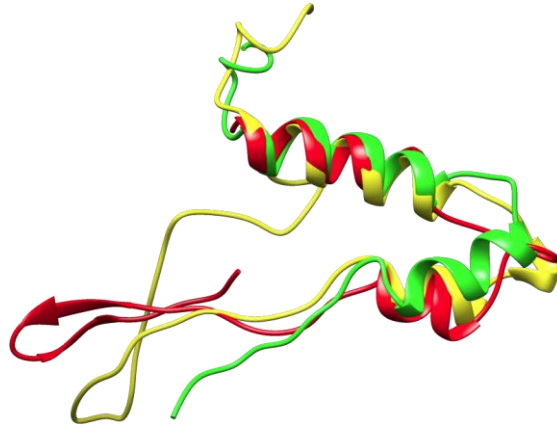
ELGILPRHIPLVAQLVDDAMVRVEREGEDDLRIADVGGFLSVTTEETV-RILVENAQFES	89
ELGVMAGHIPLVTPLKTAPV-R-IKQGDKETLIAVSGGFLEVRPDKV-NILADTAELPEE	87
RIGVLANHVPVEQLLPVV-EVM-EGSNSKKFFISGGFATVQPSQLCVTAIEAPLES	95
AFGILAAHVPTLQVLRPLGV-VVHAEDGTTSKYFVSSGSVTVNADSSVQLLAAEAVTLM	102
EYGIYPGHAYKIVQLNPSP-LTVEYTDGTTKKYFVSGGFAHINNEGSCDVNTVECTLLD	119

Mycobacterium smegmatis subunit_delta
Bacillus_sp_subunit_delta
Saccharomyces cerevisiae subunit_delta
Bos_taurus_subunit_delta
Trypanosoma brucei subunit_delta

IDADAAKEDAAASDDERTAAWGRA--RLR--ALGQID-----121
 IDVERAKKAKARHETILKRLDKTDKDYLRHKRALERAIEVRLQVANSKS--135
 FSQENIKNLLAEAKKN---VSS-----SDAREAAEAAIQVEVLENLQSVLK--138
 LDLGAAKANLEKAQSE---LLGA-----ADEATRAEIQIRIEANEALVKALE--146
 LDLAIAEKELAAQQA---LGSA-----KDDKAKSVVEIRISVIEAVIAALKHH165

Alpha-domains

F1: Epsilon structural alignment

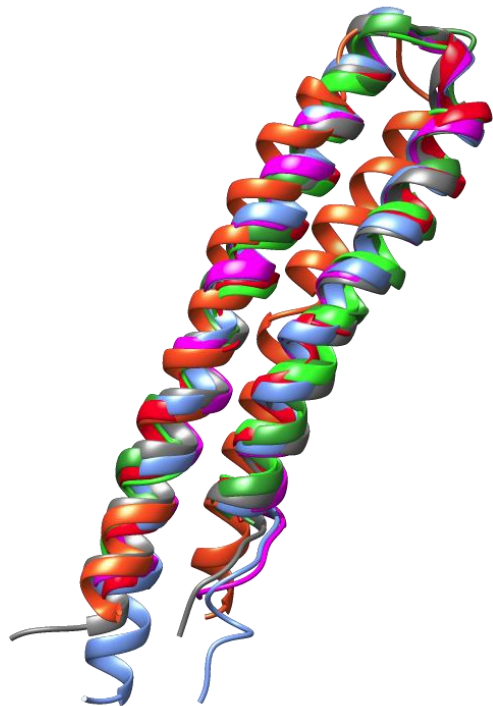


Sc: 4.11 RMS: 2.85

	W3	Y10	Y13	
Saccharomyces_cerevisiae	----	IS---	YAA	YLNVAQAIRSTELQTASVLNRSQT--DAFYTQYKNA---S-E
Bos_taurus	-VAY	WRQAGLSYIRYSQICAKAVRDALK---	TE-	FKANA-MKTSGSTIKIVK-V-----
Trypanosoma_brucei	SSSWR-	DHGISYLKYLNVCTETLHSTVK---	ES-	RRAKY-ERWSKPCYTAQR-PDGAGGQ
Saccharomyces_cerevisiae	PTP-I---	TK----		
Bos_taurus	-----			
Trypanosoma_brucei	ET-IDKVP	IHtkdy		

Alpha-helices

Fo: c structural alignment



Bos_taurus
 Arthrospira_platensis
 Mycobacterium_tuberculosis
 Polytomella_sp
 Saccharomyces_cerevisiae
 Escherichia_coli
 Ilyobacter_tartaricus

Bos_taurus
 Arthrospira_platensis
 Mycobacterium_tuberculosis
 Polytomella_sp
 Saccharomyces_cerevisiae
 Escherichia_coli
 Ilyobacter_tartaricus

```

-----IDTAAKFIGAGAAT-VGVAGSGAGIGTVFGSLII-GYARNPSLKQ-QLFSYA
-----ESNLTTAASVIAAALAVGIGSIGPLGQGQAAGQAVE-GIARQPEAEG-KIRGTL
--eIdPNALITAGALIGGGLIMGGGAIGAGIGDGIAGNALIS-GIARQPEAQG-RLFTPF
-----SVLAASKMVGAGCAT-IALAGVGAGLGVMFGSLIN-GAARNPNIAK-QLVGYA
-----QLVLAACYIGAGIST-IGLLGAGIGIAIVFAALIN-GVSRNPSTIKD-TVFPMA
-----MENLNMDLLYMAAAVMMGLAAIGAAIGIGILGGKFLE-GAARQ--PDL-IPLLRT
mdmIfAKTVVLAASAVGAGTAM-IAGIGPGVGQGYAAGKAVE-SVARQPEAKG-DIISTM
    
```

A56 E59 Loop

Alpha-helices

```

ILGFALSEAMGLFCLMVAFLILF-----
LLSLAFMEALTIYGLVVALVLLFA-NPFV---
FITVGLVEAAYFINLAFMALVFVA-TPGLq---
LLGFALTESIALFSLLVFLILF-----
ILGFALSEATGLFCLMVSFLLLF-----
QFFIVMQLVDAIPMIAVGLGLVVMFAV-A----
VLGQAVAEESTGIYSLVIALILLYA-NPFVgllg
    
```

Fo: c sequence alignment

Mycobacterium tuberculosis_subunit_c	-----ME---LDPNALITAGA	13
Escherichia_coli_subunit_c	-----MENLMDLL	9
Polytomella_sp_subunit_c	MSVQRLSLGAARCLSGVARVQASQALVAQKAVAVAPTRAQAAPAEVAQVRSMVLAASK	60
Saccharomyces_cerevisiae_subunit_c	-----MQLVLAAS	8
Bos_taurus_subunit_c	-----IDTAAS	6
Arthrospira_platensis_subunit_c	-----MESNLTTAASVIAAAL	16
Ilyobacter_tartaricus_subunit_c	-----MD--MLFAKTVVLAAS	14

Mycobacterium tuberculosis_subunit_c	LIGGGGLIMGGGAIGAGIGDGIAGNALISGIARQPEAQGRLLTPFFITVLVEAAYFINLA	73
Escherichia_coli_subunit_c	YMAAAVMMGLAAIGAAIGIGILGGKFLGAARQPLIPLRLTQFFIVMGLVDAIPMIAVG	69
Polytomella_sp_subunit_c	MVGAG-CATIALAGVGAGLGVMFGSLINGAARNPNIAKQLVGYALLGFALTESIALFSL	119
Saccharomyces_cerevisiae_subunit_c	YIGAG-ISTIGLLGAGIGIAIVFAALINGVSRNPSIKDTVFPMAILGFALTEATGLFCLM	67
Bos_taurus_subunit_c	FIGAG-AATVGVAGSGAGIGTVFGSLIIGYARNPSLKQQLFSYAILGFALTEAMGLFCLM	65
Arthrospira_platensis_subunit_c	-----AVGIGSIGPGLGQGQAAGQAVEGIARQPEAEGKIRGTLTLLSLAFMEALTIYGLV	70
Ilyobacter_tartaricus_subunit_c	AVGAG-TAMIAIGIPGVGGQYAAGKAVESVARQPEAKGDIISTMVLGQVAESTGIYSLV	73

Mycobacterium tuberculosis_subunit_c	FMALFVFRATPGLQ---	86
Escherichia_coli_subunit_c	LGLYVMFAVA-----	79
Polytomella_sp_subunit_c	VVFLILFA-----	127
Saccharomyces_cerevisiae_subunit_c	VSFLLLFGLV-----	76
Bos_taurus_subunit_c	VAFLILF-----	72
Arthrospira_platensis_subunit_c	VALVLLFANPFV----	82
Ilyobacter_tartaricus_subunit_c	IALILLYANPFVGLLG	89

Alpha-helices

Fo: a structural alignment



Sc: 2.91 RMS: 3.49

Polytomella_sp
Saccharomyces_cerevisiae
Escherichia_coli

Polytomella_sp
Saccharomyces_cerevisiae
Escherichia_coli

Polytomella_sp
Saccharomyces_cerevisiae
Escherichia_coli

Polytomella_sp
Saccharomyces_cerevisiae
Escherichia_coli

Polytomella_sp
Saccharomyces_cerevisiae
Escherichia_coli

Polytomella_sp
Saccharomyces_cerevisiae
Escherichia_coli

```

-----SVRDV-K--T--GSLPT
SPLDQFEIRTLFGLQSSFIDLSCLNLTTFSLYTIIVLLVITSLYTL-TNNNNKIIGSRWL
-----

E63 I8 D67 I53
NFLTGVMRFWRSQNPA--EKPHDPVNDRLPAVVDASDKRA----SIGTWATTFCTIIS
ISQEAIVDTIMNMT-KGQIGG-----KN--WGL--Y--FPMIFTLFMFIFIANLI
-----HG--KSKLIAPLALTIFVWVFLM-NLMDL

CNLLGLMPFNEA-----P--TS--GLGFAT-GLGVS VWATAT-ILGLSKT
SM-I--P--YS-----FALS-----AHLVFIISL-SIVIWLGNITLGL
LPID-----LLPYIAEHVLGLPALRV---VPSADVNVT-LSMAL-GVFILILFYSIK-

G---FKFPGH---F--IPG-----GTP-WPMA-FIFVPLE-TISYT-FRAVSLGVRLW
Y--KHG---WVFFSLF--VPAGTPLPLVP-LLVIIETL-SYFA-RAISLGLRLGSNIL
MKS-----LLSKPV-SLGLRLFGNMY

VNMLAGHTLLHILTGMA-----LALPFSLGFSSMVPATFGVCCLLSALVGLLEYLVAVLQS
AGHLLMVILAGLTNFN-----LIN-----L-FTLVFG-FVPLAMILAIMMLEFAIG
AGELIFILIAGLLP--WWSQWI-----LNVPWAIFILII

Q230 D244
GVFISILSTVYVG-EFNH--DKFIgpaakiv
IIQGYVWAILTA-SYLKDAVYLH-----
TLQAFIFMVLTI-----VYLS-----
    
```

Fo: a sequence alignment

Rattus_norvegicus_subunit_a
Bos_taurus_subunit_a
Ashbya_gossypii_subunit_a
Wickerhamomyces_canadensis_subunit_a
Vanderwaltozyma_polyspora
Kluyveromyces_lactis_subunit_a
Candida_glabrata_subunit_a
Saccharomyces_cerevisiae_subunit_a

Rattus_norvegicus_subunit_a
Bos_taurus_subunit_a
Ashbya_gossypii_subunit_a
Wickerhamomyces_canadensis_subunit_a
Vanderwaltozyma_polyspora
Kluyveromyces_lactis_subunit_a
Candida_glabrata_subunit_a
Saccharomyces_cerevisiae_subunit_a

Rattus_norvegicus_subunit_a
Bos_taurus_subunit_a
Ashbya_gossypii_subunit_a
Wickerhamomyces_canadensis_subunit_a
Vanderwaltozyma_polyspora
Kluyveromyces_lactis_subunit_a
Candida_glabrata_subunit_a
Saccharomyces_cerevisiae_subunit_a

---	M	N	E	N	L	F	---	A	S	F	I	T	P	T	M	---	M	G	L	P	---	I	V	T	I	I	M	F	P	S	I	L	30																									
---	M	N	E	N	L	F	---	T	S	F	I	T	P	V	I	---	L	G	L	P	---	L	V	T	L	I	V	L	F	P	S	L	30																									
M	Y	L	N	N	N	N	M	K	Y	I	N	S	P	L	E	Q	F	E	I	R	D	L	L	G	L	T	S	P	M	M	D	F	S	F	I	N	I	T	N	F	L	G	L	T	M	I	T	L	L	V	I	L	T	M	N	L	M	60
---	M	T	N	I	I	V	N	S	P	L	D	Q	F	E	I	K	V	F	I	G	F	V	S	P	F	I	D	L	T	N	I	N	I	T	T	F	V	Y	S	V	F	I	L	I	V	I	L	G	L	T	L	53						
---	M	Y	I	N	S	P	L	D	Q	F	E	I	M	T	L	L	K	F	V	T	P	F	F	D	M	S	N	L	N	I	T	T	F	L	G	L	I	I	V	L	M	V	I	S	L	N	I	L	51									
---	M	L	N	L	F	I	T	S	P	L	D	Q	F	E	I	R	V	L	M	G	F	T	S	P	L	D	F	S	S	L	N	F	T	T	F	S	L	Y	T	I	I	V	L	F	T	V	L	G	L	N	L	53						
---	M	Q	N	T	L	L	T	Y	I	N	S	P	L	E	Q	F	E	V	K	T	F	L	G	L	N	T	P	F	I	D	L	S	G	L	N	I	T	T	F	L	Y	T	I	I	V	L	L	V	S	S	L	Y	V	L	57			
---	M	F	N	L	L	N	T	Y	I	T	S	P	L	D	Q	F	E	I	R	T	L	F	G	L	Q	S	S	F	I	D	L	S	C	L	N	L	T	T	F	S	L	Y	T	I	I	V	L	L	V	I	T	S	L	Y	T	L	56	

I53
E63
D67

```

FPSSERLISNR LHSFQHWLIRLI IKQMLLIHTPKGR TWA L--MIVSLIMFIGSTNLLGL 87
FPTSNPLVSNRFVTLQDWMLQLVSKQMMSIHNSKGGQTW L--MLMSLILFIGSTNLLGL 87
TNNYNKLVGSNWYLSQEMIYDTIM--NMVK TQIGGKVWGYFPLVYTFFITIFTMNLISM 118
TDNNGRIIGNRWYVSQEMIYDTIN--NMVSGQIGGKLGGYFPLIYTF FIFIFTANLIGM 111
TTNNNTIIGSRWNLPLEMIYDTIL--NTTKGQIGGKLWGLYFPLIYTLFMFILIANLISL 109
TTNNNNKIIGSKW FVVSQEIYDTIL--NMVKGQIGGKLWGYFPLVYTF FFFIFVSNLISM 111
SNNNNKIIGSRWLLSQEVIYDTIL--NMVKGQIKGKDWGYFPFIYTLFMFILISNLISM 115
TNNNNKIIGSRWLISQEIYDTIM--NMTKGQIGGKNWGLYFPMIFTL FMFIFIANLISM 114

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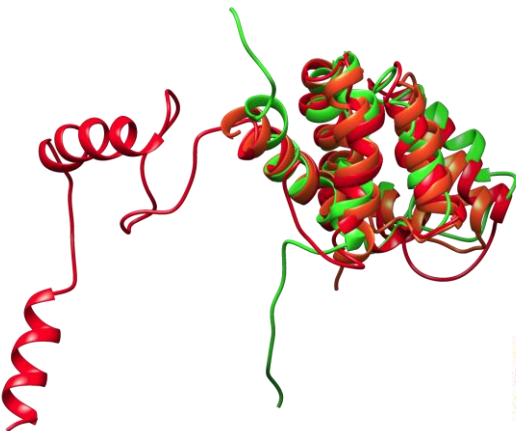
E162

LPHTFTPTTQLSMNLSMAIPLWAGAVILGFRHKLKNSLAHFLPQGTPISLIPMLIIETI	147
LPHSFTPTTQLSMNLGMAIPLWAGAVITGFRNKTASLAHFLPQGTPTPLIPMLVIIETI	147
IPYSFAMTSHVVFVVSMSMIIWLGTIIIGFYTHGLKFFGLFLPTGTPLILVPLLVSITLL	178
IPYSFAITSHMVFIISLSVVIWLGVTIIIGLYTHGLTFFALFVPAGCPLALAPLLVITLL	171
IPYSFALTAQIVFVISLSFIIWLGSTITGFNKHGWLFFSLFVPNGTPTPLVPLLVIIESL	169
IPYSFALSAHLIFIVLSVSVIWLGTIIIGLTKHGLVFFSLFVPGGTPLPLVPLLVLITLL	171
IPYSYALTAQFVFIISLSMIIWLGTIILSLFKHGWVFFSLFVPSGTALPLVPLLVIITLL	175
IPYSFALSAHLVFIISLSIVIWLGNTILGLYKHGWVFFSLFVPAGTPLPLVPLLVIITLL	174

Fo: a sequence alignment

		R176		E223	
Rattus_norvegicus_subunit_a	SLFIQPMALAVRLTANITAGHLLMHLIGGATLVLMDISPPTATITF---IILLLLTVLEF				204
Bos_taurus_subunit_a	SLFIQPMALAVRLTANITAGHLLIHLIGGATLALMSISTTTALITF---TILILLTILEF				204
Ashbya_gossypii_subunit_a	SYFARTISLGLRLSANIMAGHLLIVILGGLLFNLMAMNILTFLLGFLPMIAILGIVCLEF				238
Wickerhamomyces_canadensis_subunit_a	SYSARAISSLGLRLSANTLSGHLLMVILGGLVFNLMSSIVTFVLGFIPLAGILAIVALEF				231
Vanderwaltozyma_polyspora	SYIARAFSLGLRLTCNLAGHLLMVILGGLLLNFNINKLTLLIGIIPFAMILAILCLEF				229
Kluyveromyces_lactis_subunit_a	SYFARAISSLGLRLSSNVLSGHLLLIILGGLLFNLMSSIIITFVFGIIPGVGLLAIVVLEF				231
Candida_glabrata_subunit_a	SYVARAFSLGLRLSANIFSGHLLMAILAGLTMTFVQINIFTLLIGFIPLAIIILIMCLEF				235
Saccharomyces_cerevisiae_subunit_a	SYFARAISSLGLRLGSNLAGHLLMVILAGLTFFNFMILNLFLLVFGFVPLAMILAIMMLEF				234
	* : :*: ** * :****: :*: : : : : * : : : : : ***				
		Q230		D244	
Rattus_norvegicus_subunit_a	AVALIQAYVFTLLVSLYLHNT---				226
Bos_taurus_subunit_a	AVAMIQAYVFTLLVSLYLHNT---				226
Ashbya_gossypii_subunit_a	AITIIQAYVWCILMSSYLKDTIYLH				263
Wickerhamomyces_canadensis_subunit_a	AIAMIQSYVFAILASGYIKDGLYLH				256
Vanderwaltozyma_polyspora	AIAMIQSYVFATLTASYIKDGLYLH				254
Kluyveromyces_lactis_subunit_a	AISVIQAYVWSILTSSYLKDVLYLH				256
Candida_glabrata_subunit_a	GIAIIQAYVFSILASSYLKDGLYLH				260
Saccharomyces_cerevisiae_subunit_a	AIGIIQGYVWAILTASYLKDAVYLH				259
	: : **: **: * : **: *				

Fo: OSCP structural + sequence alignment



Sc: 5.66 RMS: 1.80

Escherichia_coli
Bos_taurus
Saccharomyces_cerevisiae

```
-----SEFIT-VARPYAKAAFDFAVEHQSVVERWQDMLAFAAEVTK-NEQMAELLSGA
FAKLVRPPVQ-IYIGIEGRYATALYSAASKQNKLEQVEKELLRVGQILK-EPKMAASLLNP
-----PPVRLFGVEGTYATALYQAAAKNSSIDAAFQSLQKVESTVKKNPKLGHLLNP
```

Escherichia_coli
Bos_taurus
Saccharomyces_cerevisiae

```
LA-PETLAESFIAVCGE--QLDENGQNLIRVMAENGRNLNALPDVLEQFIHLRAVSEA---
YVKRSVKVKSLSDMTAK-KFSPLTSNLLINLLAENGRLTNTPAVISAFSTMMSVHRG---
ALSLKDRNSVIDAIVETHKNLDGYVVNLLKVLSENNRLGCFEKIASDFGVLNDAHNGLLK
```

Escherichia_coli
Bos_taurus
Saccharomyces_cerevisiae

```
-----t-----
-----EVPCTV-----
GTVTSAEPLDPKSFKRIEKalsasklvvggkslkskikiqlnkvleds
```

Escherichia_coli_subunit_delta
Bos_taurus_subunit_oscp
Saccharomyces_cerevisiae_subunit_oscp

```
-----SEFITVARPYAKAAFDFAVEHQSVVER-WQDMLAFAAEVTKNEQMAELLSGA 50
-FAKLVRPPVQIYIGIEGRYATALYSAASKQNKLEQVEKELLRVGQ-ILKEPKMAASLLNP 58
ASKAAAPPVRLFGVEGTYATALYQAAAKNSSIDAAFQSLQKVESTVKKNPKLGHLLNP 60
.: : **.* . * : : : : : : : : : : : : : : : : *
```

Escherichia_coli_subunit_delta
Bos_taurus_subunit_oscp
Saccharomyces_cerevisiae_subunit_oscp

```
LAPETLAE--SFIIVCGEQLDENGQNLIRVMAENGRNLNALPDVLEQFIHLRAVSEATAE 107
YVKRSVKVKSLSDM-TAKEKFSPLTSNLLINLLAENGRLTNTPAVISAFSTMMSVHRGEVP 117
ALSLKDRNSVIDAIVETHKNLDGYVVNLLKVLSENNRLGCFEKIASDFGVLNDAHNGLLK 120
. : : : : : : : : : : : : : : : : : : : : *
```

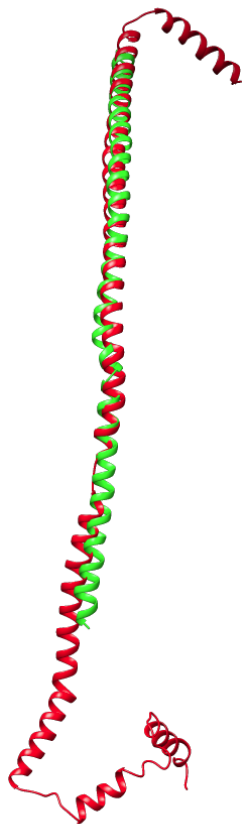
Escherichia_coli_subunit_delta
Bos_taurus_subunit_oscp
Saccharomyces_cerevisiae_subunit_oscp

```
VDVISAAALSEQQLAKISAAMEKRLSR----- 134
CTV----- 120
GTVTSAEPLDPKSFKRIEKALSASKLVGGQKSLKLENVVKPEIKGGLIVELGDKTVDL SI 180
*
```

Escherichia_coli_subunit_delta
Bos_taurus_subunit_oscp
Saccharomyces_cerevisiae_subunit_oscp

```
----- 134
----- 120
STKIQLNKVLEDSI 195
```

Fo: b structural alignment



Sc: 3.38 RMS: 2.14

Bos_taurus	-----
Saccharomyces_cerevisiae	KQTDPKAKANSIINAIPGNNILTKTGVLTSAAAVIY AISNELYVINDESILLTFLGFT
Bos_taurus	-----G-EFADKLNEQKIAQLEEVKQASIKQIQDAIDMEKSQQALVQKRHYLFD
Saccharomyces_cerevisiae	GLVAKYLAPAYKDFADARMKKVSDVLNASRNKHVEA---VD--RIDSVSQLQNV AETTK
Bos_taurus	VQRNNIAMALEVTYRERLHRVYREVKNRLDYHISVQNM MRQKEQEHMINWVEKRVVQ---
Saccharomyces_cerevisiae	VLFDVSKETVELESEAFELKQKVELAHEAKAVLDSWVRYEASLRQLEQRQLAKSVISRVQ
Bos_taurus	-----
Saccharomyces_cerevisiae	SELGNPKFQEKVLQQSISEIEQLLSK

Fo: b sequence alignment

Species	Protein	Accession	Length
Rattus norvegicus subunit b	MLSRVLSA--AATAAPCLKNAVLGPGVLQATRVFHTGQRLAPLPLPEYGGK-	53	
Bos taurus subunit b	MLSRVLSA--AAAAAPSLKNAALLGPGVLQATRVFHTGQPSLAPVPLPEHGGK-	53	
Neurospora crassa subunit b	MASRLARTAVGAARLRPSVVP--RVLPAL----STVASPRYSSGV--PSEDPKT	46	
Ashbya gossypii subunit b	MAFRALT--KAAARP--LLAL----GPR--SVAMGARYMSTP--APQDPKS	40	
Kluyveromyces lactis subunit b	MFRALT--KASARP--VVAG--LCSRQ----APIAAVRYMSTP--SPQDPKA	41	
Candida glabrata subunit b	MSFRALTM--RSAVARTALNNTIRSAARVA----TPYLGIRHSSST--PTPDPKT	46	
Saccharomyces cerevisiae subunit b	MSMSGVRGLAL--RSVS-KTLFSQ--GVRCP----SMVIGARYMSSTPEKQDPKA	48	
Rattus norvegicus subunit b	VRLGLIPEEFFQFLYPKTVGTGPYVLGTGLSLYFLSKEIYVITPETFSTISVWGLIV	110	
Bos taurus subunit b	VRFLGLIPEEFFQFLYPKTVGTGPYVLGTGLILYLLSKEIYVITPETFSAISTIGFLV	110	
Neurospora crassa subunit b	KAQSIIDSLPGS--NLMSKTAI--LSSAAGLSIYALSNEYVVNEETVVAFCLLSVWG	100	
Ashbya gossypii subunit b	KAAATLDLSPGS--TALSKTGI--LATSAAAAIYAI SNELYVLNAETILLCTFTGFSF	94	
Kluyveromyces lactis subunit b	KASSILDALPGN--TALSKTGI--LATSAAAAIYAI SNELYVLNEETILVATFTGVVL	95	
Candida glabrata subunit b	KAASLIDALPGN--TALTKTGI--LGTSAAAIYIGISNQLYVINDESIILLIFLGFSG	100	
Saccharomyces cerevisiae subunit b	KANSIINAIPGN--NILTCTGV--LGTSAAAIYAI SNELYVINDESIILLTFLGFTG	102	
Rattus norvegicus subunit b	YVIKKYGASIGEFIDKLNEEKIAQLLEEIKQSSMKIQDAINREKAQQALVQKRHYLFDVQ	170	
Bos taurus subunit b	YIVKKYGASVGEFADKLNQKIAQLLEEVKQASIKIQDAIDMEKSSQALVQKRHYLFDVQ	170	
Neurospora crassa subunit b	GLIKFGGPLYKKWADEQSDIKINILNSARADHTQAVKTRIGDVKQMSGVIDITKTLFAVS	160	
Ashbya gossypii subunit b	LIALVPAPYKEYADKRMQHVSGILNSSRNKHVAAVKERIESVSELKNVTETTKVLFVS	154	
Kluyveromyces lactis subunit b	AGIKFLAPAYNEFAENRVKQVSSILNSSRTHVDVAVKERIESVSELKNVSDTTKVLFDVS	155	
Candida glabrata subunit b	LVAKFLAPLYKDFADARIKKIGSILNSSRERHVDVAVKDRIESVSELQNVSETTKVLFDVS	160	
Saccharomyces cerevisiae subunit b	LVAKFLAPLYKDFADARMKKVSDVLNASRNKHVEAVKDRIESVSELQNVSETTKVLFDVS	162	
Rattus norvegicus subunit b	RNNIALALEVTYRERLHKAYKEVKNRLDYHISVQDMMRRKEGEHMINWVEKHVIQS---	226	
Bos taurus subunit b	RNNIAMALEVTYRERLHRVYREVKNRDLYHISVQNMRRQKEGEHMINWVEKRVVQS---	226	
Neurospora crassa subunit b	KETAKLEAEAYELEQRTALAAEAKTVLDSWVRYESQVKQRQKELAQTVIAKVKQELNP	222	
Ashbya gossypii subunit b	KETLELEAKAFELKQKVDLATEAKAVLDSWVRYEASVRLQQQKQAEISVIGKVQELANP	214	
Kluyveromyces lactis subunit b	KETVKLEAEAFELKQKVDLAAEAKSVLDSWVRYEASVRLQQQQIADSVAKVQSELNP	215	
Candida glabrata subunit b	KETVELEAKAFELKQKVELAHEAKSVLDSWVRYEASRLQKQKQAEIGISVKESELNTP	220	
Saccharomyces cerevisiae subunit b	KETVELESEAFELKQKVELAHEAKAVLDSWVRYEASRLQLEQRQKQAKSVISRVQSELGNP	222	
Rattus norvegicus subunit b	ISAQKEKETIAKICIGDKMLAKKAQAQPM	256	
Bos taurus subunit b	ISAQKEKETIAKCIADLKLSSKKAQAQPM	256	
Neurospora crassa subunit b	KVLKQILEQSVADVEKIVSKA-----	241	
Ashbya gossypii subunit b	KFQDKVLQSSVADVEKLFASLK-----	236	
Kluyveromyces lactis subunit b	KFQEKVLQSSVADVEKLLANLK-----	237	
Candida glabrata subunit b	KFQDRVLQSSIAVEQVLANK-----	242	
Saccharomyces cerevisiae subunit b	KFQEKVLQSSISEIEQLLSKLK-----	244	

Bos_taurus	KLALKT--I-DWVAFGEIIPRNQKAVANSLSKSWNETLTSRLATLPEKP--P--AIDWAYY
Saccharomyces_cerevisiae	---LDWAKVISS--LRI-----T---GSTATQLSSFKKRNDEARRQLLELQSQP-TE-V
Bos_taurus	KA---N-----VA-KAGLVDDFEKK-FNALK---VPI-PE--DKYT-AQVDAE-EK
Saccharomyces_cerevisiae	-DFSHYRSVLKNTSVIDIKIESVYVK---YKP---VKIDASKQLQVIESFEKHAMTNAK-
Bos_taurus	ED-VKSCAEFLTQSKTRIQEYEKELEKMRN-----
Saccharomyces_cerevisiae	ETES-LVSK---ELDNIQS--A-RPF-DELTVDLDTKIKPEIDAKVEEMVKKGKWDVPG
Bos_taurus	-----
Saccharomyces_cerevisiae	YKDRFGNLNVM

Rattus_norvegicus_subunit_d	-MAGRKLALKTIDWVFEIMPQNQ--KIGNALKSWNETFHTRLASLSEKPPAIDWAY	57
Bos_taurus_subunit_d	-MAGRKLALKTIDWVAFGEITPRNQ--KAVANSLSWNETLSRLATLPEKPPAIDWAY	57
Schizosaccharomyces_pombe_subunit_d	MSKVSAAGKAIOWASVASKLKLDAATASAIANFRSHAQAVAKGLTRLEQQTVDFTAY	60
Kluyveromyces_lactis_subunit_d	-MSLAKSAANKLDWAKVISLKLTKGTATLSLFFKRNDEARRQLLEQSQPTSVDFSHY	59
Saccharomyces_cerevisiae_subunit_d	-MSLAKSAANKLDWAKVISLRLITGSTATQLSLFFKRNDEARRQLLEQSQPTVEVDFSHY	59
Aspergillus_terreus_subunit_d	--MAARSAALKIDWVKVITSLGLRGQTAAQLQAFKRNDDARRKQVILSEQPTVDFAHY	58
Neurospora_crassa_subunit_d	--MAARNAALKVDWAKITSSLLDGRGTAAQLQAFKRNDDARRKQVILSELPVDFAHY	58

Rattus norvegicus subunit_d	RANVDKPLGVDDFKNKYNALKIP-VPEDKYTALVDAEEKEDVKNCQAVTGSQARVREYE	116
Bos taurus subunit_d	KANVAKAGLVDDFEKFNALKVP-IPEDKYTAQVDAEEKEDVKSCAEFLTQSKTRIQEYE	116
Schizosaccharomyces pombe subunit_d	RSVLANKTEIVNRIESMCKFPKPKVILNLSQLKANAFEAKASEGAKKNVSLKVAELQNL	120
Kluyveromyces lactis subunit_d	RSVLKNTTEVDKIEFYKYPKPSVDVSKQLSTIEAFESQAIENAAETKLVAKELDKLK	120
Saccharomyces cerevisiae subunit_d	RSVLKNTSVIDKIEISYKQYKPKVILDAKSLQLQVIESFEKHAMTNAKETSELVSKELDLQ	119
Aspergillus terreus subunit_d	RQILKNQAVVDIEISYKQYKPKATYDVSRLKAIEFAEAQAVQNAEQTKGKVEAELRLNQ	118
Neurospora crassa subunit_d	RLTKNQAVINVEIKRFTSFKPATYDVSRLKLAIEFAEVEAIKNAEATKTKVDLEKDL	118

Rattus_norvegicus_subunit_d	KQLEKIKNMIPFDQMTIDDLNEVPFETKLDKRYK---PYWPHQPI----ENL---	161
Bos_taurus_subunit_d	KELEKMRNIIPFDQMTIEDLNEVPFETKLDKKYK---PYWPHRPI----ETL---	161
Schizosaccharomyces_pombe_subunit_d	ATLKNIEQARPTTEETIEDMKQAVPEIEKIVETMTVKGKWVPGYKRFGLDSIM	175
Kluyveromyces_lactis_subunit_d	ETLNNIEARPFDELTVDELTKARPEIDAKVEEMVKKGRWDVPGYKEKFGDLTIM	174
Saccharomyces_cerevisiae_subunit_d	STLDNIQASARPFDELTVDDLTKIKPEIDAKYEEEMVKKGRWDVPGYKDRFGNLNVM	174
Aspergillus_terreus_subunit_d	KTLENIETARPFDELTVDEVAQAPEIDEKTSALVSKGRWMPAGYKRFGLDSVV	173
Neurospora_crassa_subunit_d	KTLENIETARPFDELTVDEVAQAPEIDEKTSALVSKGRWSPGYKRFGLDSLVL	173

Fo: 8 sequence alignment

Ashbya_gossypii_subunit_8	MPQ ^{Q3} MIPFFFFNQLTYGFTFILTLFLT ^{Y39} SYVFLPMILRL ^{R42} YISRLYISKL-----	48
Kluyveromyces_lactis_subunit_8	MPQLVPFYFLNQLVYGFALVTILLVLF ^{Q3} QAQYFLPQILRL ^{Y39} YSRLFISKL-----	48
Wickerhamomyces_canadensis_subunit_8	MPQLVPFYFLNQLTYGFLLLIILLVLF ^{Q3} SQFLLPRILRL ^{Y39} YISRLFISKL-----	48
Vanderwaltozyma_polyspora_subunit_8	MPQLIPFYFLNQLTYGFLMTILLVLF ^{Q3} SQFFLPMILRL ^{Y39} YLTRLFISKL-----	48
Candida_glabrata_subunit_8	MPQLIPFYFMNQLTYGLLLITVLLILF ^{Q3} SQFFLPMILRL ^{Y39} YVSRLFISKL-----	48
Saccharomyces_cerevisiae_subunit_8	MPQLVPFYFMNQLTYGFLMITLLILF ^{Q3} SQFFLPMILRL ^{Y39} YVSRLFISKL-----	48
Rattus_norvegicus_subunit_8	MPQLDTSTWFITIISSM-----ATLFI--LF-----QLKISSQTFPAPPSPKTMA	43
Bos_taurus_subunit_8	MPQLDTSTWLTMI ^{Q3} LSMF-----LTLFI--IF-----QLKVS ^{Y39} KHNFYHNPELTPTK	43
	***: :: : : :: :: :* :*,	
Ashbya_gossypii_subunit_8	-----	48
Kluyveromyces_lactis_subunit_8	-----	48
Wickerhamomyces_canadensis_subunit_8	-----	48
Vanderwaltozyma_polyspora_subunit_8	-----	48
Candida_glabrata_subunit_8	-----	48
Saccharomyces_cerevisiae_subunit_8	-----	48
Rattus_norvegicus_subunit_8	TEKTN ^{Q3} NPWESKWT ^{Y39} KT ^{R42} YLPLSLPPQ	67
Bos_taurus_subunit_8	MLKQNTPWETK ^{Q3} WT ^{Y39} KI ^{R42} YLP ^{Q3} LLLPL-	66

Fo: e, f and g sequence alignment

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Rattus_norvegicus_subunit_e      MPPVQVSPLIKFGRYALILGMAYGAKRYSYLPRAEEERRIAA-EKKRLDELKRIER      59
Bos_taurus_subunit_e            MPPVQVSPLIKLGRYSALFLGMAYGAKRYNYLPRAEEERRLAA-EKKKRDEQKRIER      59
Saccharomyces_cerevisiae_subunit_e  -----MSTVNVLRYSALGLGLFFGFRNDMILKCNAKKKKEQAYEELKLVE--EAKK      51
                                   ::. ***** *: *: .:  ** *:..... * *** : * .::

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Rattus_norvegicus_subunit_e      ELAEADVSIK-----71
Bos_taurus_subunit_e            ELAEAQEDILK-----71
Saccharomyces_cerevisiae_subunit_e EYAKLHPVTPKQVPANASFNLEDPNIDFERVILNAVESLKEAST      96
                                   * * .      *

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Rattus_norvegicus_subunit_f      -----MASIVPLKEKKLMEVKLRELPSWILMR-----DFTPSGIAGA--FRRGYDRYY      46
Bos_taurus_subunit_f            -----MASVPLKEKKLLLEVKLGLPSWILMR-----DFTPSGIAGA--FQGGYRYYY      46
Schizosaccharomyces_pombe_subunit_f -MAPFPLKSFIPPQVA--NPTALNAFPSSARMGRIVDFYSRLPHGPAPKSSNSFFSWYY      57
Saccharomyces_cerevisiae_subunit_f MIFKRAVSTLIPPQVV--SSKNIGSAPNAKRIANVVHFYKSLPQGPAPAIAKANTRLARYK      58
                                   : :.* : :      : * :      : * * *      . *

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```

Rattus_norvegicus_subunit_f      NKYINVRKGSISGINMVLAAAYVFSYCSYK-ELKHERRRKYH      88
Bos_taurus_subunit_f            NKYVNVKKGSIAGLSMVLAAYVFLNYCRSYK-ELKHERLRKYH      88
Schizosaccharomyces_pombe_subunit_f KKY-LGKNASGAPLLHLVGAVLVFSYASEYYYHIRHHEEH---96
Saccharomyces_cerevisiae_subunit_f AKYFDGDNASGKPLWHFALGIIAFGYSMEYYFHLRHHKGAEHH      101
                                   ** :.* : : .: :.* * : :.*.

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Saccharomyces_cerevisiae_subunit_g MLSRIQNYTSGLVSKANLLSSKALYYGKVGAEISKQIYLKKEGLQPPTVAQFKSVYSNLYK      60
Rattus_norvegicus_subunit_g      ----MAKFIRNLADKAPSMVAAAVTYSKPRLA-TFWHYARVELVPPTLGEIPTAIQSMKS      55
Bos_taurus_subunit_g            ----MAEFVRNLAEKAPALVNAAVTYSKPRLA-TFWYYAKVELVPPTPAEIPTAIQSLKK      55
                                   : :. *..** : *:* * : * : * *** : : . . . .

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```

Saccharomyces_cerevisiae_subunit_g QSLNFALKPTEVLSCLNKIQKNELLKYGAYGIQLIGFYSVGEIIGRRKLVGYKHH      115
Rattus_norvegicus_subunit_g      I-----I-HSAQTGNFKHLTVKEAVLNLVATEVMMWFYIGEIIGKRIGVGYDV-103
Bos_taurus_subunit_g            I-----I-NSAKTGSFKQLTVKEALLNLVATEVMMWFYVGEIIGKRIGIYDV-103
                                   : : . :.*: : * : * : : : :*****.* : :.*.

```

Reminders

- ❖ ATP synthase is involved in ATP synthesis and is composed by 17 subunits in *S. cerevisiae*.
- ❖ The alpha and beta subunits are the ones in charge of the catalytic function.
- ❖ The trimeric catalytic head of F1 has three different conformations.
- ❖ The rotation of the gamma and epsilon subunits induces the conformational change.
- ❖ Subunit a along with the c-ring form the membrane proton channel.
- ❖ Subunits a, i/j, e, k are in charge of the dimer formation. Bending occurs thanks to the further help of subunits g and b.
- ❖ Residues interacting with ATP and the responsible of the proton flux are the most conserved.

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QUESTIONS

1. Which subunits of the ATP synthase complex interact with the ATP?
 - a. Alpha
 - b. Beta
 - c. a and b are correct
 - d. C-ring
 - e. All are correct
2. Which subunits of the ATP synthase constitute the rotor?
 - a. Gamma, epsilon and delta
 - b. Gamma, alpha and beta
 - c. Delta, subunit a and c-ring
 - d. Subunits a, 8 and c-ring
 - e. All are false
3. During the ATP synthesis, the conformational changes of the Beta subunit are due to the:
 - a. Rotation of gamma subunit
 - b. Interactions with Alpha subunit
 - c. Rotation of c-ring
 - d. Concentration of ATP
 - e. Complex dimerization
4. The central stalk of the ATP synthase complex is formed by:
 - a. C-ring and subunit a
 - b. F1 subunits
 - c. a and b are correct
 - d. Subunits gamma, delta and epsilon
 - e. All are false

QUESTIONS

5. Which residues of the Beta subunit form the Catch 2?
- a. 380-406
 - b. 400-486
 - c. 1-40
 - d. 386-400
 - e. 212-276
6. Which ATPases hydrolyze ATP?
- a. V-ATPases
 - b. P-ATPases
 - c. a and b are correct
 - d. E-ATPases
 - e. All are correct
7. The peripheral stalk is composed by:
- a. Subunit a, c-ring and subunit 8
 - b. Subunit OSCP, subunit b and subunit a
 - c. Subunit b, subunit d, OSCP and subunit a
 - d. Subunit OSCP, subunit d, subunit b and subunit h
 - e. Subunit h, subunit c, subunit OSCP and subunit j
8. Which specie is the one with the simplest ATP synthase complex?
- a. *S. cerevisiae*
 - b. *E. coli*
 - c. a and b are correct
 - d. *Bos taurus*
 - e. All are false

QUESTIONS

9. Which statements are correct regarding the change of conformation of the different subunits in ATP synthesis?

1. ADP+Pi bind the protein and the conformation E changes to DP
2. When the formation of ATP is catalyzed the conformation of E changes to TP
3. When the ATP is released the conformation TP changes to E
4. The conformation changes from TP to DP when the ATP is released
 - a. 1, 2, 3
 - b. 1, 3
 - c. 2, 4
 - d. 1, 2, 3, 4

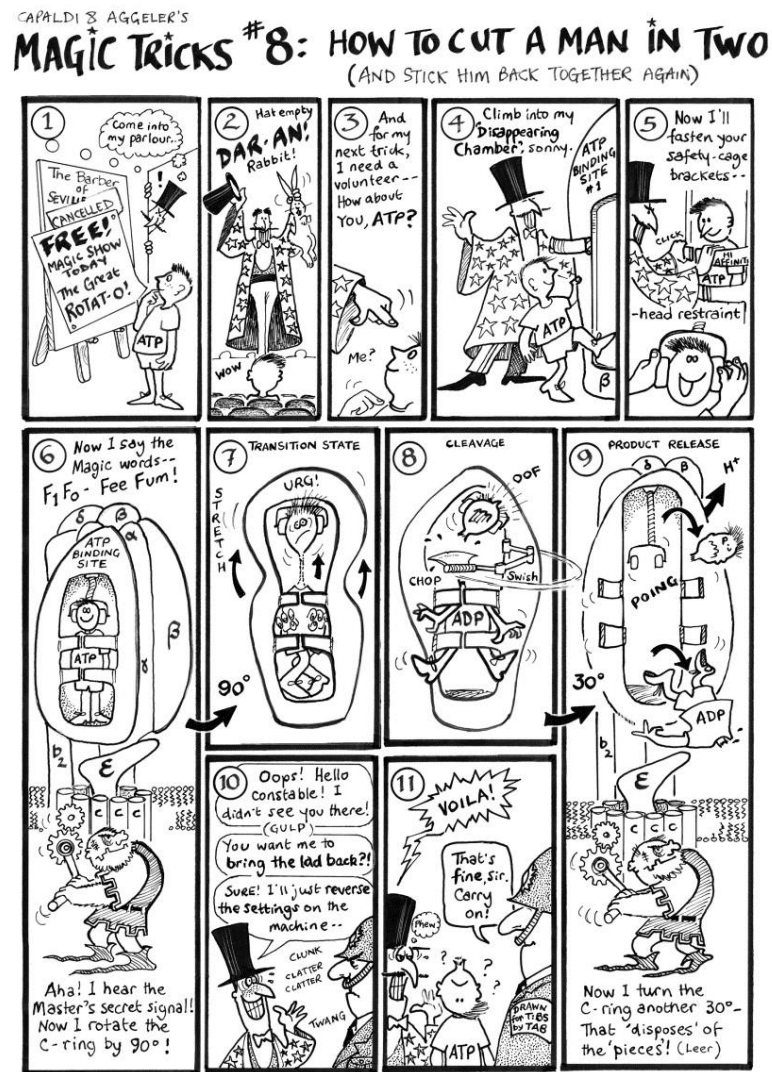
10. Which subunits hold together the dimer?

1. Subunit a
2. Subunit k
3. Subunit e
4. Subunit i/j
 - a. 1, 2, 3
 - b. 1, 3
 - c. 2, 4
 - d. 1, 2, 3, 4

THANKS FOR YOUR ATTENTION

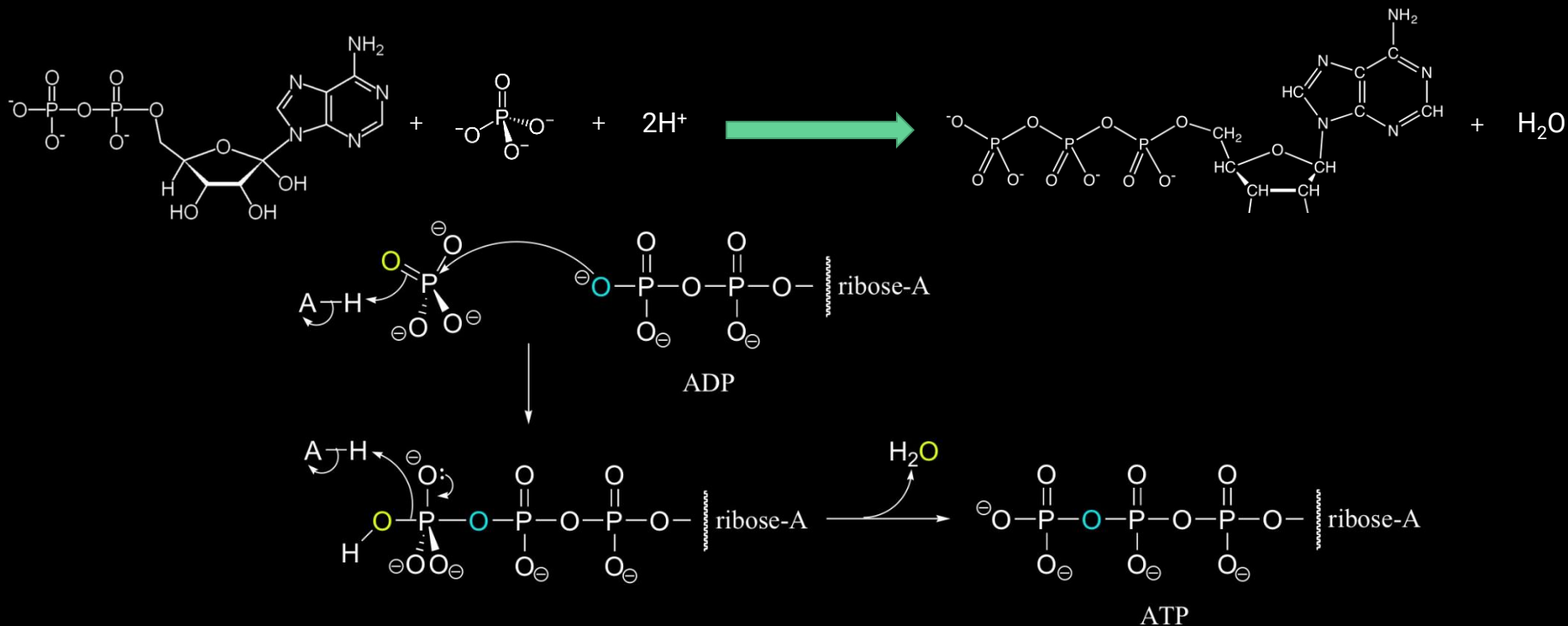
“A PICTURE IS WORTH A
THOUSAND WORDS”

From: Capaldi, R. and Aggeler, R. (2002). Mechanism of the F1F0-type ATP synthase, a biological rotary motor. *Trends in Biochemical Sciences*, 27(3), pp.154-160.



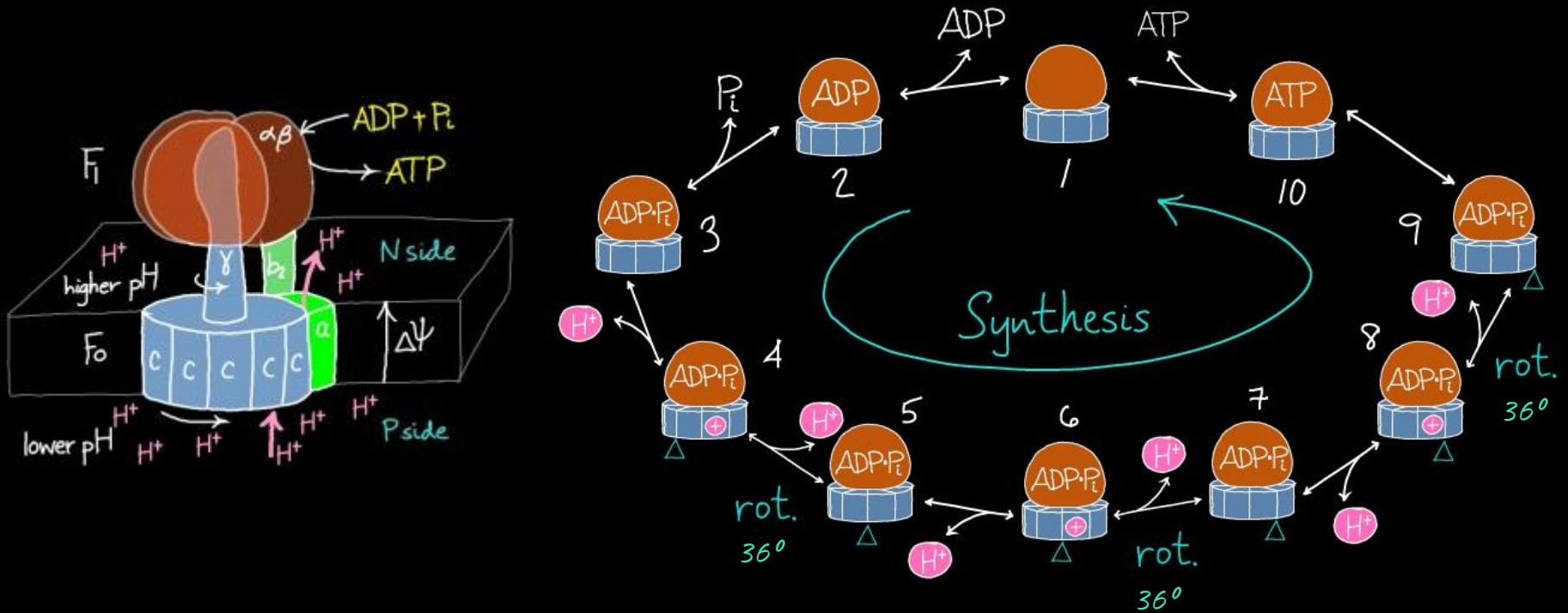
EXTRA SLIDES

ATP SYNTHESIS

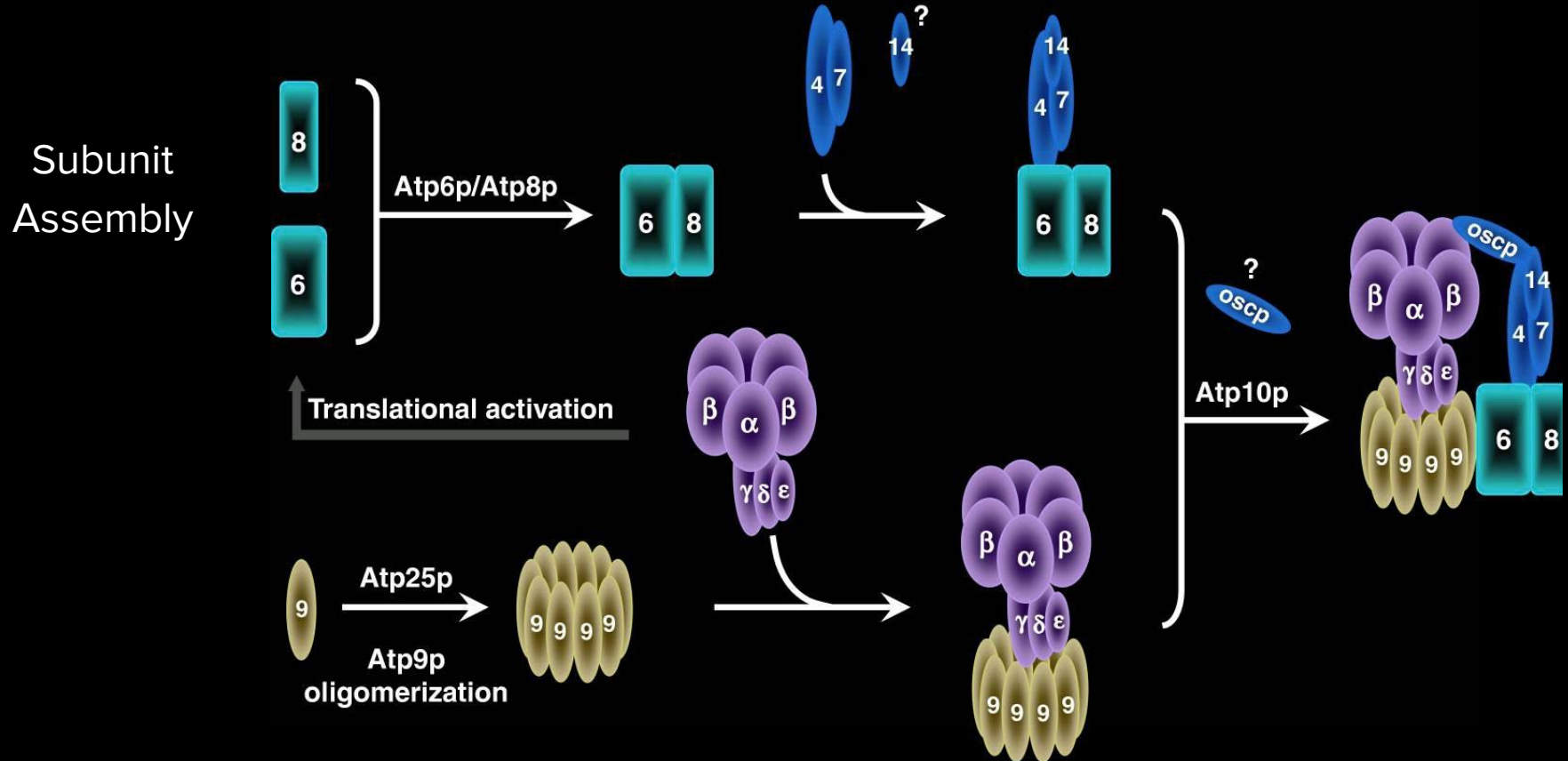


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ATP SYNTHESIS in ATP SYNTHASE



YEAST F1-F₀ ATP SYNTHASE



SUBUNIT e

- Total residues = 96
- **Polar residues = 51 - Percentage: 53.1**
- **Nonpolar residues = 45 - Percentage: 46.9**
- Acidic residues = 15 - Percentage: 15.6
- Basic residues = 14 - Percentage: 14.6
- Basic residues with His = 15 - Percentage: 15.6

SUBUNIT g

- Total residues = 115
- **Polar residues = 61 - Percentage: 53**
- **Nonpolar residues = 54 - Percentage: 46.9**
- Acidic residues = 5 - Percentage: 4.3
- Basic residues = 16 - Percentage: 13.9
- Basic residues with His = 18 - Percentage: 15.7

aminoacid%.py

```
#Open the file:
filename = input ("Insert fasta file name - if it is not in this directory, please specify the pwd: ")
file = open(filename, "r")
lines = file.readlines()
#Define variables:
counter = 0
nonpolar = 0
polar = 0
acid = 0
basic = 0
his = 0
polaratio = 0
nonpolaratio = 0

#Count the different kinds of amino acids:
for i in lines:
    res = list(i)
    if res[0] == ">":
        prot = i.split(">")
        protein = prot[1]
    if res[0] != ">":
        while counter < len(res):
            if (res[counter] == "F") or (res[counter] == "A") or (res[counter] == "L") or (res[counter] == "M") or (res[counter] == "I") or (res[counter] == "W") or (res[counter] == "P") or (res[counter] == "U") or (res[counter] == "Y"):
                nonpolar += 1
            if (res[counter] == "S") or (res[counter] == "T") or (res[counter] == "N") or (res[counter] == "Q") or (res[counter] == "C") or (res[counter] == "G") or (res[counter] == "R") or (res[counter] == "H") or (res[counter] == "K") or (res[counter] == "D") or (res[counter] == "E"):
                polar += 1
            if (res[counter] == "R") or (res[counter] == "K"):
                basic += 1
            if (res[counter] == "D") or (res[counter] == "E"):
                acid += 1
            if res[counter] == "H":
                his += 1
            counter += 1
        counter = 0

total = polar + nonpolar
basich = basic + his

#Calculate the percentages:

polaratio = (polar / total)*100
nonpolaratio = (nonpolar / total)*100
acidratio = (acid / total)*100
basicratio = (basic / total)*100
basichratio = (basich / total)*100

#Print the results:
print ("\nAMINO ACID % version 1.0\n\nSoftware developed by: Joudie-ElKaderi S, Marimon-Gilbert X, Sánchez-López R, Yagüe-Relimpio A and Herrera-Fernández V\nContact: victor.herrera01@estudiant.upf.edu\n")
print ("Protein:" ,protein,)
print ("Total residues = ", total, "\n")
print ("Polar residues = ", polar, "- Percentage: ", polaratio, "\n")
print ("Nonpolar residues = ", nonpolar, "- Percentage: ", nonpolaratio, "\n")
print ("Acidic residues = ", acid, "- Percentage: ", acidratio, "\n")
print ("Basic residues = ", basic, "- Percentage: ", basicratio, "\n")
print ("Basic residues with His = ", basich, "- Percentage: ", basichratio, "\n")
```

stamp.py

```
import os

filename = input ("Insert domains file name: ")
querysplit = filename.split(".")
query = querysplit[0]

pdbseq = 'pdbseq -f ' + query + '.domains > ' + query + '.fa'
os.system(pdbseq)

clustalw = 'clustalw ' + query + '.fa'
os.system(clustalw)

aconv = 'aconvertMod2.pl -in c -out b <' + query + '.aln> ' + query + '.block'
os.system(aconv)

alnfit = 'alignfit -f ' + query + '.block -d ' + query + '.domains -out ' + query + '.trans'
os.system(alnfit)

stamp = 'stamp -l ' + query + '.trans -prefix ' + query + '_OK > ' + query + '_OK.out'
os.system(stamp)

print("\n")

num = input("How many templates do you have? Insert a number: ")
nu = int(num)
numb = nu - 1
n = str(numb)

print("\n")

sup = 'transform -f ' + query + '_OK.' + n + ' -g -o ' + query + '_OK' + n + '_stamp.pdb'
os.system(sup)

aln = 'aconvertMod2.pl -in b -out c <' + query + '_OK.' + n + '> ' + query + '_OK' + n + '_stamp.aln'
os.system(aln)
```