# Protein Sequence



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#### HMM in PFAM

cd18182	ATP synthase F(0) complex subunit C3 (ATP5G3) and similar proteins	CDD	ATPSGS (also called ATP synthase lipid-binding protein, ATP synthase proteolipid P3, ATP synthas proton-transporting mitochondrial F(o) complex subunit C3, ATPase protein 9, or ATPase subunit of tran
cd00310	ATP synthase Fo complex, subunit 6 (eukaryotes) and subunit a (prokaryotes)	CDD	Bacterial forms are designated as ATP synthase. Fo complex, subunit a: eukaryotic (chloroplast an mitochondrial) forms are designated as ATP synthase. Fo complex, subunit 6. The F-ATP synthase (also
TIGR01131	F0F1 ATP synthase subunit A	NCBIFAM	Bacterial forms should be designated ATP synthase, F0 subunit A; eukaryotic (chloroplast an mitochondrial) forms should be designated ATP synthase, F0 subunit 6. The F1/F0 ATP synthase is multisubu
IPR032238	Putative ATP-synthase-associated protein	INTERPRO	This is a family of short highly conserved plant proteins that might be associated with ATP-synthas atp operon.
PF04627	Mitochondrial ATP synthase epsilon chain	PFAM	This family constitutes the mitochondrial ATP synthase epsilon subunit. This is not to be confuse with the bacterial epsilon subunit, which is homologous to the mitochondrial delta subun (Pfam:PF0
PF00231	ATP synthase	PFAM	
TIGR01146	ATP synthase F1 subunit gamma	NCBIFAM	This model describes the ATP synthase gamma subunit in bacteria and its equivalents in organelle namely, mitochondria and chloroplast. F1/F0-ATP synthase is a multisubunit, membrane associate enzym

We used interprot to search for ATP synthase in PFAM database.

A / Browse / By Entry / Pfam / PF00231 / Overview **PF00231** ATP synthase Member database Pfam 0 Overview Pfam type domain Proteins 50 Short name ATP-synt Domain Architectures 113 Taxonomy 448 Description # Imported from IPR000131 Proteomes 11k The ATPase F1 complex gamma subunit forms the central shaft that connects the F0 rotary motor to the F1 Structures 314 catalytic core. The gamma subunit functions as a rotary motor inside the cylinder formed by the a(3)8(3) Signature subunits in the F1 complex [2]. The most conserved region of the gamma subunit is its C terminus, which seems to be essential for assembly and catalysis. AlphaFold 418

We found an entry, so a HMM is available.

\$hmmfetch ~/Documents/databases/PFAM/Pfam-A.hmm ATP-synt\_ab > alpha.hmm

We used the hmmfetch command and the short name to get the hmm file





Now we need to try to find a model for our protein seq (example done with F1 alpha)

\$hmmscan ~/Documents/databases/PFAM/Pfam-A.hmm target\_alpha.fa > alpha\_HMM.out

Model: ATP-synt\_ab



Markov model creation

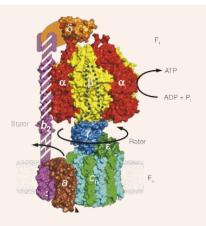
\$hmmfetch ~/Documents/databases/PFAM/Pfam-A.hmm ATP-synt\_ab > alpha.hmm

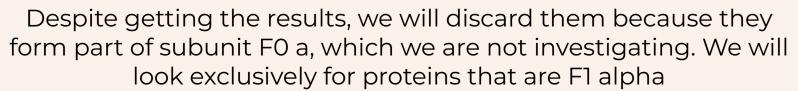
Then we look for similar proteins to create a set of protein family

\$hmmsearch alpha.hmm ~/Documents/databases/UniProt/uniprot\_sprot.fasta > prot\_fam\_ids.out

Results: Q8TWL6, A3CS71, A8AUJ7, C6A5E8, A7IAU8, O29101, Q0W363







Final Results (alpha): Q8TWL6, A3CS71, A8AUJ7, C6A5E8, A7IAU8, O29101, Q0W363

We follow the same procedure for subunit F1 beta

Final Results (beta): B7IQV8, B7HFK1, Q814W2, A9VSA3, A0RL95, C1F0M8, C3LFH9, C3P1F4





### Why Uniprot?



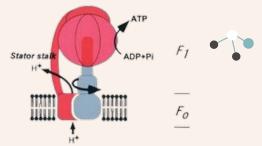




Biased and redundant

Unbiased and Non-redundant





To align subunit F1, chain alpha we did the following **\$cat seq\* >> sequences.fa** 

Align the sequences against the model we created using PFAM \$hmmalign alpha.hmm sequences\_F1\_chain\_alpha.fa > MSA\_F1\_alpha.sto

This gives us the alignment in Stockholm format, we use perl to transform it into an alignment file

\$perl ~/Documents/perl\_scripts/aconvertMod2.pl -in h -out c
<MSA\_F1\_alpha.sto > aln\_F1\_alpha.aln

We used this steps for both subunit F1 alpha and beta



## Alignment (alpha)



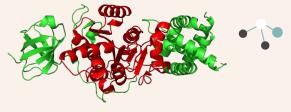
In red the region that better fits the model

3 sp Q8TWL6 VATA METKA	-msnsvkgeivkiagpvveavgcegakmyevfrvgdegligeviniesdratigvyeett
4 SP A3CS71 VATA METMJ	mdkgkenraggvlkrisgpvvtavgldahmydvvkvgneelmgevikiggeniiigv
5 sp A8AUJ7 VATA STRGC	msqqkiikvsqplvlasqmqeaniqdicrvqdlqliqeiiemrrdqasiqvyeets
6 sp   C6A5E8   VATA THESM	mgkivrvtgplvvademrgsrmyevvrvgelgligeiirlegdkavigvyeeta
7 sp A7IAU8 VATA METB6	mevkangaketkkgvlkriagpvvtavnldahmydvvrvgnealmgevikiggdnviigv
8 sp   029101   VATA ARCFU	mevkeagyvgeiyrisgplvvaeglkarmydlckvgeeglmgevvglvgqkvliqvy
9 sp   00W363   VATA METAR	msqqqtiyrvaqpvvtavqlnarmydvvkvqneqlmqevieidndkaiiqvy
10	
11 sp Q8TWL6 VATA_METKA	glqpgepvkgtgellsvelgpglltqifdgiqrplpeirkevgdfvergilvsaldrkkk
12 sp A3CS71 VATA METMJ	yedtagirpgesvgntglslavelgpglltsiydgiqrplevlvdkmgnfiergvsapgl
13 sp A8AUJ7 VATA_STRGC	glgpgepvittgsplsvelgpglisqmfdgiqrplerfqtitesdflvrgvqlpnldret
14 sp C6A5E8 VATA_THESM	gikpgepvmgtgaslsvelgpglltsiydgiqrpleilrsqsgdfigrgltapalsrdkk
15 sp A7IAU8 VATA_METB6	yedttgikpgepvsntglslavelgpglltsiydgiqrplevlvnkmgnfiergvsapgl
16 sp 029101 VATA_ARCFU	edtegvkpgdkventgmplsvelgpglirniydgvqrplpvlkevsgdfigrgieapgld
17 sp Q0W363 VATA_METAR	edtsgvrpgepventgmplsvelgpglltsiydgiqrplevlkekmgnfitrgvsapgls
18	
19 sp Q8TWL6 VATA_METKA	weftpkvkegekveegdvlgtvpetefiehkimvppgvsgevieiaadgeytvedtiavi
20 sp A3CS71 VATA_METMJ	shekkwefvptvkkgdevkagdilgtvqetnivhkvmvppkakggkikkisggsftvdet
21 sp A8AUJ7 VATA_STRGC	kwnfvpslsvgdaveagdilgtvqetnlvehrimvpvgvsgrlanisagsftveetvyei
22 sp C6A5E8 VATA_THESM	whftpkvkvgdkvvggdiigvvpetsiiehkimippeiegeiieivgegdytieeviakv
23 sp A7IAU8 VATA_METB6	shekkwtfkpvvkagdkvepgailgevqetnivhkvmlppnvkagvvktikagdftvdei
24 sp 029101 VATA_ARCFU	rkakwefkplvkkgekvkpgeiigtvqetevveqkilvppnvkegviaeiyegsftvedt
25 sp Q0W363 VATA_METAR	rtkkwkfvpvvkagdkvkggivigtvqetktivhkimvppnvgettikdikegeftvedv
26	
27 sp Q8TWL6 VATA_METKA	edeegeehevtmmqewpvrkprpykrkldpeepliTGQRVIDTFFPVAKGGTAAIPGPFG
28 sp A3CS71 VATA_METMJ	vcvledgteiamlqrwpvrvprpvtqklnpdipliTGQRILDGLFPIAKGGTAAIPGPFG
29 sp A8AUJ7 VATA_STRGC	eqaegsifkgtlmqkwpvrrgrpfaqklipveplvTGQRVIDTFFPVTKGGAAAVPGPFG
30 sp C6A5E8 VATA_THESM	kapngeikevrmyqrwpvrmkrpykqklppevplvTGQRTIDTFFPQAKGGTAAIPGPFG
31 sp A7IAU8 VATA_METB6	iviledgreypmiqrwpvrvprpvkekknptipllTGQRILDGLFPIAKGGTAAIPGPFG
32 sp 029101 VATA_ARCFU	iavledgtelklyhkwpvriprpyveklppvvpliTGQRILDTFFPVAKGGTAAIPGPFG
33 sp Q0W363 VATA_METAR	ighlengtelklmhkwpvrvprpyveklrpdipliTGQRVLDGLFPIAKGGTAAIPGPFG
34	
35 sp Q8TWL6 VATA_METKA	SGKTVTQQQLAKWADAQVVVYIGCGERGNEMTEVLEDFpeledprTGRPLMERTILVANT
36 sp A3CS71 VATA_METMJ	SGKTVTQQQLAKWSDAEIVVYIGCGERGNEMTEVLTEFpeledpkTGKPLMERTVLIANT
37 sp A8AUJ7 VATA_STRGC	AGKTVVQHQVAKFANVDIVIYVGCGERGNEMTDVLNEFpelidpsTGQSIMQRTVLIANT
38 sp C6A5E8 VATA_THESM	SGKTVTQHQLAKWSDAEVVVYIGCGERGNEMTDVLEEFpklkdprTGKPLMERTVLIANT
39 sp A7IAU8 VATA_METB6	SGKTVTQQQLAKWSDAKIVVYIGCGERGNEMTEVLTEFphledptSGKPLMERTVLIANT
10 sp 029101 VATA_ARCFU	SGKTVTQHQLAKWSDAQIVVYIGCGERGNEMTEVLEEFpeledprTGKPLMERTVLVANT
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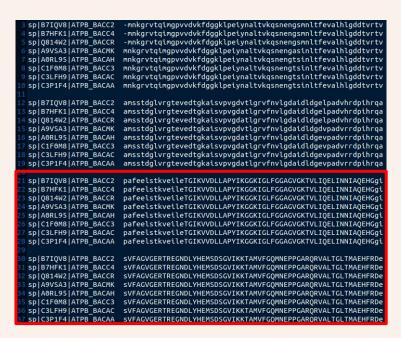
43 sp Q8TWL6 VATA_METKA	SNMPVAAREACIYTGITMAEYYRDMGYDVALMADSTSRWAEALREISGRLEEMPGEEGYP
44 sp A3CS71 VATA_METMJ	SNMPVAAREASVYTGITIAEYFRDMGYDVSLMADSTSRWAEAMREISSRLEEMPGEEGYP
45 sp A8AUJ7 VATA_STRGC	SNMPVAAREASIYTGITIAEYFRDMGYSVAIMADSTSRWAEALREMSGRLEEMPGDEGYP
46 sp C6A5E8 VATA_THESM	SNMPVAAREASIYTGITIAEYFRDMGYNVALMADSTSRWAEALREISGRLEEMPGEEGYP
47 sp A7IAU8 VATA_METB6	SNMPVAAREASVYTGITIAEYFRDMGYDVSLMADSTSRWAEAMREISSRLEEMPGEEGYP
48 sp 029101 VATA_ARCFU	SNMPVAAREASVYTGITIAEYFRDMGYDVAIQADSTSRWAEAMREISGRLEEMPGEEGYP
49 sp Q0W363 VATA_METAR	SNMPVAAREASCYTGITIAEYYRDMGYGVSLMADSTSRWAEAMREISSRLEEMPGEEGYP
50	
51 sp Q8TWL6 VATA_METKA	AYLASRLAEFYERAGRVvclGSDDRVGSVTVVGAVSPPGGDFSEPVTQNTLRIVKVFWAL
52 sp A3CS71 VATA_METMJ	AYLAARLSEFYERAGRViSLNGEGGSVSVIGAVSPPGGDFSEPVTQNTLRIVKVFWAL
53 sp A8AUJ7 VATA_STRGC	AYLGSRIAEYYERAGRVktlGSTAREGSITAIGAVSPPGGDISEPVTQNTLRIVKVFWGL
54 sp C6A5E8 VATA_THESM	AYLASKVAEFYERAGRVrtlGSDDRIGSVSVIGAVSPPGGDLSDPVVQNTLRVVKVFWAL
55 sp A7IAU8 VATA_METB6	AYLAARLSEFYERAGLVeTLNHQSGSVSVIGAVSPPGGDFSEPVTQNTLRIVKVFWAL
56 sp 029101 VATA_ARCFU	AYLASRLAEFYERAGRVkTLAGNIGSVTVVGAVSPPGGDFSEPVTQNTLRIVKVFWAL
57 sp Q0W363 VATA_METAR	AYLAARLSEFYERAGRVITPIGKEGSVTVIGAVSPAGGDISEPVTQNTLRIVKVFWAL
58	The state of the s
59 sp Q8TWL6 VATA_METKA	DSKLADRRHFPAINWLQSYSlylddvekwwheeiggdwrelrdeameilqreseleeivq
60 sp A3CS71 VATA_METMJ	DAKLSQRRHFPAINWLNSYSlyldalnewydkevspewnplrawamgvlqkeaelqeivq
61 sp A8AUJ7 VATA_STRGC	DAQLAQRRHFPAINWLSSYSlyldevgayidqhekiawaekvtkamnilqkeselqeivr
62 sp C6A5E8 VATA_THESM	DADLARRRHFPAINWLTSYSlyvdsikdwwqnnvdpewkamrdeamallqkeseleeivr
63 sp A7IAU8 VATA_METB6	DAKLSQRRHFPAINWLNSYSlyldalhdwydknvspdwnklrswamgvlqkeaelqeivq
64 sp 029101 VATA_ARCFU	DAKLAARRHFPAINWLQSYSlyvdtlkdwfaenvseewnelrrwamevlqeeanlqeivq
65 sp Q0W363 VATA_METAR	DAKLAQRRHFPSINWLNSYSlyqdslkdwydknispewnqlkaesmellqreselqeivq
67 sp Q8TWL6 VATA_METKA	lvgpdalpeserlilevarmiredflqqnafhevdtycppekqyemlktilhfkeraeea
68 sp A3CS71 VATA_METMJ	lvgs dalp de eqv tie var mire if lqqnay dav dtfc pmsk qyd mm kaikhyadlarta
69 sp A8AUJ7 VATA_STRGC	lvgldslsekdrltmnaakmiredylqqnafddvdtytsfkkqvallsniltfdaeanra
70 sp C6A5E8 VATA_THESM	ivgpdalperekaillvarmlredylqqdafhevdtyclpkkqvtmmrvilnfyrhtmra
71 sp A7IAU8 VATA_METB6	lvgsdalpeteqitievarmireiflqqnaydavdtfcdmqkqydmmkairlysdlanta
72 sp 029101 VATA_ARCFU	lvgsdalpesqrvllevariirevyliqyayhpvdtycsvqkqydmlkaikqindwfyqa
73 sp Q0W363 VATA_METAR	lvgsdalpedqqltieiarmireiflqqnayhevdtycsldkqlkmlksimqfgayarta
74	
75 sp Q8TWL6 VATA_METKA	vdkgvpvdeilkldviddiarmkvipneeakekiqeirkkideqfeelieeas
76 sp A3CS71 VATA_METMJ	qtggatpqqvigirsknelpqikfirdyepelakimkdmeaefdamrav
77 sp A8AUJ7 VATA_STRGC	lelgayfreimegtvelrdriarskfvhedqlekiqalsqtieetlhqilaqggldnerh idagipveeiaklpvreeigrmkvnpnieeiavlmektkegfeelfkkvge
78 sp C6A5E8 VATA_THESM	
79 sp A7IAU8 VATA_METB6	qaagvspaqittikaknelpqikfvkdykqplakiekdmdaefnalrsaa
80 sp 029101 VATA_ARCFU	leagktideiagvegleefarakfeedykpameaalekirknllge lasgvpmskilnlnskndlakvkfeanydayltkvnddmkkefksleaa
81 sp Q0W363 VATA_METAR	tasgvpmskttmtnsknotakvkreanydayttkvnodmkkerksteaa



#### Alignment (beta)



In red the region that better fits the model



```
sp|B7HFK1|ATPB BACC4 OGODVLLFIDNIFRFTOAGSEVSALLGRMPSAVGYOPTLATEMGOLOERITST----NKG
sp|Q814W2|ATPB_BACCR
                   OGODVLLFIDNIFRFTOAGSEVSALLGRMPSAVGYOPTLATEMGOLOERITST----NKG
sp|A0RL95|ATPB_BACAH QGQDVLLFIDNIFRFTQAGSEVSALLGRMPSAVGYQPTLATEMGQLQERITST----NKG
SDIC3LFH9|ATPB BACAC
                   OGODVLLFIDNIFRFTOAGSEVSALLGRMPSAVGYOPTLATEMGOLOERITST----NKG
splC3P1F4|ATPB BACAA OGODVLLFIDNIFRFTOAGSEVSALLGRMPSAVGYOPTLATEMGOLOERITST----NKG
sp|B7IQV8|ATPB BACC2 SITSIQAVYVPADDYTDPAPATTFAHLDATTNLERRLTQMGIYPAVDPLASTSralspei
sp|B7HFK1|ATPB_BACC4 SITSIQAVYVPADDYTDPAPATTFAHLDATTNLERRLTQMGIYPAVDPLASTSralspei
sp|0814W2|ATPB BACCR SITSIOAVYVPADDYTDPAPATTFAHLDATTNLERRLTOMGIYPAVDPLASTSralspei
sp|A9VSA3|ATPB BACMK SITSIQAVYVPADDYTDPAPATTFAHLDATTNLERRLTQMGIYPAVDPLASTSralspei
sp|A0RL95|ATPB BACAH SITSIOAVYVPADDYTDPAPATTFAHLDATTNLERRLTOMGIYPAVDPLASTSralspei
sp|C1F0M8|ATPB BACC3 SITSIOAVYVPADDYTDPAPATTFAHLDATTNLERRLTOMGIYPAVDPLASTSralspei
sp|C3LFH9|ATPB BACAC SITSIQAVYVPADDYTDPAPATTFAHLDATTNLERRLTQMGIYPAVDPLASTSralspei
splC3P1F4|ATPB_BACAA_SITSIOAVYVPADDYTDPAPATTFAHLDATTNLERRLTOMGIYPAVDPLASTSralspei
sp|B7IQV8|ATPB BACC2 vgeehyevarqvqqtlqrykelqdiiailgmdelseedklvvhrarriqfflsqnfhvae
SD|B7HFK1|ATPB BACC4
                   vgeehvevargvggtlgrykelgdiiailgmdelseedklyvhrarrigfflsgnfhvae
sp|0814W2|ATPB BACCR
                   vgeehyevarqvqqtlqrykelqdiiailqmdelseedklvvhrarriqfflsqnfhvae
SDIA9VSA3IATPB BACKK
                   vaeehvevaravaatlarvkeladiiailamdelseedklvvhrarriafflsanfhvae
                   vgeehyevarqvqqtlqrykelqdiiailgmdelseedklvvhrarriqfflsqnfhvae
SDIAORL95|ATPB BACAH
                   vgeehyevargvggtlgrykelgdiiailgmdelseedklvvhrarrigfflsgnfhvae
sp|C1F0M8|ATPB BACC3
sp|C3LFH9|ATPB BACAC
                   vgeehyevarqvqqtlqrykelqdiiailgmdelseedklvvhrarriqfflsqnfhvae
SD|C3P1F4|ATPB BACAA
                   vgeehvevargvggtlgrykelgdiiailgmdelseedklvvhrarrigfflsgnfhvae
sp|B7IQV8|ATPB BACC2 qftgqkgsyvpvkntvsgfkeilegkyddlpedafrlvggieevienakkmma
sp|B7HFK1|ATPB BACC4 qftqqkqsvvpvkntvsqfkeileqkyddlpedafrlyqqieevienakkmma
sp|0814W2|ATPB BACCR
                   qftqqkqsyvpvkntvsqfkeileqkyddlpedafrlvqqieevienakkmma
SDIA9VSA3IATPB BACMK
                   qftgqkgsyvpvkntvsgfkeilegkyddlpedafrlvgsieevienakkmma
SPIAORL95|ATPB BACAH
                   gftggkgsyvpvketvrgfkeilegkyddlpedafrlyggieevienakkmma
sp|C1F0M8|ATPB BACC3
                   qftqqkqsyvpvketvrqfkeilegkyddlpedafrlvqqieevienakkmma
splC3LFH9lATPB BACAC aftaakasvypyketyrafkeileakyddlpedafrlyggieevienakkmma
sp|C3P1F4|ATPB BACAA qftqqkqsyvpvketvrqfkeileqkyddlpedafrlyqqieevienakkmma
```





#### Alpha and beta

#### Hypothesis of conservation:

- Active site (F1 alpha and beta are in charge of ATP synthesis)
- Vital zone for protein-protein interaction



In red the region that better fits the model