Δομική Βιοχημεία και στοιχεία Βιοπληροφορικής

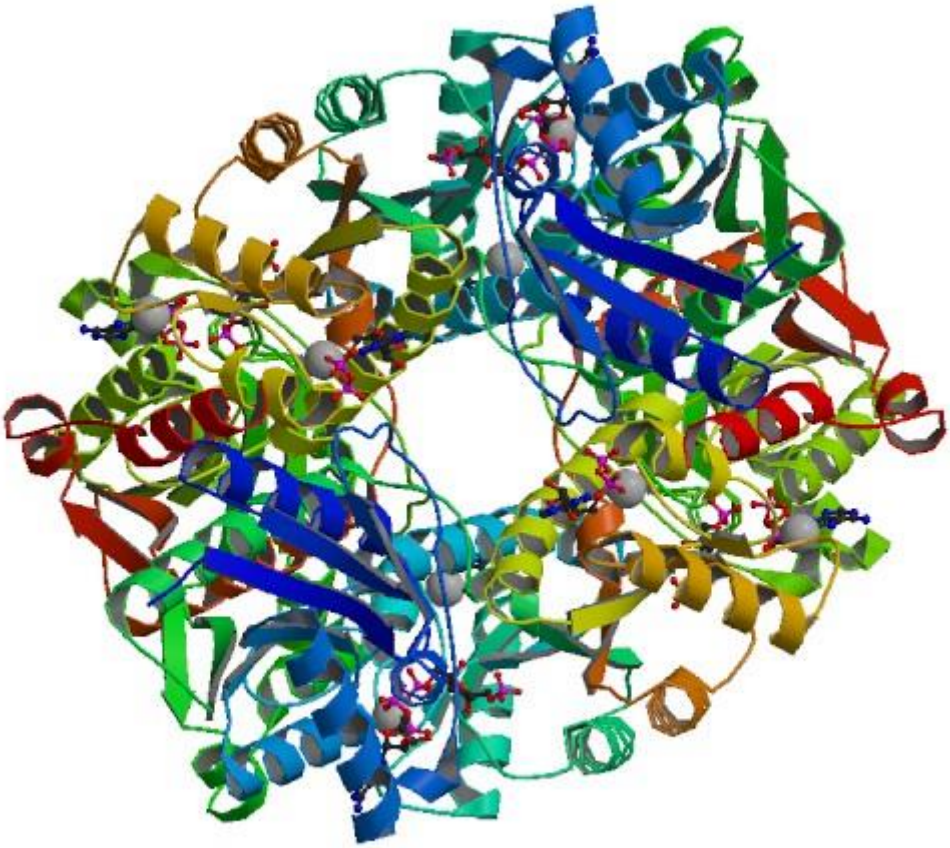
Ονοματεπώνυμο : Καβαρατζή Κωνσταντίνα

Α.Ε.Μ. : 8309

Υπεύθυνη Καθηγήτρια : κ. Χολή Θ.

Πρωτεϊνη : PHOSPHOFRUCTOKINASE 1

Κωδικός πρωτεϊνης στην PDB : 1PFK



- **Κωδικός 1PFK από PDB : P0A796**

- **Expasy: κάνω αναζήτηση τον κωδικό της 1PFK και επιλέγω το 1hit της UniProt και αποθηκεύω το Fasta**

FASTA UNIPROT:

>sp|P0A796|PFKA_ECOLI ATP-dependent 6-phosphofructokinase isozyme 1 OS=Escherichia coli (strain K12) GN=pfkA PE=1 SV=1

MIKKIGVLTSGGDAPGMNAAIRGVVRSALTEGLEVMGIYDGYLGLYEDRMVQLDRYSVSD
MINRGGTFLGSARFPEFRDENIRAVAIENLKKRGIDALVVIGGDGSYMGAMRLTEMGFPC
IGLPGTIDNDIKGTDYTIGFFTALSTVVEAIDRLRDTSSSHQRISVVEVMGRYCGDLTLA
AAIAGGCEFVVVPEVEFSREDLVNEIKAGIAKGKKHAIVAITEHMCDVDELAHFIEKETG
RETRATVLGHIQRGGSPVPYDRILASRMGAYAIDLLLAGYGGRCVGIQNEQLVHHDIIDA
IENMKRPFKGDWLDCAKKLY

- **Εισάγω το Fasta του 1PFK στην αναζήτηση στην ProtParam και παίρνω τα εξής δεδομένα**

ProtParam

User-provided sequence:

1 0 2 0 3 0 4 0 5 0 6 0
MIKKIGVLTS GGDAPGMNAA IRGVVRSALT EGLEVMGIYD GYLGLYEDRM VQLDRYSVSD

7 0 8 0 9 0 10 0 11 0 12 0
MINRGGTFLG SARFPEFRDE NIRAVAIENL KKRGIDALVV IGGDGSYMGA MRLTEMGFPC

13 0 14 0 15 0 16 0 17 0 18 0
IGLPGTIDND IKGTDYTIGF FTALSTVVEA IDRLRDTSSS HQRISVVEVM GRYCGDLTLA

19 0 20 0 21 0 22 0 23 0 24 0
AAIAGGCEFV VVPEVEFSRE DLVNEIKAGI AKGKKHAIVA ITEHMCDVDE LAHFIEKETG

25 0 26 0 27 0 28 0 29 0 30 0
RETRATVLGH IQRGGSPVPY DRILASRMGA YAIDLLLAGY GGRCVGIQNE QLVHHDIIDA

31 0 32 0
IENMKRPFKG DWLDCAKKLY

References and documentation are available.

Number of amino acids: 320

Molecular weight: 34842.0

Theoretical pI: 5.47

Amino acid composition: CSV format

Ala (A)	27	8.4%			
Arg (R)	22	6.9%			
Asn (N)	8	2.5%			
Asp (D)	23	7.2%			
Cys (C)	6	1.9%			
Gln (Q)	5	1.6%			
Glu (E)	21	6.6%			
Gly (G)	38	11.9%			
His (H)	7	2.2%			
Ile (I)	28	8.8%			
Leu (L)	25	7.8%			
Lys (K)	14	4.4%			
Met (M)	12	3.8%			
Phe (F)	10	3.1%			
Pro (P)	8	2.5%			
Ser (S)	14	4.4%			
Thr (T)	15	4.7%			
Trp (W)	1	0.3%			
Tyr (Y)	11	3.4%			
Val (V)	25	7.8%			
Pyl (O)	0	0.0%			
Sec (U)	0	0.0%			
(B)	0	0.0%			
(Z)	0	0.0%			
(X)	0	0.0%			

Total number of negatively charged residues (Asp + Glu): 44
Total number of positively charged residues (Arg + Lys): 36

Atomic composition:

Carbon	C	1532
Hydrogen	H	2458
Nitrogen	N	428
Oxygen	O	462
Sulfur	S	18

Formula: $C_{1532}H_{2458}N_{428}O_{462}S_{18}$
Total number of atoms: 4898

Extinction coefficients:

Extinction coefficients are in units of M^{-1} cm^{-1}, at 280 nm measured in water.

Ext. coefficient 22265
Abs 0.1% (=1 g/l) 0.639, assuming all pairs of Cys residues form cystines

Ext. coefficient 21890
Abs 0.1% (=1 g/l) 0.628, assuming all Cys residues are reduced

Estimated half-life:

The N-terminal of the sequence considered is M (Met).

The estimated half-life is: 30 hours (mammalian reticulocytes, in vitro).
>20 hours (yeast, in vivo).
>10 hours (Escherichia coli, in vivo).

Instability index:

The instability index (II) is computed to be 30.68
This classifies the protein as stable.

Aliphatic index: 95.69

Grand average of hydropathicity (GRAVY): 0.000

- **Στη συνέχεια λαμβάνω επιπλέον πληροφορίες από το ProDom**

database: multiple alignments

Program: ncbi-blastp

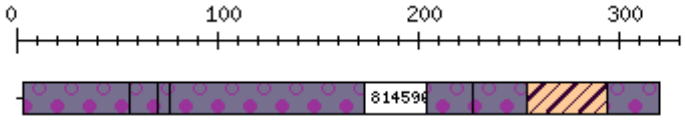
Matrix: BLOSUM62

Expect: 0.01

Filter: seg

Graphical results and forms to other applications

The following is the graphical representation of the HSP found by BLAST.
Please note that HSPs are sorted from highest to lowest scores, so that lower scoring HSPs may be hidden.



Align subsequence with ProDom domains, using Multalin

Domain ID	BEGIN	END	
PDA1E662	3	55	Submit
PDA1N274	76	172	Submit
PD814596	156	203	Submit
PDC6E7U1	17	69	Submit
PD017880	254	293	Submit
PD000707	118	155	Submit
PDA1M1Q4	173	226	Submit
PDA1Z4Z4	120	155	Submit
PDC63680	56	90	Submit
PDB003C6	222	253	Submit
PDC65645	119	158	Submit
PDC8C8N0	4	104	Submit
PDB003F8	294	319	Submit
PDA7Y619	235	269	Submit
PDA1L5G2	3	73	Submit

PDB9B5J4	7	151	Submit
PDB6C0S6	296	319	Submit
PDB002U4	229	253	Submit
PDB2C5T7	121	205	Submit
PDD2A5S9	222	279	Submit
PDD34781	4	103	Submit
PD814606	222	276	Submit
PDC636Q6	94	117	Submit
PDB20112	101	139	Submit
PDD26876	242	271	Submit
PDD0K4X9	235	266	Submit
PDC678Z0	151	172	Submit
PDD1I220	244	283	Submit
PDC1J7X6	246	286	Submit
PDC649Z0	119	157	Submit
PDB1Q9A7	87	115	Submit
PDC64702	100	119	Submit

PDB7X7P1	122	168	Submit
PDA0Y6P9	163	202	Submit
PDD08718	28	70	Submit

Domain 3D modelling using Swiss-Model

Domain ID	BEGIN	END	
PDA1E662	3	55	Submit
PD814596	156	203	Submit
PD017880	254	293	Submit
PD000707	118	155	Submit
PDA1M1Q4	173	226	Submit
PDA1Z4Z4	120	155	Submit
PDC63680	56	90	Submit
PDB003C6	222	253	Submit
PDC65645	119	158	Submit
PDB003F8	294	319	Submit
PDA7Y619	235	269	Submit
PDB002U4	229	253	Submit

PDC636Q6	94	117	Submit
PDC678Z0	151	172	Submit
PDB1Q9A7	87	115	Submit
PDC64702	100	119	Submit

Domain 3D modelling using Geno3D

Domain ID	BEGIN	END	
PDA1E662	3	55	Submit
PD814596	156	203	Submit
PD017880	254	293	Submit
PD000707	118	155	Submit
PDA1M1Q4	173	226	Submit
PDA1Z4Z4	120	155	Submit
PDC63680	56	90	Submit
PDB003C6	222	253	Submit
PDC65645	119	158	Submit
PDB003F8	294	319	Submit
PDA7Y619	235	269	Submit

PDB002U4	229	253	Submit
PDC636Q6	94	117	Submit
PDC678Z0	151	172	Submit
PDB1Q9A7	87	115	Submit
PDC64702	100	119	Submit

HSP Results

Warning: Original output has been filtered to yield non-redundant similarities

blastp 2.2.26 [Sep-21-2011]

Reference: Altschul, Stephen F., Thomas L. Madden, Alejandro A. Schaffer,
Jinghui Zhang, Zheng Zhang, Webb Miller, and David J. Lipman (1997),
_quot;Gapped BLAST and PSI-BLAST: a new generation of protein database search
programs_quot;, Nucleic Acids Res. 25:3389-3402.

Query: unkwown
(320 letters)

Database: prodom2010.1 multiple alignments
45,292,438 sequences; 2,147,483,647 total letters

ProDom domains producing High-scoring Segment Pairs:

Position	ProDom domain	Score	E value
3-55	#PDA1E662	265	3e-26
3-73	#PDA1L5G2	136	5e-08
4-104	#PDC8C8N0	162	3e-11
4-103	#PDD34781	118	8e-05
7-151	#PDB9B5J4	136	2e-07
17-69	#PDC6E7U1	223	2e-20
28-70	#PDD08718	100	0.003
56-90	#PDC63680	181	1e-14
76-172	#PDA1N274	254	4e-24
87-115	#PDB1Q9A7	104	0.0008
94-117	#PDC636Q6	114	3e-05
100-119	#PDC64702	102	0.001
101-139	#PDB20112	114	3e-05
118-155	#PD000707	197	6e-17

119-157	#PDC649Z0	104 0.0008
119-158	#PDC65645	166 2e-12
120-155	#PDA1Z4Z4	184 5e-15
121-205	#PDB2C5T7	125 3e-06
122-168	#PDB7X7P1	102 0.002
151-172	#PDC678Z0	107 0.0003
156-203	#PD814596	245 2e-23
163-202	#PDA0Y6P9	100 0.004
173-226	#PDA1M1Q4	190 9e-16
222-253	#PDB003C6	172 2e-13
222-276	#PD814606	116 3e-05
222-279	#PDD2A5S9	124 3e-06
229-253	#PDB002U4	129 3e-07
235-269	#PDA7Y619	136 3e-08
235-266	#PDD0K4X9	110 0.0001
242-271	#PDD26876	112 7e-05
244-283	#PDD1I220	106 0.0004
246-286	#PDC1J7X6	105 0.0006
254-293	#PD017880	205 4e-18
294-319	#PDB003F8	156 4e-11
296-319	#PDB6C0S6	133 7e-08

>**PDA1E662** (Closest domain: Q1R403_ECOUT 35-87)
Number of domains in family: 1878
Commentary (automatic):
KINASE ATP-BINDING GLYCOLYSIS FULL=6-PHOSPHOFRUCTOKINASE NUCLEOTIDE-BINDING EC=2.7.1.11 ALTNAME: RECNAME: FULL=PHOSPHOHEXOKINASE CYTOPLASM
Length = 53
Score = 265 (106.7 bits), Expect = 3e-26
Identities = 53/53 (100%), Positives = 53/53 (100%)

```
Query:     3 KKIGVLTSGGDAPGMNAAIRGVVRSALTEGLEVMGIYDGYLGLYEDRMVQLDR 55
           KKIGVLTSGGDAPGMNAAIRGVVRSALTEGLEVMGIYDGYLGLYEDRMVQLDR
Sbjct:    35 KKIGVLTSGGDAPGMNAAIRGVVRSALTEGLEVMGIYDGYLGLYEDRMVQLDR 87
```

>**PDA1N274** (Closest domain: D9SST4_CLOC7 86-189)
Number of domains in family: 31
Commentary (automatic):
KINASE SUBNAME: TRANSFERASE NUCLEOTIDE-BINDING ATP-BINDING GLYCOLYSIS CYTOPLASM FULL=PHOSPHOFRUCTOKINASE FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11
Length = 104
Score = 254 (102.4 bits), Expect = 4e-24
Identities = 49/97 (50%), Positives = 65/97 (67%)

```
Query:     76 EFRDENIRAVAIENLKKRGIDALVVIGGDGSYMGAMRLTEMGFPCIGLPGTIDNDIKGTD
135
           E  +++  VAIENLKK G+DA+VVIGGDG+  A  + G  IG+P TIDND+  T+
Sbjct:    92 EIVKKDVSDVAIENLKKEGVDAIVVIGGDGTLTSARDFSRKGINVIGVPKTIDNDLPATE 151

Query:    136 YTIGFFTALSTVVEAIDRLRDTSSSHQRISVVEVMGR 172
           T GF TA+    EA+DRL  T+ SH R+ ++EVMGR
Sbjct:    152 VTFGFNTAVEVATEALDRLHTTAESHHRVMLLEVMGR 188
```

>**PD814596** (Closest domain: K6PF_SHIBS 156-203)
Number of domains in family: 1391

Commentary (automatic):
KINASE ATP-BINDING FULL=6-PHOSPHOFRUCTOKINASE GLYCOLYSIS NUCLEOTIDE-BINDING ALTNAME: EC=2.7.1.11 RECNAME: FULL=PHOSPHOHEXOKINASE TRANSFERASE
Length = 48
Score = 245 (99.0 bits), Expect = 2e-23
Identities = 48/48 (100%), Positives = 48/48 (100%)

```
Query:   156 DTSSSHQRISVVEVMGRYCGDLTLAAAIAGGCEFVVVPEVEFSREDLV 203
             DTSSSHQRISVVEVMGRYCGDLTLAAAIAGGCEFVVVPEVEFSREDLV
Sbjct:   156 DTSSSHQRISVVEVMGRYCGDLTLAAAIAGGCEFVVVPEVEFSREDLV 203
```

>**PDC6E7U1** (Closest domain: A4MW46_HAEIF 1-53)
Number of domains in family: 36
Commentary (automatic):
ALTNAME: EC=2.7.1.11 KINASE NUCLEOTIDE-BINDING FULL=6-PHOSPHOFRUCTOKINASE ATP-BINDING TRANSFERASE RECNAME: GLYCOLYSIS FULL=PHOSPHOHEXOKINASE
Length = 53
Score = 223 (90.5 bits), Expect = 2e-20
Identities = 43/53 (81%), Positives = 48/53 (90%)

```
Query:    17 MNAAIRGVVRSALTEGLEVMGIYDGYLGLYEDRMVQLDRYSVSDMINRGGTFL 69
            MNAAIRGVVRSAL EGLEV GIYDGY GLY +++ QL+RYSVSD+INRGGTFL
Sbjct:     1 MNAAIRGVVRSALAEGLEVFGIYDGYQGLYNNKIKQLNRYSVSDVINRGGTFL 53
```

>**PD017880** (Closest domain: K6PF_ECOSM 254-293)
Number of domains in family: 1521
Commentary (automatic):
KINASE ATP-BINDING GLYCOLYSIS FULL=6-PHOSPHOFRUCTOKINASE NUCLEOTIDE-BINDING EC=2.7.1.11 CYTOPLASM MAGNESIUM ALTNAME: METAL-BINDING
Length = 40
Score = 205 (83.6 bits), Expect = 4e-18
Identities = 40/40 (100%), Positives = 40/40 (100%)

```
Query:   254 GGSPVPYDRILASRMGAYAIDLLLAGYGGRCVGIQNEQLV 293
             GGSPVPYDRILASRMGAYAIDLLLAGYGGRCVGIQNEQLV
Sbjct:   254 GGSPVPYDRILASRMGAYAIDLLLAGYGGRCVGIQNEQLV 293
```

>**PD000707** (Closest domain: F4MBD2_ECOLX 118-155)
Number of domains in family: 1359
Commentary (automatic):
KINASE ATP-BINDING FULL=6-PHOSPHOFRUCTOKINASE GLYCOLYSIS EC=2.7.1.11 ALTNAME: NUCLEOTIDE-BINDING RECNAME: FULL=PHOSPHOHEXOKINASE CYTOPLASM
Length = 38
Score = 197 (80.5 bits), Expect = 6e-17
Identities = 38/38 (100%), Positives = 38/38 (100%)

```
Query:   118 FPCIGLPGTIDNDIKGTDYTIGFFTALSTVVEAIDRLR 155
             FPCIGLPGTIDNDIKGTDYTIGFFTALSTVVEAIDRLR
Sbjct:   118 FPCIGLPGTIDNDIKGTDYTIGFFTALSTVVEAIDRLR 155
```

>**PDA1M1Q4** (Closest domain: E0QZ63_ECOLX 173-226)
Number of domains in family: 601
Commentary (automatic):
KINASE ATP-BINDING GLYCOLYSIS NUCLEOTIDE-BINDING FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11
CYTOPLASM MAGNESIUM ALTNAME: FULL=PHOSPHOHEXOKINASE
Length = 54
Score = 190 (77.8 bits), Expect = 9e-16
Identities = 38/54 (70%), Positives = 38/54 (70%)

Query: 173 YCGDLTLAAAIAGGCEFVVVPEVEFSREDLVNEXXXXXXXXXXXXXXXXXTEHMC 226
YCGDLTLAAAIAGGCEFVVVPEVEFSREDLVNE TEHMC
Sbjct: 173 YCGDLTLAAAIAGGCEFVVVPEVEFSREDLVNEIKAGIAKGKKHAIVAITEHMC 226

>**PDA1Z4Z4** (Closest domain: K6PF_ECOSM 120-155)
Number of domains in family: 487
Commentary (automatic):
KINASE ATP-BINDING NUCLEOTIDE-BINDING GLYCOLYSIS TRANSFERASE FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11 SUBNAME: ALTNAME: RECNAME:
Length = 36
Score = 184 (75.5 bits), Expect = 5e-15
Identities = 36/36 (100%), Positives = 36/36 (100%)

Query: 120 CIGLPGTIDNDIKGTDYTIGFFTALSTVVEAIDRLR 155
CIGLPGTIDNDIKGTDYTIGFFTALSTVVEAIDRLR
Sbjct: 120 CIGLPGTIDNDIKGTDYTIGFFTALSTVVEAIDRLR 155

>**PDC63680** (Closest domain: F0JXJ6_ESCFE 56-90)
Number of domains in family: 1491
Commentary (automatic):
KINASE ATP-BINDING FULL=6-PHOSPHOFRUCTOKINASE GLYCOLYSIS ALTNAME: EC=2.7.1.11
NUCLEOTIDE-BINDING RECNAME: FULL=PHOSPHOHEXOKINASE CYTOPLASM
Length = 35
Score = 181 (74.3 bits), Expect = 1e-14
Identities = 35/35 (100%), Positives = 35/35 (100%)

Query: 56 YSVSDMINRGGTFLGSARFPEFRDENIRAVAIENL 90
YSVSDMINRGGTFLGSARFPEFRDENIRAVAIENL
Sbjct: 56 YSVSDMINRGGTFLGSARFPEFRDENIRAVAIENL 90

>**PDB003C6** (Closest domain: G7RUM4_ECOC1 238-285)
Number of domains in family: 773
Commentary (automatic):
KINASE ATP-BINDING GLYCOLYSIS FULL=6-PHOSPHOFRUCTOKINASE NUCLEOTIDE-BINDING EC=2.7.1.11
CYTOPLASM MAGNESIUM ALTNAME: METAL-BINDING
Length = 48
Score = 172 (70.9 bits), Expect = 2e-13
Identities = 32/32 (100%), Positives = 32/32 (100%)

Query: 222 TEHMCDVDELAHFIEKETGRETRATVLGHIQR 253
TEHMCDVDELAHFIEKETGRETRATVLGHIQR

Sbjct: 254 TEHMCDVDELAHFIEKETGRETRATVLGHIQR 285

>**PDC65645** (Closest domain: K6PF_BACCQ 118-157)
Number of domains in family: 141
Commentary (automatic):
KINASE ATP-BINDING GLYCOLYSIS NUCLEOTIDE-BINDING FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11 CYTOPLASM ALTNAME: TRANSFERASE FULL=PHOSPHOHEXOKINASE
Length = 40
Score = 166 (68.6 bits), Expect = 2e-12
Identities = 29/40 (72%), Positives = 38/40 (95%)

Query: 119 PCIGLPGTIDNDIKGTDYTIGFFTALSTVVEAIDRLRDTS 158
PC+G+PGTIDNDI GTD+TIGF TAL+TV++AID++RDT+
Sbjct: 118 PCVGVPGTIDNDIPGTDFTIGFDTALNTVIDAIDKIRDTA 157

>**PDC8C8N0** (Closest domain: F0QYN6_VULM7 1-105)
Number of domains in family: 5
Commentary (automatic):
SUBNAME: KINASE NUCLEOTIDE-BINDING TRANSFERASE ATP-BINDING GLYCOLYSIS FULL=PYROPHOSPHATE-DEPENDENT FULL=6-PHOSPHOFRUCTOKINASE PHOSPHOFRUCTOKINASE PRECURSOR
Length = 105
Score = 162 (67.0 bits), Expect = 3e-11
Identities = 37/101 (36%), Positives = 58/101 (57%), Gaps = 1/101 (0%)

Query: 4 KIGVLTSGGDAPGMNAAIRGVVRSALTEGLEVMGIYDGYLGLYEDRMVQLDRYSVSDMIN 63
+IG+LT GGDAPG+N A+ + + L EV I+ G+ G+ + + ++ + D
Sbjct: 2 RIGILTGGGDAPGLNIAVYTLTK-LLERKHEVYAIFHGWRGILDKEVRRVTSKDLIDFAF 60

Query: 64 RGGTFLGSARFPEFRDENIRAVAIENLKKRGIDALVVIGGD 104
GGTF+ ++R F+DE NLK+ G+D +V IGGD
Sbjct: 61 TGGTFIRTSRTNPFKDEARVETFARNLKELGLDVIVAIGGD 101

>**PDB003F8** (Closest domain: K6PF_ECOSM 294-319)
Number of domains in family: 334
Commentary (automatic):
FULL=6-PHOSPHOFRUCTOKINASE ATP-BINDING ALTNAME: METAL-BINDING MAGNESIUM KINASE GLYCOLYSIS CYTOPLASM EC=2.7.1.11 FULL=PHOSPHOHEXOKINASE
Length = 26
Score = 156 (64.7 bits), Expect = 4e-11
Identities = 26/26 (100%), Positives = 26/26 (100%), Gaps = 1/26 (3%)

Query: 294 HHDIIDAIENMKRPFKGDWLDCAKKL 319
HHDIIDAIENMKRPFKGDWLDCAKKL
Sbjct: 294 HHDIIDAIENMKRPFKGDWLDCAKKL 319

>**PDA7Y619** (Closest domain: G8RQD0_MYCRN 258-293)

Number of domains in family: 314
Commentary (automatic):
ALTNAME: ATP-BINDING KINASE EC=2.7.1.11 NUCLEOTIDE-BINDING FULL=6-PHOSPHOFRUCTOKINASE TRANSFERASE RECNAME: GLYCOLYSIS FULL=PHOSPHOHEXOKINASE
Length = 36
Score = 136 (57.0 bits), Expect = 3e-08
Identities = 23/35 (65%), Positives = 28/35 (80%), Gaps = 1/35 (2%)

Query: 235 IEKETGRETRATVLGHIQRGGSPVPYDRILASRMG 269
+EK +E R TVLGH+QRGG+P PYDRILA+R G
Sbjct: 258 VEKRINKEVRVTVLGHVQRGGTPTPYDRILATRFG 292

>**PDA1L5G2** (Closest domain: F5Y7R7_TREAZ 10-81)
Number of domains in family: 63
Commentary (automatic):
SUBNAME: KINASE TRANSFERASE 1-PHOSPHOTRANSFERASE EC=2.7.1.90 PRECURSOR FLAGS: SIGNAL FULL=PHOSPHOFRUCTOKINASE FULL=PYROPHOSPHATE--FRUCTOSE-6-PHOSPHATE
Length = 72
Score = 136 (57.0 bits), Expect = 5e-08
Identities = 33/72 (45%), Positives = 43/72 (59%), Gaps = 1/72 (1%)

Query: 3 KKIGVLTSGGDAPGMNAAIRGVVRSALTE-GLEVMGIYDGYLGLYEDRMVQLDRYSVSDM 61
K G+LT+GGD PG+NAAIRGV R+A + +GI G+ GL E L S +
Sbjct: 10 KTFGILTAGGDCPGLNAAIRGVCRAAHDRYNMTALGIAYGFRGLIEGDSRVLSPDDFSGI 69

Query: 62 INRGGTFLGSAR 73
+ RGGT LG+ R
Sbjct: 70 LTRGGTILGAGR 81

>**PDB9B5J4** (Closest domain: B3QRP9_CHLT3 151-327)
Number of domains in family: 24
Commentary (automatic):
SUBNAME: KINASE TRANSFERASE REFERENCE FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11 FULL=PYROPHOSPHATE-DEPENDENT EC=2.7.1.90 PYROPHOSPHATE-DEPENDENT FULL=6-PHOSPHOFRUCTOKINASE
Length = 177
Score = 136 (57.0 bits), Expect = 2e-07
Identities = 48/165 (29%), Positives = 70/165 (42%), Gaps = 21/165 (12%)

Query: 7 VLTSGGDAPGMNAAIRGVVRSALTEGLEVMGIYDGYLGLYEDRMVQLDRYSVSDMINR-- 64
V+ GG APG N+ + G V +G+ L + R S + R
Sbjct: 157 VVQDGGCAPGYNSVTAFLTEFLEKSGRRVFAASEGFRSLVSGDLRDFRRVVYSGSLYRLI 216

Query: 65 ----------GGTFLGSARFPEFRDENIRAVAIENLKKRGIDALVVIGGDGSYMG 109
G S R+P+F++ + A EN+KKR + A++ IGGDG+ G
Sbjct: 217 EDFHGVVFTPPLREARGADFRSERYPDFKELENQKRAAENIKKRKVKAIIGIGGDGTLAG 276

Query: 110 AMRLTEM---GFPCIGLPGTIDNDIKGTDYTIGFFTALSTVVEAI 151
L E+ +P TID+DI GTD IG +T + E I
Sbjct: 277 MQSLGELLPDEIQMFFVPVTIDSDIYGTD-CIGQYTGVEVGAEKI 320

>**PDB6C0S6** (Closest domain: K6PF_KLEP3 296-319)
Number of domains in family: 314
Commentary (automatic):
KINASE FULL=6-PHOSPHOFRUCTOKINASE MAGNESIUM ATP-BINDING GLYCOLYSIS CYTOPLASM METAL-BINDING EC=2.7.1.11 NUCLEOTIDE-BINDING SHORT=PHOSPHOFRUCTOKINASE
Length = 24
Score = 133 (55.8 bits), Expect = 7e-08
Identities = 23/24 (95%), Positives = 23/24 (95%), Gaps = 1/24 (4%)

Query: 296 DIIDAIENMKRPFKGDWLDCAKKL 319
DIIDAIENMKRPFK DWLDCAKKL
Sbjct: 296 DIIDAIENMKRPFKNDWLDCAKKL 319

>**PDB002U4** (Closest domain: F4MBD2_ECOLX 229-253)
Number of domains in family: 372
Commentary (automatic):
KINASE ATP-BINDING FULL=6-PHOSPHOFRUCTOKINASE GLYCOLYSIS NUCLEOTIDE-BINDING EC=2.7.1.11 ALTNAME: FULL=PHOSPHOHEXOKINASE RECNAME: TRANSFERASE
Length = 25
Score = 129 (54.3 bits), Expect = 3e-07
Identities = 25/25 (100%), Positives = 25/25 (100%), Gaps = 2/25 (8%)

Query: 229 DELAHFIEKETGRETRATVLGHIQR 253
DELAHFIEKETGRETRATVLGHIQR
Sbjct: 229 DELAHFIEKETGRETRATVLGHIQR 253

>**PDB2C5T7** (Closest domain: D4IYH6_BUTFI 128-230)
Number of domains in family: 3
Commentary (automatic):
SUBNAME: FULL=PUTATIVE UNCHARACTERIZED FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11 REFERENCE TRANSFERASE KINASE
Length = 103
Score = 125 (52.8 bits), Expect = 3e-06
Identities = 34/96 (35%), Positives = 54/96 (56%), Gaps = 15/96 (15%)

Query: 121 IGLPGTIDNDIKGTDYTIGF-----FTALSTVVEAID-RLRDTSSSHQRISVVEVMGRYC 174
+G+P T+DND+ TD+T GF + A ST+ D ++ D S ++++EVMGR
Sbjct: 136 VGVPKTVDNDLCVTDHTPGFGSAAKYIATSTMEVIFDAQIYDNPS----VTIIEVMGRDA 191

Query: 175 GDLTLAAAIA-----GGCEFVVVPEVEFSREDLVNE 205
G LT A A+A G + + +PEV F R+ + +
Sbjct: 192 GWLTAATALAKNECCDGPDLIYLPEVPFDRDKFIED 227

>**PDD2A5S9** (Closest domain: K6PF_AQUAE 219-313)
Number of domains in family: 2
Commentary (automatic):
ENZYME METAL-BINDING MAGNESIUM SUBNAME: SHORT=PHOSPHOFRUCTOKINASE ALLOSTERIC FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11 ALTNAME: ATP-BINDING

Length = 95
Score = 124 (52.4 bits), Expect = 3e-06
Identities = 27/61 (44%), Positives = 37/61 (60%), Gaps = 3/61 (4%)

```
Query:  222 TEHMCDVDELAHFIEKETGR---ETRATVLGHIQRGGSPVPYDRILASRMGAYAIDLLLA 278
            E  C   EL  F+ ++ G    E R+TVLGHIQRGG P  +DRI+ ++ G  A + L+A
Sbjct:  221 AEGYCRAKELEDFLLEKIGDKYGEIRSTVLGHIQRGGIPTHFDRIMGTKFGVVAYESLIA 280

Query:  279 G 279
           G
Sbjct:  281 G 281
```

>**PDD34781** (Closest domain: Q8SSA3_ENCCU 494-703)
Number of domains in family: 2
Commentary (automatic):
NUCLEOTIDE-BINDING FULL=6-PHOSPHOFRUCTOKINASE TRANSFERASE ATP-BINDING KINASE SUBNAME: EC=2.7.1.11 ALTNAME: REFERENCE FULL=PHOSPHOHEXOKINASE
Length = 210
Score = 118 (50.1 bits), Expect = 8e-05
Identities = 32/101 (31%), Positives = 55/101 (54%), Gaps = 6/101 (5%)

```
Query:    4 KIGVLTSGGDAPGMNAAIRGVVRSALTEGLEVMGIYDGYLGLYEDRMVQLDRYSVSDMIN 63
           +IG++  G  + GMNAA+   V+ +L  G E   I +G+ GL   ++++   Y  S  +N
Sbjct:  594 RIGIMQFGQRSSGMNAALNAAVQYSLMVGAEPFYIPNGFEGLVNSQLIRPRLYEFSSDVN 653

Query:   64 RGGTFLGSARFPEFRDENIRAVAIE-NLKKRGIDALVVIGG 103
            GG+ +G       +E + A  I+  L +  +D+L+VIGG
Sbjct:  654 NGGSAIGVG-----SNEEVDAGLIQKKLDESKLDSLIVIGG 689
```

>**PD814606** (Closest domain: K6PF2_SYNY3 254-323)
Number of domains in family: 8
Commentary (automatic):
KINASE SUBNAME: ATP-BINDING NUCLEOTIDE-BINDING TRANSFERASE GLYCOLYSIS FULL=6-PHOSPHOFRUCTOKINASE FULL=PHOSPHOFRUCTOKINASE ALTNAME: CYTOPLASM
Length = 70
Score = 116 (49.3 bits), Expect = 3e-05
Identities = 22/55 (40%), Positives = 38/55 (69%), Gaps = 2/55 (3%)

```
Query:  222 TEHMCDVDELAHFIEKETGRETRATVLGHIQRGGSPVPYDRILASRMGAYAIDLL 276
           ++H+CD+ + A F +     + RAT LGH+QR G+P+ +DR+LA+  G  A++L+
Sbjct:  271 SQHLCDIKDPA-FCDL-ISLDIRATTLGHLQRSGTPLSFDRLLATVFGIRAVELI 323
```

>**PDC636Q6** (Closest domain: F4U1K6_ECOLX 94-117)
Number of domains in family: 921
Commentary (automatic):
KINASE FULL=6-PHOSPHOFRUCTOKINASE ATP-BINDING GLYCOLYSIS CYTOPLASM EC=2.7.1.11 NUCLEOTIDE-BINDING MAGNESIUM METAL-BINDING ALTNAME:

Length = 24
Score = 114 (48.5 bits), Expect = 3e-05
Identities = 24/24 (100%), Positives = 24/24 (100%), Gaps = 1/24 (4%)

```
Query:    94 GIDALVVIGGDGSYMGAMRLTEMG 117
            GIDALVVIGGDGSYMGAMRLTEMG
Sbjct:    94 GIDALVVIGGDGSYMGAMRLTEMG 117
```

>**PDB20112** (Closest domain: F6ENH8_AMYSD 101-139)
Number of domains in family: 113
Commentary (automatic):
SUBNAME: KINASE TRANSFERASE FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11 ATP-BINDING FULL=PHOSPHOFRUCTOKINASE GLYCOLYSIS NUCLEOTIDE-BINDING FULL=PUTATIVE
Length = 39
Score = 114 (48.5 bits), Expect = 3e-05
Identities = 22/39 (56%), Positives = 27/39 (69%), Gaps = 1/39 (2%)

```
Query:   101 IGGDGSYMGAMRLTEMGFPCIGLPGTIDNDIKGTDYTIG 139
           IGG+G+   A  L+E G P +G+P TIDNDI  TDYT G
Sbjct:   101 IGGEGTLTAAHWLSESGVPVVGVPKTIDNDIACTDYTFG 139
```

>**PDD26876** (Closest domain: F6B1J1_DELSC 252-296)
Number of domains in family: 2
Commentary (automatic):
SUBNAME: NUCLEOTIDE-BINDING DOMAIN-ASSOCIATED FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11 TRANSFERASE ATP-BINDING KINASE GLYCOLYSIS CYTOPLASM
Length = 45
Score = 112 (47.8 bits), Expect = 7e-05
Identities = 18/30 (60%), Positives = 24/30 (80%), Gaps = 1/30 (3%)

```
Query:   242 ETRATVLGHIQRGGSPVPYDRILASRMGAY 271
           E R TVLGH+QRGG P P+DR+LA++ G +
Sbjct:   267 EVRTTVLGHVQRGGDPTPFDRVLATQYGHH 296
```

>**PDD0K4X9** (Closest domain: C7QQX2_CYAP0 269-300)
Number of domains in family: 2
Commentary (automatic):
NUCLEOTIDE-BINDING METAL-BINDING MAGNESIUM SUBNAME: SHORT=PHOSPHOFRUCTOKINASE FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11 ALTNAME: REFERENCE ATP-BINDING
Length = 32
Score = 110 (47.0 bits), Expect = 0.0001
Identities = 22/32 (68%), Positives = 24/32 (75%), Gaps = 1/32 (3%)

```
Query:   235 IEKETGRETRATVLGHIQRGGSPVPYDRILAS 266
           I  +TG ETR TVLGHIQRGG P P DR+L S
Sbjct:   269 IALKTGAETRVTVLGHIQRGGMPSPVDRLLGS 300
```

>**PDC678Z0** (Closest domain: E0QZ63_ECOLX 151-172)

Number of domains in family: 80
Commentary (automatic):
KINASE ATP-BINDING GLYCOLYSIS NUCLEOTIDE-BINDING FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11 METAL-BINDING MAGNESIUM CYTOPLASM SHORT=PHOSPHOFRUCTOKINASE
Length = 22
Score = 107 (45.8 bits), Expect = 0.0003
Identities = 22/22 (100%), Positives = 22/22 (100%), Gaps = 1/22 (4%)

Query: 151 IDRLRDTSSSHQRISVVEVMGR 172
IDRLRDTSSSHQRISVVEVMGR
Sbjct: 151 IDRLRDTSSSHQRISVVEVMGR 172

>**PDD1I220** (Closest domain: B8HKT9_CYAP4 276-317)
Number of domains in family: 2
Commentary (automatic):
SUBNAME: NUCLEOTIDE-BINDING FULL=GP75 FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11 TRANSFERASE ATP-BINDING KINASE GLYCOLYSIS CYTOPLASM
Length = 42
Score = 106 (45.4 bits), Expect = 0.0004
Identities = 19/40 (47%), Positives = 29/40 (72%), Gaps = 3/40 (7%)

Query: 244 RATVLGHIQRGGSPVPYDRILASRMGAYAIDLLLAGYGGR 283
R +VLGHIQRGG P+ +DR++A+ G A+D+L+ G+
Sbjct: 277 RVSVLGHIQRGGIPLAFDRLMAAAFGKAAVDVLVPKISGQ 316

>**PDC1J7X6** (Closest domain: D1BMZ7_VEIPT 244-290)
Number of domains in family: 4
Commentary (automatic):
KINASE NUCLEOTIDE-BINDING METAL-BINDING MAGNESIUM SUBNAME: SHORT=PHOSPHOFRUCTOKINASE FULL=6-PHOSPHOFRUCTOKINASE EC=2.7.1.11 ALTNAME: ATP-BINDING
Length = 47
Score = 105 (45.1 bits), Expect = 0.0006
Identities = 21/41 (51%), Positives = 29/41 (70%), Gaps = 23/41 (56%)

Query: 246 TVLGHIQRGGSPVPYDRILASRMGAYAIDLLLAGYGGRCVG 286
TVLG++QRGG P +D ILA+RM ++LL++G R VG
Sbjct: 245 TVLGYLQRGGGPSAFDAILAARMSEACLNLLMSGVDNRLVG 285

>**PDC649Z0** (Closest domain: A7NKE6_ROSCS 510-549)
Number of domains in family: 183
Commentary (automatic):
ALTNAME: ATP-BINDING KINASE FULL=6-PHOSPHOFRUCTOKINASE NUCLEOTIDE-BINDING TRANSFERASE EC=2.7.1.11 FULL=PHOSPHOHEXOKINASE RECNAME: GLYCOLYSIS
Length = 40
Score = 104 (44.7 bits), Expect = 0.0008
Identities = 18/39 (46%), Positives = 30/39 (76%), Gaps = 23/39 (58%)

Query: 119 PCIGLPGTIDNDIKGTDYTIGFFTALSTVVEAIDRLRDT 157
P I LP +I+ND+ G++ +IG TAL+ +VEA+DR++ +
Sbjct: 511 PIICLPASINNDLPGSELSIGADTALNAIVEALDRIKQS 549

>**PDB1Q9A7** (Closest domain: K6PF_BACCQ 86-114)
Number of domains in family: 95
Commentary (automatic):
SUBNAME: TRANSFERASE KINASE EC=2.7.1.90 1-PHOSPHOTRANSFERASE ATP-BINDING GLYCOLYSIS NUCLEOTIDE-BINDING FULL=6-PHOSPHOFRUCTOKINASE PRECURSOR
Length = 29
Score = 104 (44.7 bits), Expect = 0.0008
Identities = 22/29 (75%), Positives = 24/29 (82%), Gaps = 23/29 (79%)

```
Query:    87 IENLKKRGIDALVVIGGDGSYMGAMRLTE 115
          IE LKK GI+ LVVIGGDGSY GA +LTE
Sbjct:    86 IEQLKKHGIEGLVVIGGDGSYQGAKKLTE 114
```

>**PDC64702** (Closest domain: K6PF_SHIBS 100-119)
Number of domains in family: 215
Commentary (automatic):
FULL=6-PHOSPHOFRUCTOKINASE KINASE EC=2.7.1.11 ATP-BINDING GLYCOLYSIS MAGNESIUM CYTOPLASM SHORT=PHOSPHOFRUCTOKINASE ALTNAME: FULL=PHOSPHOHEXOKINASE
Length = 20
Score = 102 (43.9 bits), Expect = 0.001
Identities = 20/20 (100%), Positives = 20/20 (100%), Gaps = 1/20 (5%)

```
Query:   100 VIGGDGSYMGAMRLTEMGFP 119
         VIGGDGSYMGAMRLTEMGFP
Sbjct:   100 VIGGDGSYMGAMRLTEMGFP 119
```

>**PDB7X7P1** (Closest domain: F0ZKK2_DICPU 515-561)
Number of domains in family: 6
Commentary (automatic):
NUCLEOTIDE-BINDING TRANSFERASE ATP-BINDING KINASE SUBNAME: FULL=6-PHOSPHOFRUCTOKINASE GLYCOLYSIS EC=2.7.1.11 ALTNAME: REFERENCE
Length = 47
Score = 102 (43.9 bits), Expect = 0.002
Identities = 18/47 (38%), Positives = 35/47 (74%), Gaps = 3/47 (6%)

```
Query:   122 GLPGTIDNDIKGTDYTIGFFTALSTVVEAIDRLRDTSSSHQRISVVE 168
         G PGTI N++ GT+ +IG  T+L+  ++A+D+++ ++ + +R+ VVE
Sbjct:   515 GAPGTIANNVPGTNISIGADTSLNNTLDALDKIKQSAVASRRLFVVE 561
```

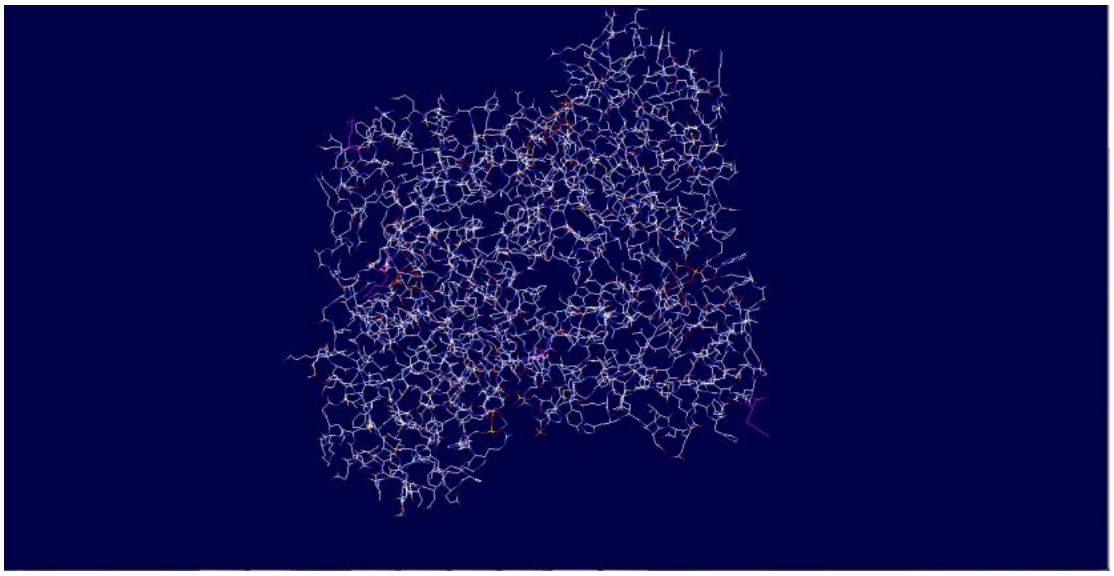
>**PDA0Y6P9** (Closest domain: E6WEH1_PANSA 151-241)
Number of domains in family: 20
Commentary (automatic):
NUCLEOTIDE-BINDING SUBNAME: TRANSFERASE ATP-BINDING KINASE GLYCOLYSIS CYTOPLASM FULL=PUTATIVE FULL=PHOSPHOFRUCTOKINASE 6-PHOSPHOFRUCTOKINASE
Length = 91
Score = 100 (43.1 bits), Expect = 0.004
Identities = 16/40 (40%), Positives = 29/40 (72%), Gaps = 23/40 (57%)

Query: 163 RISVVEVMGRYCGDLTLAAAIAGGCEFVVVPEVEFSREDL 202
R+ +VE++G YCG+LTL +AI +F ++PE + + ++L
Sbjct: 159 RVFMVELLGGYCGELTLQSAIKSNADFALIPECQIATQEL 198

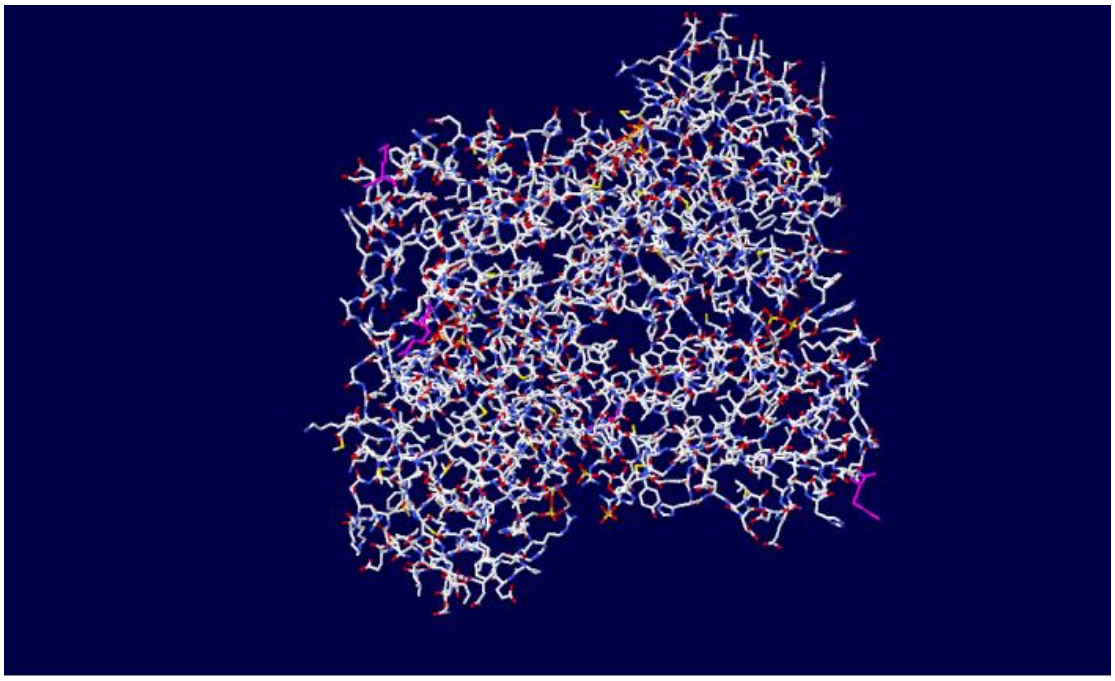
>**PDD08718** (Closest domain: Q09B24_STIAD 4-46)
Number of domains in family: 3
Commentary (automatic):
NUCLEOTIDE-BINDING FULL=6-PHOSPHOFRUCTOKINASE ATP-BINDING KINASE GLYCOLYSIS METAL-BINDING MAGNESIUM SHORT=PHOSPHOFRUCTOKINASE EC=2.7.1.11 ALTNAME:
Length = 43
Score = 100 (43.1 bits), Expect = 0.003
Identities = 20/43 (46%), Positives = 28/43 (65%), Gaps = 23/43 (53%)

Query: 28 ALTEGLEVMGIYDGYLGLYEDRMVQLDRYSVSDMINRGGTFLG 70
A G E+MG+ DG+ GL ED +L R + S +++RGGT LG
Sbjct: 4 ATEHGFEMMGLRDGWKGLLEDNHFRLTRETTSGILHRGGTILG 46

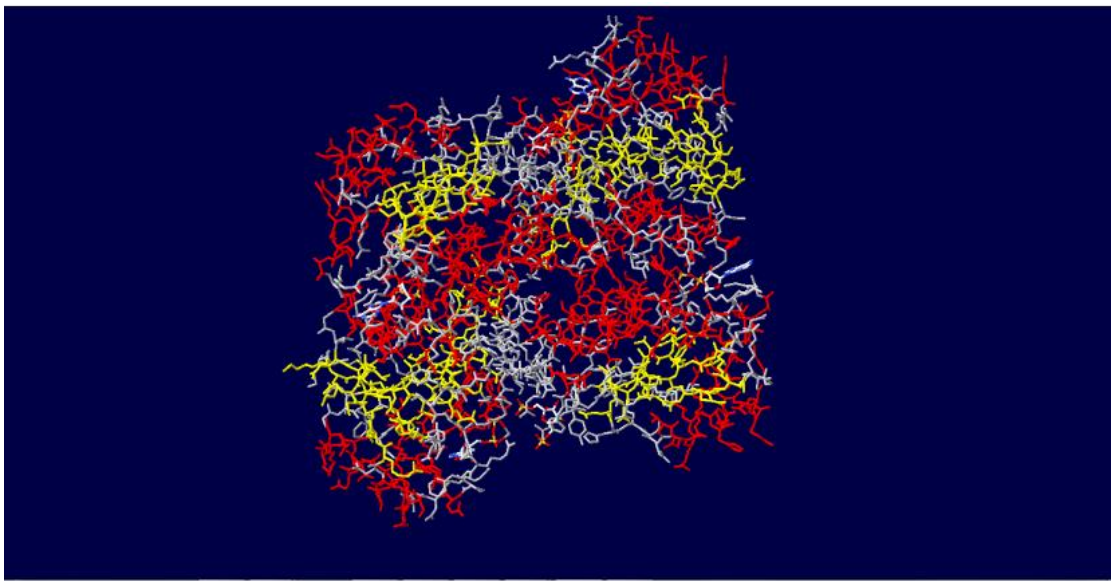
- **Από το πρόγραμμα SwissPdbViewer λαμβάνουμε την παρακάτω απεικόνιση της πρωτεΐνης 1PFK.pdb**



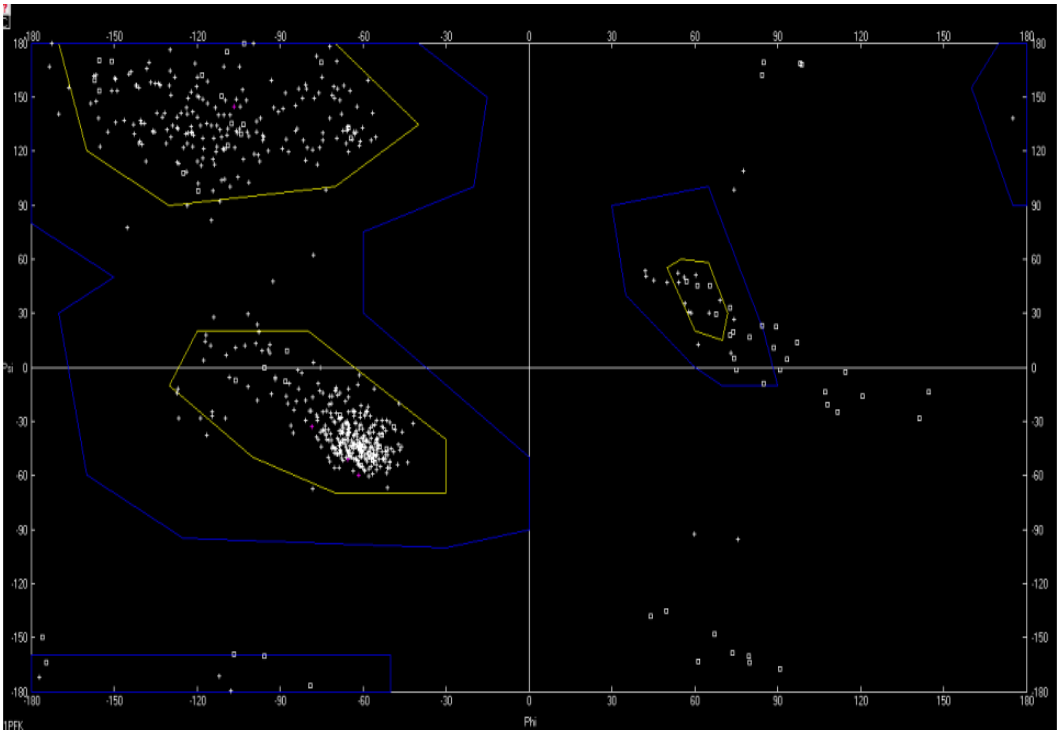
- **Μορφοποιώ την εικόνα με την επιλογή Render in Solid 3D:**



- **Χρωματίζω την πρωτεΐνη σύμφωνα με τη δευτεροταγή δομή της και έτσι εμφανίζονται με κίτρινο χρώμα τα β-φύλλα και με κόκκινο οι α-έλικες**



- **Τέλος εμφανίζω το Ramachandran plot και τα αμινοξέα που η περιστροφή των δεσμών γύρω από τον άνθρακα Ca δεν είναι επιτρεπτή.**



- **Τα αμινοξέα αυτά είναι τα εξής:**

Αλυσίδα Α

ILE1

GLY170

GLY40

GLY69

GLY254

GLY171

GLY15

GLY10

GLY138

GLY248

GLY278

GLY65

GLY212

Αλυσίδα Β

GLY 101

GLY15

GLY65

GLY69

GLY116

GLY10

GLY254

GLY138

GLY102

ILE1

GLY170

GLY132

GLY171

GLY278

GLY40

GLY212

GLY248