

Εργασία στη δομική βιοχημεία και στοιχεία βιοπληροφορικής

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1PFK:

**CRYSTAL STRUCTURE OF THE COMPLEX OF
PHOSPHOFRUCTOKINASE FROM ESCHERICHIA
COLI WITH ITS REACTION PRODUCTS**



1PFK

Από την *PDB* λαμβάνουμε τον κωδικό της πρωτεΐνης 1PFK ο οποίος είναι P0A796 και μέσω της *swiss prot* μπαίνουμε στην *expasy* όπου κάνουμε αναζήτηση βάσει κωδικού και επιλέγουμε από τα αποτελέσματα της αναζήτησης το *1hit* της *uniprot* το οποίο μας εμφανίζει μια σελίδα με στοιχεία για την συγκεκριμένη πρωτεΐνη όπως το *fasta* που επακολουθεί:

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
IGLPGTIDNDIKGTDYTI GFFFTALSTVVEAIDRLRDTSSSHQRI SVVEVMGRYCGDLTLA
AAIAGGCEFVVPEVEFSREDLVNEIKAGIAKGGKHAIVAITEHMC DVDELAHFIEKETG
RETRATVLGHIQRGGSPVPYDRILASRMGAY AIDL LLAGYGGRCVGIQNEQLVHHDIIDA
IENMKRPFKGDWLDCAKKLY
```

- Εισάγοντας το *fasta* της 1 φωσφοφρουκτοκινάσης στην αναζήτηση βάσει της αλληλουχίας του ενζύμου από την **ProtParam** λαμβάνουμε τα υποφανόμενα δεδομένα:

ProtParam

User-provided sequence:

```
      10      20      30      40      50      60
MIKKIGVLTSGGDAPGMNAAIRGVVRSALT EGGLEVMGIYD GYLGLYEDRM VQLDRYSVSD
      70      80      90     100     110     120
MINRGGTFLG SARFPEFRDE NIRAVAIENL KKR GIDALVV IGGDGSYMGÄ MRLTEMGFPC
     130     140     150     160     170     180
IGLPGTIDND IKGTDYTI GF FTALSTVVEA IDRLRDTSSS HQRI SVVEVM GRYCGDLTLA
     190     200     210     220     230     240
AAIAGGCEFV VVPEVEFSRE DLVNEIKAGI AKGGKHAIVA ITEHMC DVDE LAHFIEKETG
     250     260     270     280     290     300
RETRATVLGH IQRGGSPVPY DRILASRMGA YAIDL LLAGY GGRCVGIQNE QLVHHDIIDA
     310     320
IENMKRPFKG DWLDCAKKLY
```

References and documentation are available.

Number of amino acids: 320

Molecular weight: 34842.0

Theoretical pI: 5.47

Amino acid composition:

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: C₁₅₃₂H₂₄₅₈N₄₂₈O₄₆₂S₁₈

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

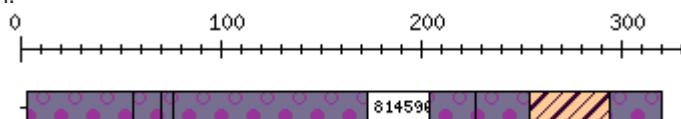
- Επίσης μέσω της επιλογής *proteomics* στην σελίδα του *expasy* μπορούμε και από το **ProDom** να αντλήσουμε πληροφορίες για την πρωτεΐνη, οι οποίες και παραθέτονται παρακάτω:

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
PDA1L5G2	3	73
PDB9B5J4	7	151
PDB6C0S6	296	319
PDB002U4	229	253
PDB2C5T7	121	205
PDD2A5S9	222	279
PDD34781	4	103
PD814606	222	276
PDC636Q6	94	117
PDB20112	101	139
PDD26876	242	271
PDD0K4X9	235	266
PDC678Z0	151	172
PDD1I220	244	283
PDC1J7X6	246	286
PDC649Z0	119	157
PDB1Q9A7	87	115
PDC64702	100	119
PDB7X7P1	122	168
PDA0Y6P9	163	202
PDD08718	28	70

Domain 3D modelling using Swiss-Model

Domain ID	BEGIN	END
PDA1E662	3	55

PD814596	156	203
PD017880	254	293
PD000707	118	155
PDA1M1Q4	173	226
PDA1Z4Z4	120	155
PDC63680	56	90
PDB003C6	222	253
PDC65645	119	158
PDB003F8	294	319
PDA7Y619	235	269
PDB002U4	229	253
PDC636Q6	94	117
PDC678Z0	151	172
PDB1Q9A7	87	115
PDC64702	100	119

Domain 3D modelling using Geno3D

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

PDA7Y619	235	269
PDB002U4	229	253
PDC636Q6	94	117
PDC678Z0	151	172
PDB1Q9A7	87	115
PDC64702	100	119

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

>**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 GGSPVPYDRILASRMGAY AIDLLLAGYGGRCVGIQNEQLV 293
GGSPVPYDRILASRMGAY AIDLLLAGYGGRCVGIQNEQLV
Sbjct: 254 GGSPVPYDRILASRMGAY AIDLLLAGYGGRCVGIQNEQLV 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 FPCIGLPGTIDNDIKGTDYTIGFF TALSTVVE AIDRLR 155
FPCIGLPGTIDNDIKGTDYTIGFF TALSTVVE AIDRLR
Sbjct: 118 FPCIGLPGTIDNDIKGTDYTIGFF TALSTVVE AIDRLR 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 YCGDLTLAAA IAGGCE FVVVPEVEFSREDLVNXXXXXXXXXXXXXXXXXXXXTEHMC
226
YCGDLTLAAA IAGGCE FVVVPEVEFSREDLVN TEHMC
Sbjct: 173 YCGDLTLAAA IAGGCE FVVVPEVEFSREDLVNEIKAGIAKGGKHAIVAITEHMC
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 CIGLPGTIDNDIKGTDYTIGFFFTALSTVVEAIDRLR 155
CIGLPGTIDNDIKGTDYTIGFFFTALSTVVEAIDRLR
Sbjct: 120 CIGLPGTIDNDIKGTDYTIGFFFTALSTVVEAIDRLR 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 RECNAM: 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 PCIGLPGTIDNDIKGTDYTIGFFFTALSTVVEAIDRLRDT 158
PC+G+PGTIDNDI GTD+TIGF TAL+TV++AID++RDT+
Sbjct: 118 PCVGVPGTIDNDIPGTDFDTIGFDTALNTVIDAIDKIRDTA 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-
LLERKHEVYAI FHGWRGILDKEVRRVTSKDLIDFAF 60

Query: 64 RGGTFLGSARFPEFRDENIRAVAIENLKKRGIDALVVIGGD 104
GGTF+ ++R F+DE NLK+ G+D +V IGGD
Sbjct: 61 TGGTFIRTSRTNPFKDEARVETFARNLKLGLDVIVAIGGD 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 RECNAM: 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 IEKETGRETRATVVLGHIQRGGSPVPYDRILASRMG 269
+EK +E R TVLGH+QRGG+P PYDRILA+R G
Sbjct: 258 VEKRINKEVRVTVLGHVQRGGTPTPYDRILATRF 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
VVQDGGCAPGYNVTAFLTEFLEKSGRRVFAASEGFRSLVSGDLRDFRRVVYSGSLYRLI 216

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

Query: 110 AMRLTEM---GFPCIGLPGTIDNDIKGTDYTGFFFTALSTVVEAI 151
L E+ +P TID+DI GTD IG +T + E I
Sbjct: 277 MQSLGELLPDEIQMFFVPTIDSDIYGTD-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 ALTNAM: FULL=PHOSPHOHEXOKINASE RECNAM: 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 IGLPGTIDNDIKGTDYTGIF-----FTALSTVVEAID-
RLRDTSSSHQRISVVEVMGRYC 174
+G+P T+DND+ TD+T GF + A ST+ D ++ D S
++++EVMGR

Sbjct: 136 VGVPKTVDNDLDCVTDHTPGFGSAAKYIATSTMEVIFDAQIYDNPS-----
VTIIEVMGRDA 191

Query: 175 GDLTLAAAIA-----GGCEFVVVPEVEFSREDLVNE 205
G LT A A+A G + + +PEV F R+ + +

Sbjct: 192 GWLTAATALAKNECCDGPDLIYLPVFPDRDKFIED 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+TVLGHQIRGG 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

RIGIMQFGQRSSGMNAAALNAAVQYSLMVGAEFPFYIPNGFEGLVNSQLIRPRLYEFSSDVN 653

Query: 64 RGGTFLGSARFPEFRDENIRAVAIE-NLKKRGIDALVVIGG 103

GG+ +G +E + A I+ L + +D+L+VIGG

Sbjct: 654 NGSAGVVG-----SNEEVDAGLIQKLDLDESKLDSLIVIGG 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-
ISLDIRATTLGHLQSRGTPLSFDRLLATVFGIRAVELI 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 IGGEGTLTAAHWLSESGVPVVGVPKTIDNDIACDITYTFG 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: C7QX2_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 TVLGH+QRGG P P DR+L S
Sbjct: 269 IALKTGAETRVTVLGH+QRGGMPSPVDRLG 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 IDRLRDTSSSSHQRISVVEVMGR 172
IDRLRDTSSSSHQRISVVEVMGR
Sbjct: 151 IDRLRDTSSSSHQRISVVEVMGR 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 RATVLGHIQRGGSPVPYDRILASRMGAYAIDLLLAGYGGGR 283
R +VLGHIQRGG P+ +DR++A+ G A+D+L+ G+
Sbjct: 277 RVSVLGHIQRGGIPLAFDRLMAAAFVKAAVDVLPKISGQ 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 ALTNAM:
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 TVLGYLQRGGPSAFDAILAARMSEACLNLLMSGVDNRLVG 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 RECNAM: 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 PCIGLPGTIDNDIKGTDYTGFFFTALSTVVEAIDRLRDT 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 GLPGTIDNDIKGTDYITIGFFFTALSTVVEAIDRLRDTSSSHQRISVVE 168
G PGTI N++ GT+ +IG T+L+ ++A+D+++ ++ + +R+ VVE
Sbjct: 515 GAPGTIANNVPGTNISIGADTSLNNTLDALDKIKQSAVASRRLFFVVE 561

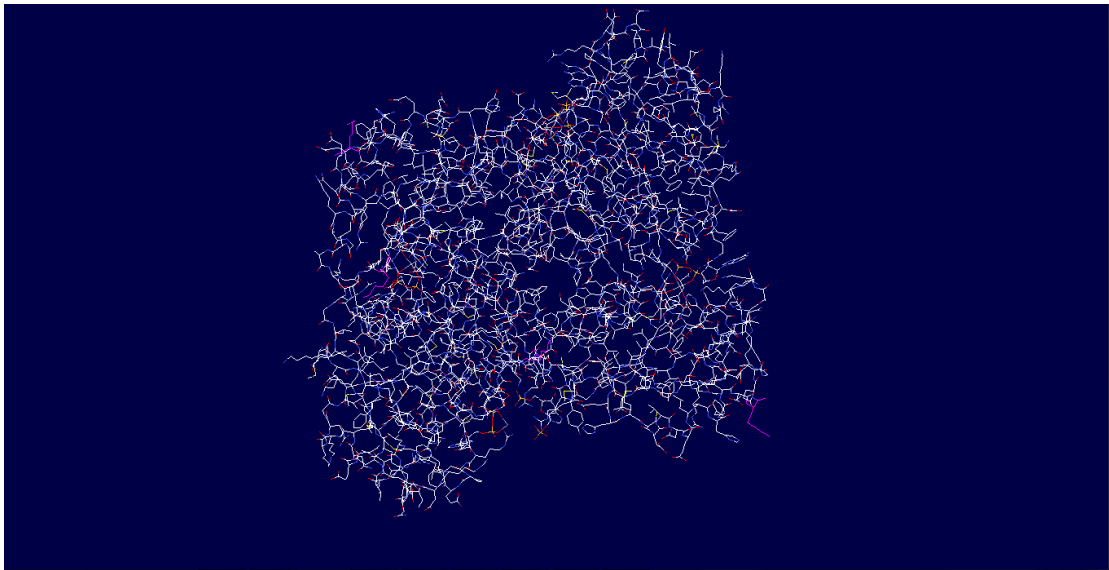
>**PDA0Y6P9** (Closest domain: E6WEH1_PANSA 151-241)
Number of domains in family: 20
Commentary (automatic):
NUCLEOTIDE-BINDING SUBNAME: TRANSFERASE ATP-BINDING KINASE GLYCOLYSIS
CYTOPLASM FULL=PUTATIVE FULL=PHOSPHOFRUCTOKINASE 6-PHOSPHOFRUCTOKINASE
Length = 91
Score = 100 (43.1 bits), Expect = 0.004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

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

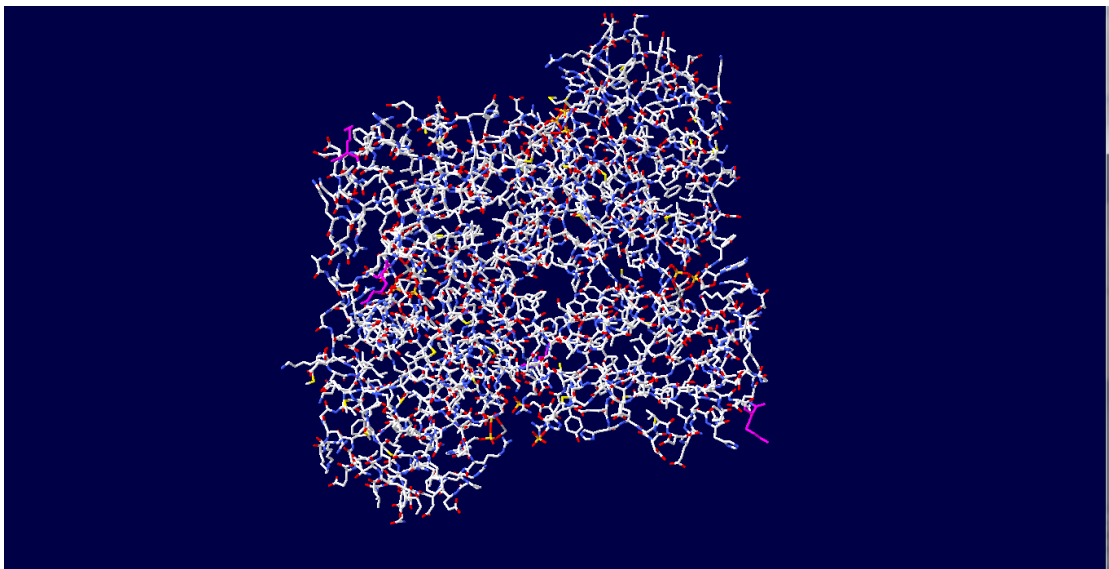
>**PDD08718** (Closest domain: Q09B24_STIAD 4-46)
Number of domains in family: 3
Commentary (automatic):
NUCLEOTIDE-BINDING FULL=6-PHOSPHOFRUCTOKINASE ATP-BINDING KINASE GLYCOLYSIS
METAL-BINDING MAGNESIUM SHORT=PHOSPHOFRUCTOKINASE EC=2.7.1.11 ALTNAME:
Length = 43
Score = 100 (43.1 bits), Expect = 0.003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

Οπτικοποιούμε το αρχείο της πρωτεΐνης (1PFK.pdb) μέσω του προγράμματος *Swiss-PdbViewer* και αρχικά λαμβάνουμε την παρακάτω απεικόνιση:

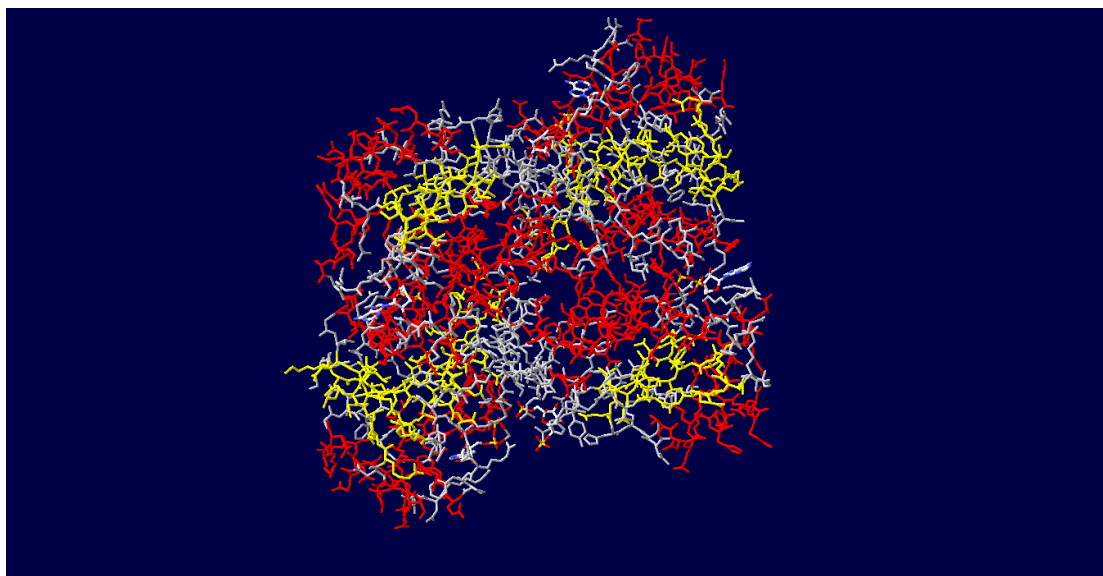


Επιλέγοντας από τη γραμμή εργαλείων το *Display* και έπειτα *Render in Solid 3D* λαμβάνουμε την παρακάτω εικόνα:

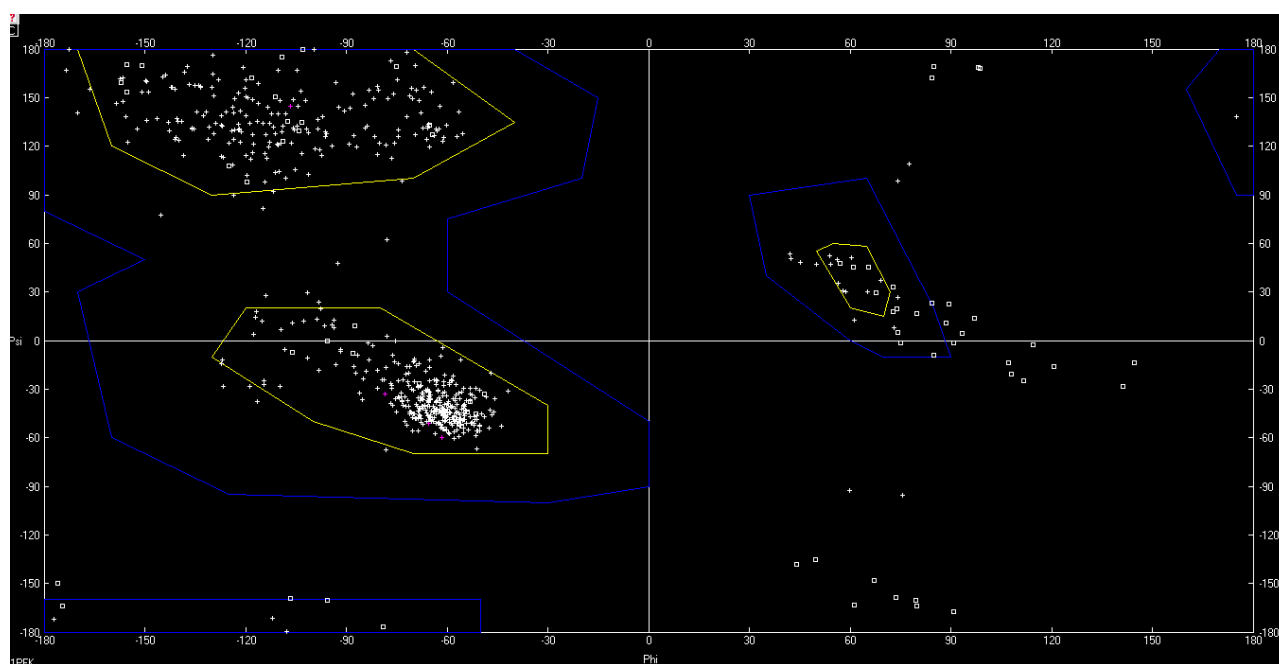


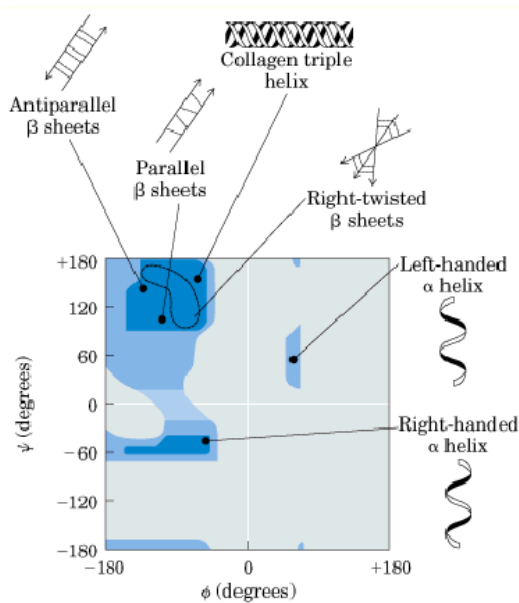
Ακόμα το πρόγραμμα μας δίνει την δυνατότητα να χρωματίσουμε την πρωτεΐνη με διαφορετικό τρόπο σύμφωνα με την δευτεροταγή δομή όπως φαίνεται παρακάτω

μέσω της επιλογής *Color* και ακολούθως *Secondary structure*, όπου με κίτρινο χρώμα εμφανίζονται τα β-φυλλά και με κόκκινο οι έλικες:



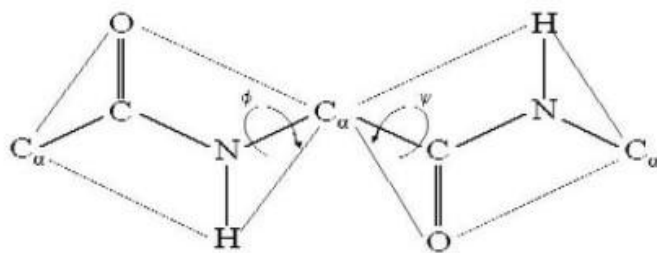
Μαρκάροντας όλα τα αμινοξέα που παρουσιάζονται στο *Control Panel* το οποίο υπάρχει ως υπο-επιλογή του *Window* μπορούμε να εμφανίσουμε το *Ramachandran plot* το οποίο μας γνωστοποιεί σε ποια αμινοξέα είναι επιτρεπτή η περιστροφή στην τελική μορφή της πρωτεΐνης. Ανάλογα λοιπόν με την περιοχή που εμφανίζεται το κάθε αμινοξύ μπορούμε να αντλήσουμε την συγκεκριμένη πληροφορία. Παρακάτω φαίνεται το *Ramachandran plot* για την 1PFK :





Στην εικόνα φαίνεται αναλυτικά ποιες είναι οι επιτρεπτές περιοχές του *Ramachandran plot* και τι διαμόρφωση παρουσιάζει σε κάθε σημείο η πεπτιδική αλυσίδα ανάλογα με την θέση των αμινοξέων, που βρίσκονται σ' αυτό, στο διάγραμμα .

Στον υποφαινόμενο πίνακα σημειώνονται όλα εκείνα τα αμινοξέα που η περιστροφή των δεσμών γύρω από τον άνθρακα C_{α} δεν είναι επιτρεπτή, δηλαδή τα αμινοξέα που βρίσκονται εκτός των χρωματισμένων περιοχών της παραπάνω απεικόνισης του *Ramachandran plot* για την 1



φωσφοφρουκτοκινάση. Πρέπει ακόμα να επισημανθεί ότι η γλυκίνη που είναι το αμινοξύ με την μικρότερη πλευρική ομάδα, μόνο ένα άτομο υδρογόνου, συνήθως λαμβάνει μη επιτρεπτές διαμορφώσεις ακριβώς εξαιτίας αυτού του χαρακτηριστικού της. Προφανώς επειδή το συγκεκριμένο ένζυμο αποτελείται από δύο ίδιες αλυσίδες είναι αναμενόμενο τα πιο πολλά αμινοξέα, των οποίων η περιστροφή δεν λαμβάνει επιτρεπτές διαμορφώσεις, να είναι κοινά και στις δυο όπως και διαπιστώθηκε τελικώς. Σε παρενθέσεις βρίσκονται μόνο κάποια αμινοξέα που δεν ήταν ξεκάθαρο αν βρίσκονται εντός των πλαισίων των περιοχών όπου η περιστροφή είναι επιτρεπτή.

Αλυσίδα A		Αλυσίδα B		
GLY69	GLY170	GLY 101	GLY15	GLY65
GLY254	GLY171	GLY69	GLY116	GLY10
ILE1	GLY40	GLY254	GLY138	(GLY102)
GLY132	GLY248	ILE1	GLY170	
GLY278	GLY65	GLY132	GLY171	
GLY15	GLY10	GLY278	GLY40	
GLY138	(GLY212)	GLY212	GLY248	

Εικόνες :

<http://www.huichun.tcu.edu.tw/MMP/Protein%20structure/doc/Protein%20Structure-46.htm>

<http://www.cerm.unifi.it/ramachandran-potentials>

<http://www.rcsb.org/pdb/explore/jmol.do?structureId=1PFK&bionumber=1>

Πηγή :

RCSB PDB: RCSB Protein Data Bank - <http://www.rcsb.org/pdb/home/home.do>