Λαγού Χρυσαφούλα-Ειρήνη, ΑΕΜ:8328

Εργασία Βιοπληροφορικής, κ. Χολή

1H6M

FASTA:

>sp|P00698|LYSC_CHICK Lysozyme C OS=Gallus gallus GN=LYZ PE=1 SV=1

MRSLLILVLCFLPLAALGKVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQA

TNRNTDGSTDYGILQINSRWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCAKKIVSDG

NGMNAWVAWRNRCKGTDVQAWIRGCRL

ProtParam:

User-provided sequence:

```
        10         20         30         40         50         60
MRSLLILVLC FLPLAALGKV FGRCELAAAM KRHGLDNYRG YSLGNWVCAA KFESNFNTQA

        70         80         90        100        110        120
TNRNTDGSTD YGILQINSRW WCNDGRTPGS RNLCNIPCSA LLSSDITASV NCAKKIVSDG

       130        140
NGMNAWVAWR NRCKGTDVQA WIRGCRL
```

References and documentation are available.

Number of amino acids: 147

Molecular weight: 16238.6

Theoretical pI: 9.36

Amino acid composition: CSV format

Ala (A)	14	9.5%
Arg (R)	12	8.2%
Asn (N)	14	9.5%
Asp (D)	7	4.8%
Cys (C)	9	6.1%
Gln (Q)	3	2.0%
Glu (E)	2	1.4%
Gly (G)	13	8.8%
His (H)	1	0.7%
Ile (I)	7	4.8%
Leu (L)	15	10.2%
Lys (K)	6	4.1%
Met (M)	3	2.0%
Phe (F)	4	2.7%
Pro (P)	3	2.0%
Ser (S)	11	7.5%
Thr (T)	7	4.8%
Trp (W)	6	4.1%
Tyr (Y)	3	2.0%
Val (V)	7	4.8%
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): 9

Total number of positively charged residues (Arg + Lys): 18

Atomic composition:

Carbon	C	705
Hydrogen	H	1116
Nitrogen	N	214
Oxygen	O	204
Sulfur	S	12

Formula: C705H1116N214O204S12

Total number of atoms: 2251

Extinction coefficients:

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

Ext. coefficient 37970

Abs 0.1% (=1 g/l) 2.338, assuming all pairs of Cys residues form cystines

Ext. coefficient   37470

Abs 0.1% (=1 g/l)   2.307, 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 19.86

This classifies the protein as stable.

Aliphatic index: 81.70

Grand average of hydropathicity (GRAVY): -0.150

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

PD000577

19

147

Υποβολή

PDC5E2N9

45

145

Υποβολή

PDC1J6J2

42

134

Υποβολή

Domain 3D modelling using Swiss-Model

Domain ID BEGIN END

PD000577

19

147

Υποβολή

Domain 3D modelling using Geno3D

Domain ID BEGIN END

PD000577

19

147

Υποβολή

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
        (147 letters)
PRODOM:
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


  19-147  #PD000577                               678 3e-89
  42-134  #PDC1J6J2                              180 2e-14
  45-145  #PDC5E2N9                               202 1e-17



>PD000577 (Closest domain: LYSC_CHICK 19-147)
Number of domains in family: 566
Commentary (automatic):
DISULFIDE BOND SUBNAME: FULL=LYSOZYME C RECNAME: ALTNAME: EC=3.2.1.17
GLYCOSIDASE PRECURSOR
Length = 129
Score = 678  (265.8 bits), Expect = 3e-89
Identities = 129/129 (100%), Positives = 129/129 (100%)
```

```
 Query:     19
KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINS 78

            KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINS

 Sbjct:     19
KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINS 78


 Query:     79
RWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGTDV 138

            RWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGTDV

 Sbjct:     79
RWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGTDV 138


 Query:    139 QAWIRGCRL 147

            QAWIRGCRL

 Sbjct:    139 QAWIRGCRL 147
```

>PDC5E2N9 (Closest domain: Q7Q6R2_ANOGA 366-501)

Number of domains in family: 2

Commentary (automatic):

SUBNAME: DISULFIDE BOND FULL=LYSOZYME FULL=AGAP005717-PA REFERENCE C-6

Length = 136

Score = 202 (82.4 bits), Expect = 1e-17

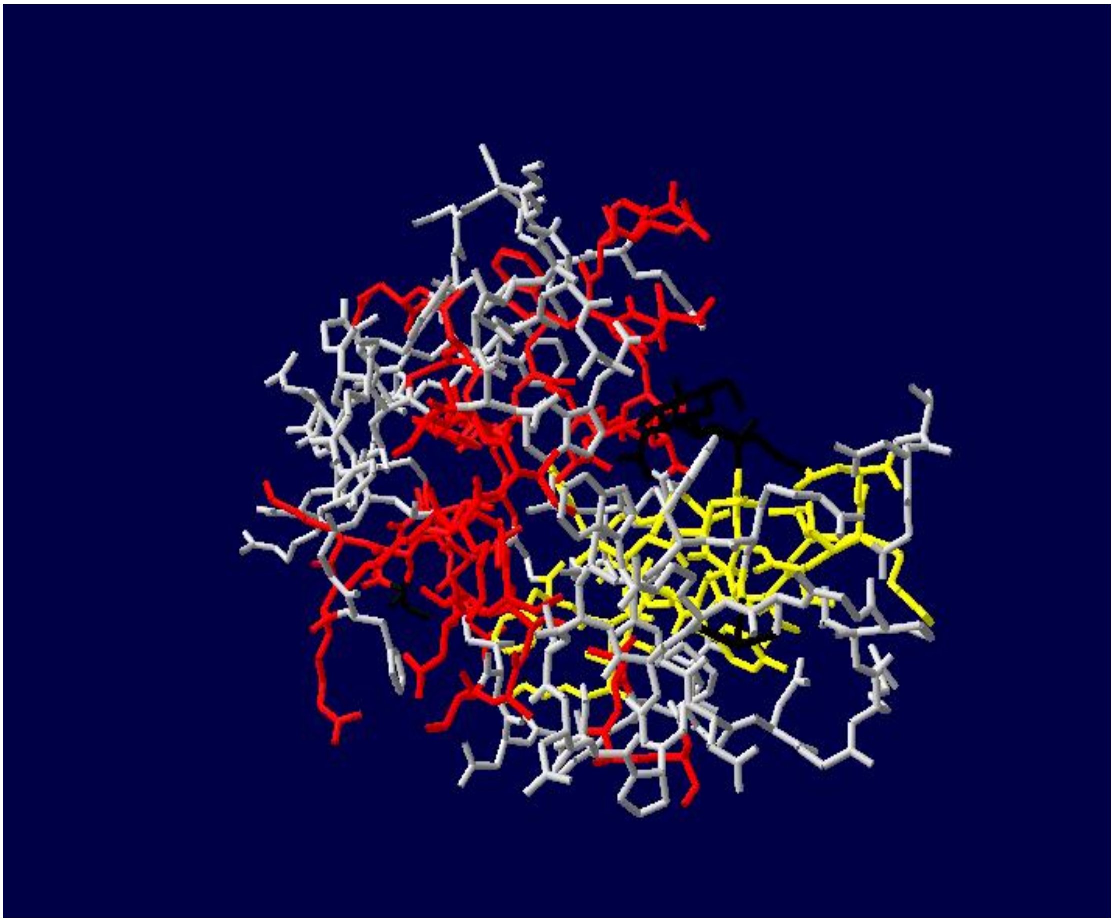
Identities = 44/107 (41%), Positives = 59/107 (55%), Gaps = 9/107 (8%)

```
 Query:     45 NWVCAAKFESNFNTQATNR-
NTDGSTDYGILQINSRWWCNDGRTPGSRNLCNIPCSALLS 103

              WVC A  ES FNT A  R N DGS D+G+ QI+  +WC+    PG+   C + C AL

 Sbjct:    366 TWVCIAYHESRFNTSAEGRLNADGSGDHGLFQISDIYWCS---PPGNGWACGVSCDALKD
422


 Query:    104 SDITASVNCAKKIVSD-----GNGMNAWVAWRNRCKGTDVQAWIRGC 145

             SDI+  V C K I  +     G+G NAW  ++  C+   V  ++RGC

 Sbjct:    423 SDISDDVQCVKTIYEEHQRLSGDGFNAWSVYKPYCQRDAVDTFVRGC 469
```

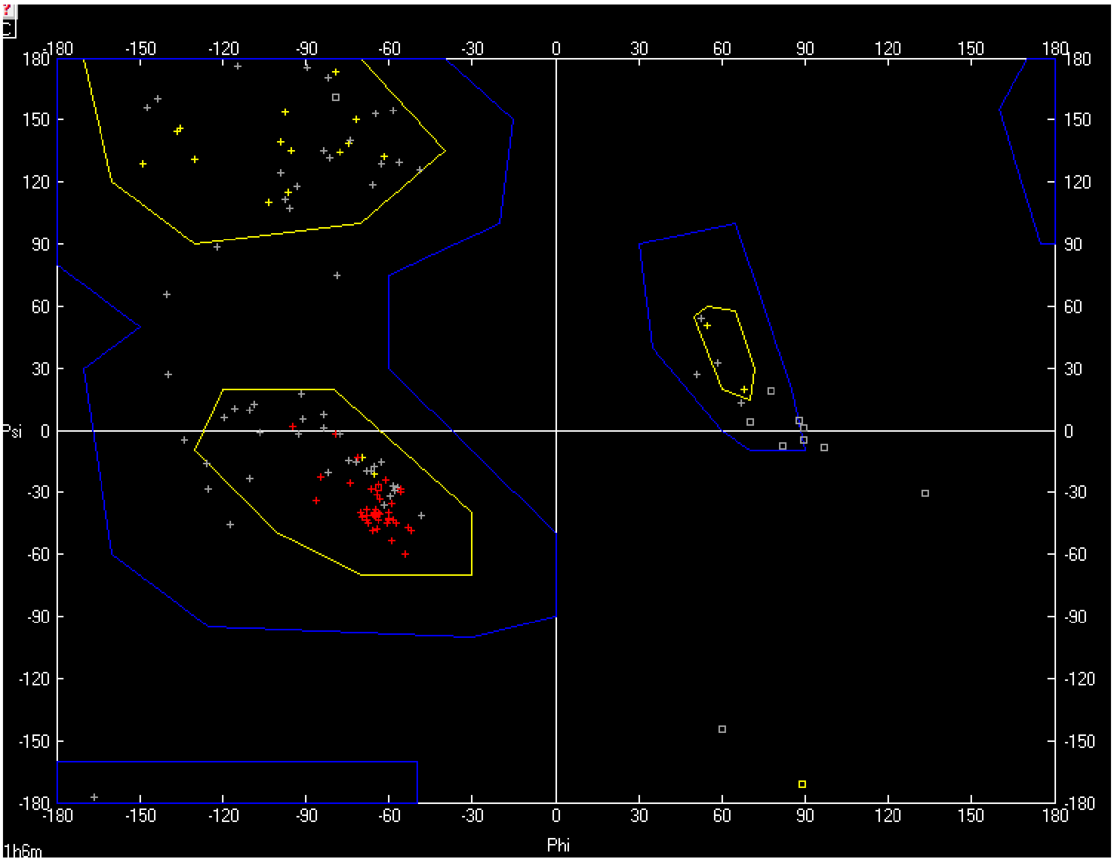
```
>PDC1J6J2 (Closest domain: B4IWP9_DROGR 949-1127)

Number of domains in family: 3

Commentary (automatic):

SUBNAME: DISULFIDE BOND FULL=GI13315 FULL=GH16162

Length = 179

Score = 180  (73.9 bits), Expect = 2e-14

Identities = 38/100 (38%), Positives = 55/100 (55%), Gaps = 10/100 (10%)


 Query:     42 SLGNWVCAAKFESNFNTQATNR-NTDGSTDYGILQINSRWWC-
NDGRTPGSRNLCNIPCS 99

              +  WVC A+ ES+++T A  R NTD S D+G+ QI+  +WC +DG    S   C+I C

 Sbjct:    960 EIPTWVCIAQHESSYSTAAVGRLNTDSSEDHGLFQISDLYWCTHDG---SSGKACHIECD
1016


 Query:    100 ALLSSDITASVNCAKKIVSD-----GNGMNAWVAWRNRCK 134
```

```
             LL SDI+  + C K I  +     G+G  AW  +   C+
Sbjct:   1017 RLLDSDISDDIECIKTIYKEHTRISGDGFTAWTVYNGHCR 1056
```

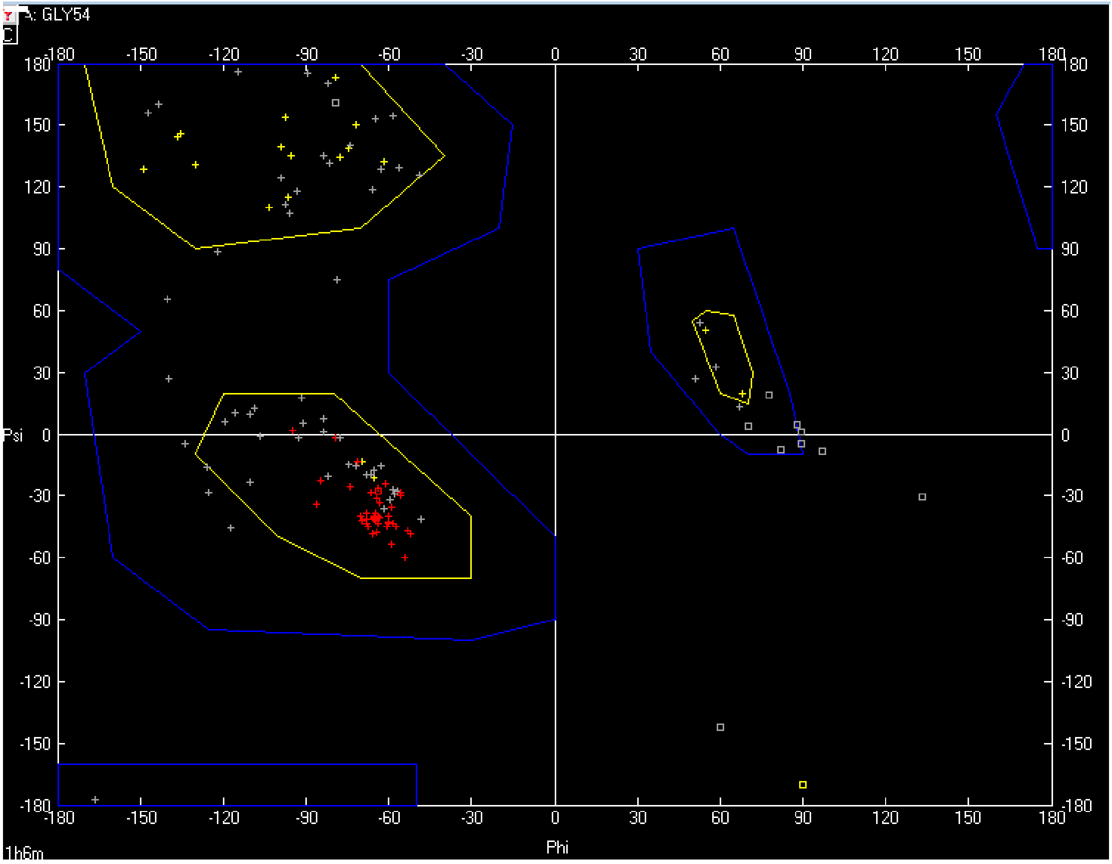
Rendered by 3D/Colored by secondary structrure

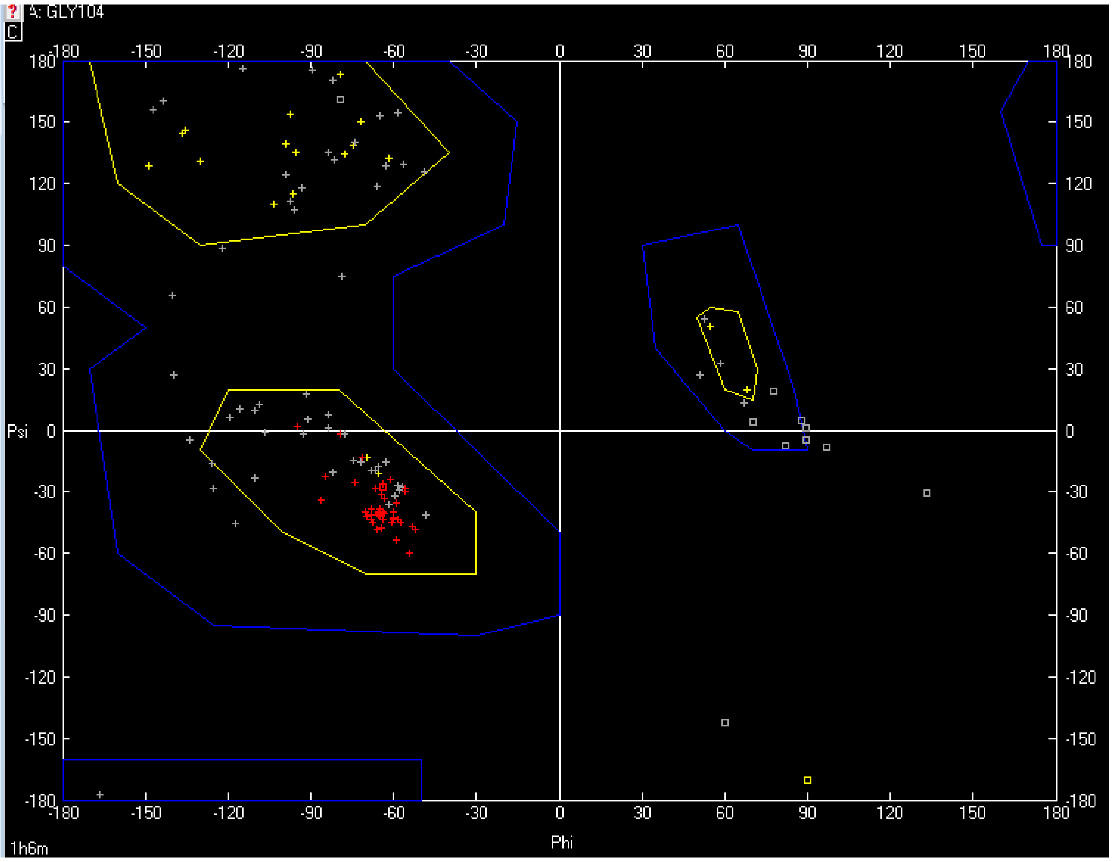


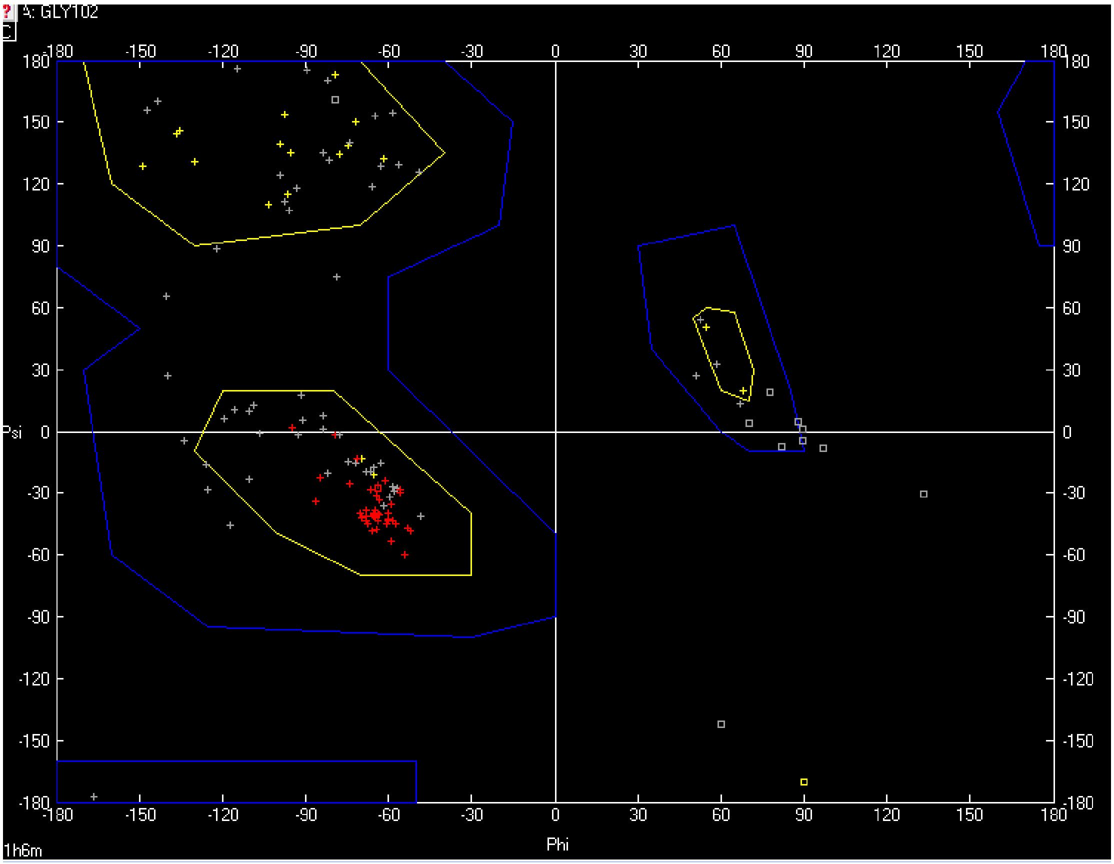
Ramachandran Plot



Αμινοξέα που εμφανίζονται εκτός επιτρεπτών ορίων: GLY54,GLY104,GLY102


A: GLY54
C
-180 -150 -120 -90 -60 -30 0 30 60 90 120 150 180
180 150 120 90 60 30 0 -30 -60 -90 -120 -150 -180
Psi
Phi
1h6m


A: GLY104
C
-180 -150 -120 -90 -60 -30 0 30 60 90 120 150 180
180 150 120 90 60 30 0 -30 -60 -90 -120 -150 -180
Psi
Phi
1h6m


?
A: GLY102
-180
-150
-120
-90
-60
-30
0
30
60
90
120
150
180
Psi
Phi
1h6m