ΑΣΚΗΣΗ ΒΙΟΠΛΗΡΟΦΟΡΙΚΉΣ

06/01/2016

ΛΕΟΝΙΔΗΣ ΓΕΩΡΓΙΟΣ 8329

2HHB protein

Subunit one:

```
>sp|P69905|HBA_HUMAN Hemoglobin subunit alpha OS=Homo sapiens GN=HBA1 PE=1
SV=2

MVLSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTTKTYFPHFDLSHGSAQVKGHG
KKVADALTNAVAHVDDMPNALSALSDLHAHKLRVDPVNFKLLSHCLLVTLAAHLPAEFTP
AVHASLDKFLASVSTVLTSKYR
```

Number of amino acids: 142

Molecular weight: 15257.5

Theoretical pI: 8.72

Amino acid composition:

```
Ala (A)  21     14.8%
Arg (R)   3      2.1%
Asn (N)   4      2.8%
Asp (D)   8      5.6%
Cys (C)   1      0.7%
Gln (Q)   1      0.7%
Glu (E)   4      2.8%
Gly (G)   7      4.9%
His (H)  10      7.0%
Ile (I)   0      0.0%
Leu (L)  18     12.7%
Lys (K)  11      7.7%
Met (M)   3      2.1%
Phe (F)   7      4.9%
Pro (P)   7      4.9%
Ser (S)  11      7.7%
Thr (T)   9      6.3%
Trp (W)   1      0.7%
Tyr (Y)   3      2.1%
Val (V)  13      9.2%
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): 12
Total number of positively charged residues (Arg + Lys): 14

Atomic composition:

```
Carbon      C          690
Hydrogen    H         1080
Nitrogen    N          188
Oxygen      O          195
Sulfur      S            4
```

Formula: $C_{690}H_{1080}N_{188}O_{195}S_4$
Total number of atoms: 2157

Extinction coefficients:

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

```
Ext. coefficient     9970
Abs 0.1% (=1 g/l)   0.653, assuming all pairs of Cys residues form cystines


Ext. coefficient     9970
Abs 0.1% (=1 g/l)   0.653, 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 6.97
This classifies the protein as stable.

Aliphatic index: 90.77

Grand average of hydropathicity (GRAVY): 0.048

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
        (142 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

      1-40  #PD820594                                             212 3e-20
      3-38  #PD859957                                             191 4e-17
      6-71  #PDA8N7E0                                              97 0.001
      6-76  #PD559047                                              97 0.001
     34-90  #PDA1I509                                             189 1e-16
     41-67  #PDA9Z7D9                                             140 7e-10
     43-68  #PDA9Z7D5                                             136 3e-09
     68-88  #PDB0N2Z0                                              99 0.0004
    70-100  #PD748724                                             155 5e-12
    89-111  #PD000377                                             115 2e-06
    92-141  #PD688662                                             194 2e-17
   102-141  #PD000054                                             193 2e-17
   113-141  #PDA1F6T7                                             141 5e-10
   114-141  #PDC64954                                             135 4e-09


>PD820594 (Closest domain: HBA_HUMAN 1-40)
Number of domains in family: 643
Commentary (automatic):
FULL=HEMOGLOBIN HEME IRON METAL-BINDING OXYGEN ALTNAME: SUBUNIT SUBNAME:
ALPHA CHAIN
Length = 40
Score = 212  (86.3 bits), Expect = 3e-20
Identities = 40/40 (100%), Positives = 40/40 (100%)

 Query:      1 MVLSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTT 40
               MVLSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTT
 Sbjct:      1 MVLSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTT 40




>PD688662 (Closest domain: HBPI_CHICK 91-141)
Number of domains in family: 19
Commentary (automatic):
```

```
HEME OXYGEN FULL=HEMOGLOBIN ALTNAME: METAL-BINDING IRON RECNAME: SUBNAME:
SEQUENCING DIRECT
Length = 51
Score = 194  (79.3 bits), Expect = 2e-17
Identities = 35/50 (70%), Positives = 44/50 (88%)

 Query:     92 LRVDPVNFKLLSHCLLVTLAAHLPAEFTPAVHASLDKFLASVSTVLTSKY 141
               LRVDPVNFKLLSHC+L ++AA  P++FTP VHA+ DKFL+S+S+VLT KY
 Sbjct:     92 LRVDPVNFKLLSHCILCSVAARYPSDFTPEVHAAWDKFLSSISSVLTEKY 141




>PD000054 (Closest domain: G3V1N2_HUMAN 70-109)
Number of domains in family: 776
Commentary (automatic):
FULL=HEMOGLOBIN ALTNAME: HEME IRON METAL-BINDING OXYGEN BETA SUBUNIT CHAIN
SUBNAME:
Length = 40
Score = 193  (79.0 bits), Expect = 2e-17
Identities = 40/40 (100%), Positives = 40/40 (100%)

 Query:    102 LSHCLLVTLAAHLPAEFTPAVHASLDKFLASVSTVLTSKY 141
               LSHCLLVTLAAHLPAEFTPAVHASLDKFLASVSTVLTSKY
 Sbjct:     70 LSHCLLVTLAAHLPAEFTPAVHASLDKFLASVSTVLTSKY 109




>PD859957 (Closest domain: HBA_PANTR 3-38)
Number of domains in family: 1137
Commentary (automatic):
FULL=HEMOGLOBIN HEME IRON METAL-BINDING OXYGEN ALTNAME: SUBUNIT SUBNAME: BETA
CHAIN
Length = 36
Score = 191  (78.2 bits), Expect = 4e-17
Identities = 36/36 (100%), Positives = 36/36 (100%)

 Query:      3 LSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFP 38
               LSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFP
 Sbjct:      3 LSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFP 38




>PDA1I509 (Closest domain: HBPI_CHICK 34-90)
Number of domains in family: 66
Commentary (automatic):
HEME OXYGEN SUBNAME: METAL-BINDING IRON RECNAME: ALTNAME: FULL=CYTOGLOBIN
FULL=HEMOGLOBIN REFERENCE
Length = 57
Score = 189  (77.4 bits), Expect = 1e-16
Identities = 33/57 (57%), Positives = 45/57 (78%)
```

```
 Query:     34 FLSFPTTKTYFPHFDLSHGSAQVKGHGKKVADALTNAVAHVDDMPNALSALSDLHAH 90
               F S+P TKTYFPHFD+S GS Q++GHG KV +A+  AV ++DD+  AL+ LS+LHA+
 Sbjct:     34 FASYPQTKTYFPHFDVSQGSVQLRGHGSKVLNAIGEAVKNIDDIRGALAKLSELHAY 90
```

```
>PD748724 (Closest domain: HBA_PANTR 70-100)
Number of domains in family: 1213
Commentary (automatic):
FULL=HEMOGLOBIN ALTNAME: HEME IRON METAL-BINDING OXYGEN SUBUNIT SUBNAME:
CHAIN BETA
Length = 31
Score = 155  (64.3 bits), Expect = 5e-12
Identities = 31/31 (100%), Positives = 31/31 (100%)

 Query:     70 AVAHVDDMPNALSALSDLHAHKLRVDPVNFK 100
               AVAHVDDMPNALSALSDLHAHKLRVDPVNFK
 Sbjct:     70 AVAHVDDMPNALSALSDLHAHKLRVDPVNFK 100
```

```
>PDA1F6T7 (Closest domain: HBA_PANPA 113-141)
Number of domains in family: 714
Commentary (automatic):
FULL=HEMOGLOBIN HEME IRON METAL-BINDING OXYGEN ALTNAME: SUBUNIT SUBNAME:
ALPHA CHAIN
Length = 29
Score = 141  (58.9 bits), Expect = 5e-10
Identities = 29/29 (100%), Positives = 29/29 (100%)

 Query:    113 HLPAEFTPAVHASLDKFLASVSTVLTSKY 141
               HLPAEFTPAVHASLDKFLASVSTVLTSKY
 Sbjct:    113 HLPAEFTPAVHASLDKFLASVSTVLTSKY 141
```

```
>PDA9Z7D9 (Closest domain: HBA_MACSP 40-66)
Number of domains in family: 713
Commentary (automatic):
FULL=HEMOGLOBIN HEME IRON METAL-BINDING OXYGEN SUBNAME: SUBUNIT ALTNAME:
ALPHA CHAIN
Length = 27
Score = 140  (58.5 bits), Expect = 7e-10
Identities = 27/27 (100%), Positives = 27/27 (100%)

 Query:     41 KTYFPHFDLSHGSAQVKGHGKKVADAL 67
               KTYFPHFDLSHGSAQVKGHGKKVADAL
 Sbjct:     40 KTYFPHFDLSHGSAQVKGHGKKVADAL 66
```

```
>PDA9Z7D5 (Closest domain: HBA_PANTR 43-68)
Number of domains in family: 931
Commentary (automatic):
FULL=HEMOGLOBIN ALTNAME: HEME IRON METAL-BINDING OXYGEN SUBUNIT BETA CHAIN
SUBNAME:
Length = 26
Score = 136  (57.0 bits), Expect = 3e-09
Identities = 26/26 (100%), Positives = 26/26 (100%)

 Query:     43 YFPHFDLSHGSAQVKGHGKKVADALT 68
               YFPHFDLSHGSAQVKGHGKKVADALT
 Sbjct:     43 YFPHFDLSHGSAQVKGHGKKVADALT 68
```

```
>PDC64954 (Closest domain: G7Q017_MACFA 114-141)
Number of domains in family: 191
Commentary (automatic):
FULL=HEMOGLOBIN METAL-BINDING IRON HEME OXYGEN SUBNAME: ALTNAME: SUBUNIT
ALPHA CHAIN
Length = 28
Score = 135  (56.6 bits), Expect = 4e-09
Identities = 28/28 (100%), Positives = 28/28 (100%)

 Query:    114 LPAEFTPAVHASLDKFLASVSTVLTSKY 141
               LPAEFTPAVHASLDKFLASVSTVLTSKY
 Sbjct:    114 LPAEFTPAVHASLDKFLASVSTVLTSKY 141
```

```
>PD000377 (Closest domain: HBA_ERIEU 88-110)
Number of domains in family: 544
Commentary (automatic):
FULL=HEMOGLOBIN IRON HEME METAL-BINDING OXYGEN SUBNAME: SUBUNIT ALPHA
ALTNAME: CHAIN
Length = 23
Score = 115  (48.9 bits), Expect = 2e-06
Identities = 23/23 (100%), Positives = 23/23 (100%), Gaps = 1/23 (4%)

 Query:     89 AHKLRVDPVNFKLLSHCLLVTLA 111
               AHKLRVDPVNFKLLSHCLLVTLA
 Sbjct:     88 AHKLRVDPVNFKLLSHCLLVTLA 110
```

```
>PDB0N2Z0 (Closest domain: HBA_CEBCA 67-87)
Number of domains in family: 90
Commentary (automatic):
```

```
FULL=HEMOGLOBIN ALTNAME: METAL-BINDING IRON HEME OXYGEN SUBUNIT ALPHA CHAIN
RECNAME:
Length = 21
Score = 99  (42.7 bits), Expect = 0.0004
Identities = 20/21 (95%), Positives = 21/21 (100%), Gaps = 1/21 (4%)

 Query:     68 TNAVAHVDDMPNALSALSDLH 88
               +NAVAHVDDMPNALSALSDLH
 Sbjct:     67 SNAVAHVDDMPNALSALSDLH 87




>PDA8N7E0 (Closest domain: E3TEM7_ICTPU 2-78)
Number of domains in family: 172
Commentary (automatic):
HEME OXYGEN METAL-BINDING IRON MUSCLE FULL=MYOGLOBIN RECNAME: SEQUENCING
DIRECT SUBNAME:
Length = 77
Score = 97  (42.0 bits), Expect = 0.001
Identities = 25/71 (35%), Positives = 36/71 (50%), Gaps = 5/71 (7%)

 Query:      6 ADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTTKTYFPHFDL-----SHGSAQVKGHG
60
               +D   V  +WG V A+    G E L R+F+  P T+ +FP FD      + G+  VK HG
 Sbjct:      2 SDFDTVLTSWGSVEANYAAIGGEVLGRLFVEHPETQKHFPKFDGISAADAAGNPAVKAHG
61

 Query:     61 KKVADALTNAV 71
               + V   L + V
 Sbjct:     62 ETVLKKLGDLV 72




>PD559047 (Closest domain: GLB2A_SCAIN 14-91)
Number of domains in family: 65
Commentary (automatic):
HEME OXYGEN ALTNAME: SUBNAME: IRON METAL-BINDING RECNAME: SEQUENCING DIRECT
FULL=GLOBIN
Length = 78
Score = 97  (42.0 bits), Expect = 0.001
Identities = 25/74 (33%), Positives = 37/74 (50%), Gaps = 3/74 (4%)

 Query:      6 ADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTTKTYFPHF-DLSHGSA--QVKGHGKK
62
               A K N++ +WG + A     G   +  +F   P TKTYF    D+  G A  +++GH
 Sbjct:     14 AIKANLRRSWGVLSADIEATGLMLMSNLFTLRPDTKTYFTRLGDVQKGKANSKLRGHAIT
73

 Query:     63 VADALTNAVAHVDD 76
               +  AL N V  +DD
 Sbjct:     74 LTYALNNFVDSLDD 87
```

Subunit two:

```
>sp|P68873|HBB_PANTR Hemoglobin subunit beta OS=Pan troglodytes GN=HBB PE=1
SV=2

MVHLTPEEKSAVTALWGKVNVDEVGGEALGRLLVVYPWTQRFFESFGDLSTPDAVMGNPK
VKAHGKKVLGAFSDGLAHLDNLKGTFATLSELHCDKLHVDPENFRLLGNVLVCVLAHHFG
KEFTPPVQAAYQKVVAGVANALAHKYH
```

Number of amino acids: 147

Molecular weight: 15998.4

Theoretical pI: 6.74

Amino acid composition:

```
Ala (A)  15      10.2%
Arg (R)   3       2.0%
Asn (N)   6       4.1%
Asp (D)   7       4.8%
Cys (C)   2       1.4%
Gln (Q)   3       2.0%
Glu (E)   8       5.4%
Gly (G)  13       8.8%
His (H)   9       6.1%
Ile (I)   0       0.0%
Leu (L)  18      12.2%
Lys (K)  11       7.5%
Met (M)   2       1.4%
Phe (F)   8       5.4%
Pro (P)   7       4.8%
Ser (S)   5       3.4%
Thr (T)   7       4.8%
Trp (W)   2       1.4%
Tyr (Y)   3       2.0%
Val (V)  18      12.2%
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): 15
Total number of positively charged residues (Arg + Lys): 14

Atomic composition:

```
Carbon      C         729
Hydrogen    H        1128
Nitrogen    N         196
Oxygen      O         202
```

Sulfur	S	4

Formula: $C_{729}H_{1128}N_{196}O_{202}S_4$
Total number of atoms: 2259

Extinction coefficients:

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

Ext. coefficient	15595
Abs 0.1% (=1 g/l)	0.975, assuming all pairs of Cys residues form cystines

Ext. coefficient	15470
Abs 0.1% (=1 g/l)	0.967, 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 6.16
This classifies the protein as stable.

Aliphatic index: 93.47

Grand average of hydropathicity (GRAVY): 0.014

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)

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

      1-18  #PDD359J6                                             90 0.008
      1-38  #PD859957                                            196 7e-18
      4-39  #PD820594                                            101 0.0002
     12-74  #PDA8N7E0                                            133 1e-08
     36-94  #PDA1I509                                            107 4e-05
     40-72  #PDA9Z7D5                                            172 2e-14
     54-78  #PD792899                                            100 0.002
    76-105  #PD748724                                            158 2e-12
    97-146  #PD688662                                            119 9e-07
   107-146  #PD000054                                            203 7e-19
   119-146  #PDC64954                                            110 1e-05

>PD000054 (Closest domain: HBB_PROLO 106-145)
Number of domains in family: 776
Commentary (automatic):
FULL=HEMOGLOBIN ALTNAME: HEME IRON METAL-BINDING OXYGEN BETA SUBUNIT CHAIN
SUBNAME:
Length = 40
Score = 203  (82.8 bits), Expect = 7e-19
Identities = 40/40 (100%), Positives = 40/40 (100%)

 Query:    107 LGNVLVCVLAHHFGKEFTPPVQAAYQKVVAGVANALAHKY 146
               LGNVLVCVLAHHFGKEFTPPVQAAYQKVVAGVANALAHKY
 Sbjct:   106 LGNVLVCVLAHHFGKEFTPPVQAAYQKVVAGVANALAHKY 145



>PD859957 (Closest domain: HBB_PANTR 1-38)
Number of domains in family: 1137
Commentary (automatic):
FULL=HEMOGLOBIN HEME IRON METAL-BINDING OXYGEN ALTNAME: SUBUNIT SUBNAME: BETA
CHAIN
Length = 38
Score = 196  (80.1 bits), Expect = 7e-18
Identities = 38/38 (100%), Positives = 38/38 (100%)

 Query:      1 MVHLTPEEKSAVTALWGKVNVDEVGGEALGRLLVVYPW 38
               MVHLTPEEKSAVTALWGKVNVDEVGGEALGRLLVVYPW
 Sbjct:      1 MVHLTPEEKSAVTALWGKVNVDEVGGEALGRLLVVYPW 38



>PDA9Z7D5 (Closest domain: HBB_PANTR 40-72)
Number of domains in family: 931
Commentary (automatic):
```

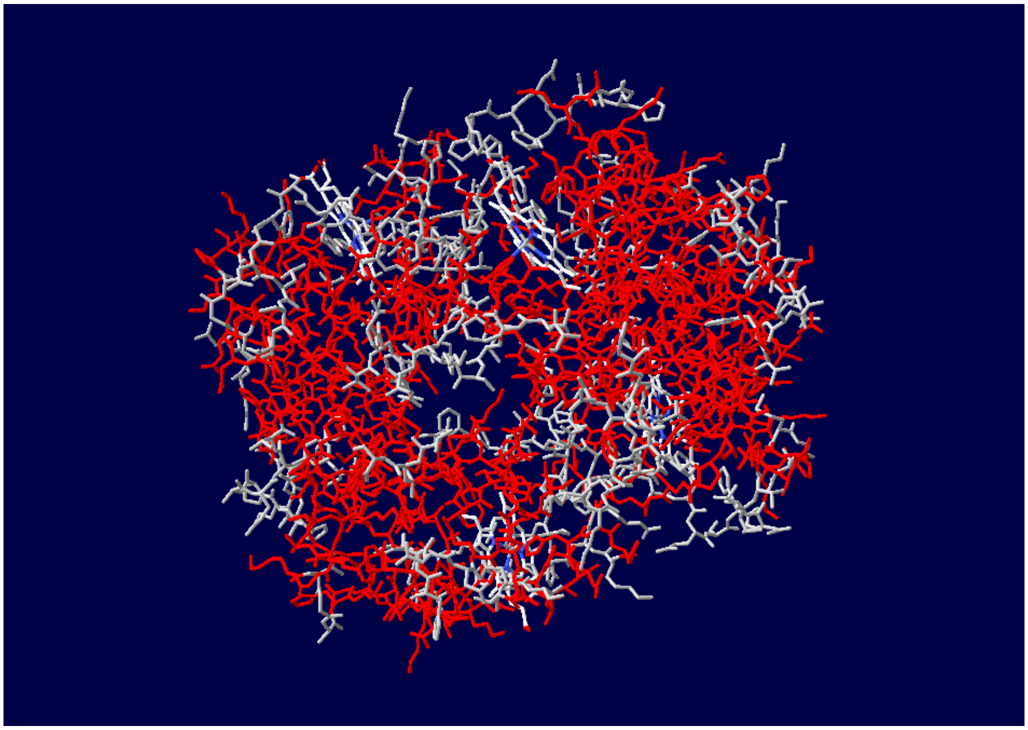
```
FULL=HEMOGLOBIN ALTNAME: HEME IRON METAL-BINDING OXYGEN SUBUNIT BETA CHAIN
SUBNAME:
Length = 33
Score = 172  (70.9 bits), Expect = 2e-14
Identities = 33/33 (100%), Positives = 33/33 (100%), Gaps = 4/33 (12%)

 Query:     40 QRFFESFGDLSTPDAVMGNPKVKAHGKKVLGAF 72
               QRFFESFGDLSTPDAVMGNPKVKAHGKKVLGAF
 Sbjct:     40 QRFFESFGDLSTPDAVMGNPKVKAHGKKVLGAF 72




>PD748724 (Closest domain: D9YZU5_HUMAN 76-105)
Number of domains in family: 1213
Commentary (automatic):
FULL=HEMOGLOBIN ALTNAME: HEME IRON METAL-BINDING OXYGEN SUBUNIT SUBNAME:
CHAIN BETA
Length = 30
Score = 158  (65.5 bits), Expect = 2e-12
Identities = 30/30 (100%), Positives = 30/30 (100%), Gaps = 4/30 (13%)

 Query:     76 LAHLDNLKGTFATLSELHCDKLHVDPENFR 105
               LAHLDNLKGTFATLSELHCDKLHVDPENFR
 Sbjct:     76 LAHLDNLKGTFATLSELHCDKLHVDPENFR 105




>PDA8N7E0 (Closest domain: E3TEM7_ICTPU 2-78)
Number of domains in family: 172
Commentary (automatic):
HEME OXYGEN METAL-BINDING IRON MUSCLE FULL=MYOGLOBIN RECNAME: SEQUENCING
DIRECT SUBNAME:
Length = 77
Score = 133  (55.8 bits), Expect = 1e-08
Identities = 32/65 (49%), Positives = 37/65 (56%), Gaps = 3/65 (4%)

 Query:     12 VTALWGKV--NVDEVGGEALGRLLVVYPWTQRFFESFGDLSTPDAVMGNPKVKAHGKKVL
69
               V   WG V  N   +GGE LGRL V +P TQ+ F  F  +S  DA  GNP VKAHG+ VL
 Sbjct:      7 VLTSWGSVEANYAAIGGEVLGRLFVEHPETQKHFPKFDGISAADAA-GNPAVKAHGETVL
65

 Query:     70 GAFSD 74
                   D
 Sbjct:     66 KKLGD 70




>PD688662 (Closest domain: HBPI_CHICK 91-141)
Number of domains in family: 19
Commentary (automatic):
```

```
HEME OXYGEN FULL=HEMOGLOBIN ALTNAME: METAL-BINDING IRON RECNAME: SUBNAME:
SEQUENCING DIRECT
Length = 51
Score = 119  (50.4 bits), Expect = 9e-07
Identities = 20/50 (40%), Positives = 33/50 (66%), Gaps = 3/50 (6%)

 Query:     97 LHVDPENFRLLGNVLVCVLAHHFGKEFTPPVQAAYQKVVAGVANALAHKY 146
               L VDP NF+LL + ++C +A  +  +FTP V AA+ K ++ +++ L  KY
 Sbjct:     92 LRVDPVNFKLLSHCILCSVAARYPSDFTPEVHAAWDKFLSSISSVLTEKY 141




>PDC64954 (Closest domain: Q03903_MACMU 119-146)
Number of domains in family: 191
Commentary (automatic):
FULL=HEMOGLOBIN METAL-BINDING IRON HEME OXYGEN SUBNAME: ALTNAME: SUBUNIT
ALPHA CHAIN
Length = 28
Score = 110  (47.0 bits), Expect = 1e-05
Identities = 20/28 (71%), Positives = 26/28 (92%), Gaps = 2/28 (7%)

 Query:    119 FGKEFTPPVQAAYQKVVAGVANALAHKY 146
               FGKEFTP VQA++QK+VAGVA+AL+ +Y
 Sbjct:    119 FGKEFTPEVQASWQKMVAGVASALSSRY 146




>PDA1I509 (Closest domain: HBPI_CHICK 34-90)
Number of domains in family: 66
Commentary (automatic):
HEME OXYGEN SUBNAME: METAL-BINDING IRON RECNAME: ALTNAME: FULL=CYTOGLOBIN
FULL=HEMOGLOBIN REFERENCE
Length = 57
Score = 107  (45.8 bits), Expect = 4e-05
Identities = 21/59 (35%), Positives = 34/59 (57%), Gaps = 6/59 (10%)

 Query:     36 YPWTQRFFESFGDLSTPDAVMGNPKVKAHGKKVLGAFSDGLAHLDNLKGTFATLSELHC 94
               YP T+ +F  F      D   G+ +++ HG KVL A  + + ++D+++G  A LSELH
 Sbjct:     37 YPQTKTYFPHF------DVSQGSVQLRGHGSKVLNAIGEAVKNIDDIRGALAKLSELHA 89




>PD820594 (Closest domain: C0H805_SALSA 93-132)
Number of domains in family: 643
Commentary (automatic):
FULL=HEMOGLOBIN HEME IRON METAL-BINDING OXYGEN ALTNAME: SUBUNIT SUBNAME:
ALPHA CHAIN
Length = 40
Score = 101  (43.5 bits), Expect = 0.0002
Identities = 21/38 (55%), Positives = 24/38 (63%), Gaps = 2/38 (5%)
```

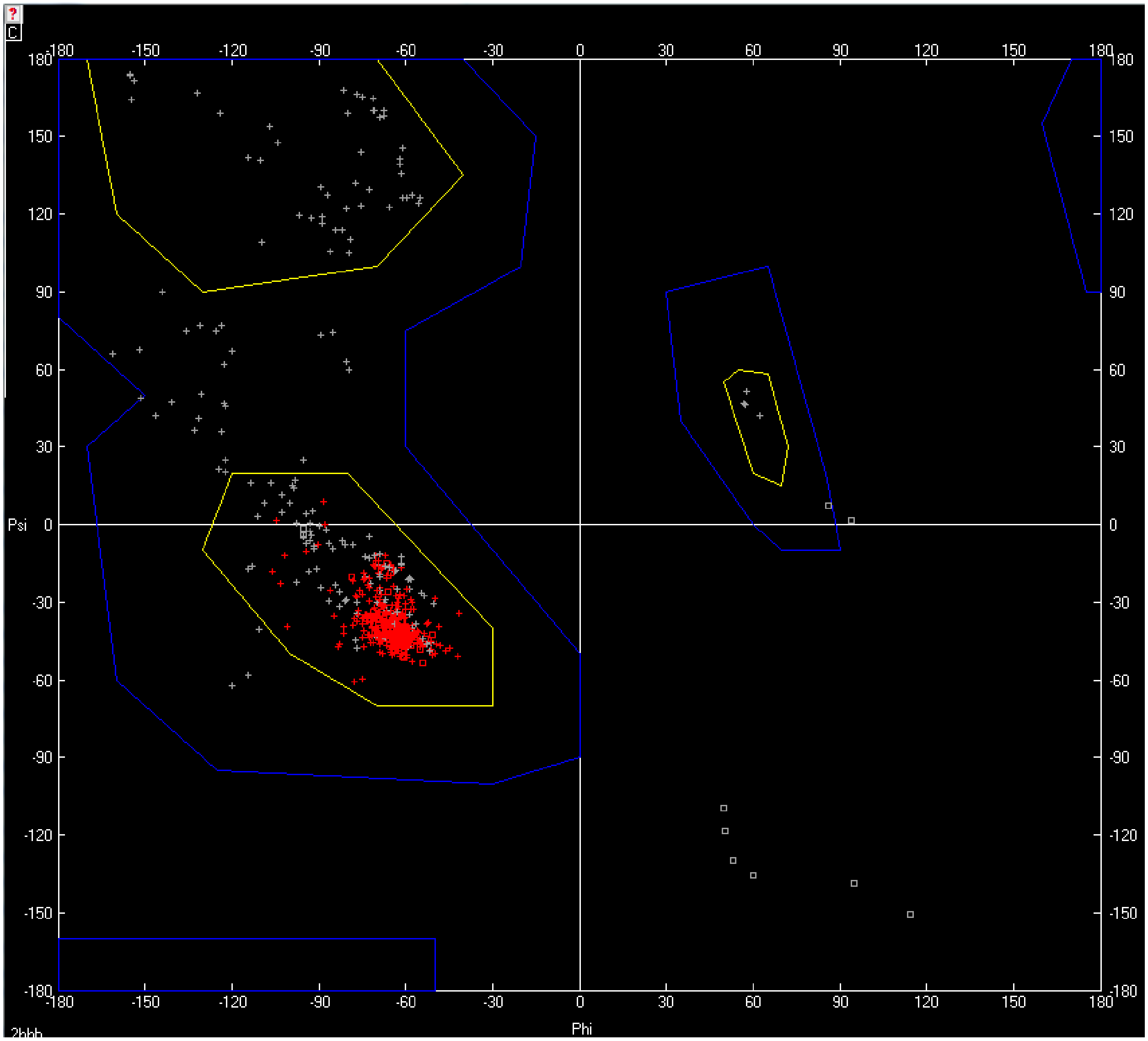
```
 Query:      4 LTPEEKSAVTALWGKVN--VDEVGGEALGRLLVVYPWT 39
               LT  +KS V A WGK+    D VG EALGR+L  YP T
 Sbjct:     95 LTARDKSVVNAFWGKIKGKADVVGAEALGRMLTAYPQT 132
```

```
>PD792899 (Closest domain: Q86QI8_PLABE 1-159)
Number of domains in family: 1
Commentary (automatic):
HEME OXYGEN SUBNAME: ANTIGEN FULL=31
Length = 159
Score = 100  (43.1 bits), Expect = 0.002
Identities = 19/25 (76%), Positives = 22/25 (88%), Gaps = 2/25 (8%)

 Query:     54 AVMGNPKVKAHGKKVLGAFSDGLAH 78
               A+MGN KVKAHGKKV+ AF+DGL H
 Sbjct:    135 AIMGNAKVKAHGKKVITAFNDGLNH 159
```

```
>PDD359J6 (Closest domain: Q2XP30_HUMAN 1-22)
Number of domains in family: 1
Commentary (automatic):
BETA-GLOBIN SUBNAME: FULL=MUTANT
Length = 22
Score = 90  (39.3 bits), Expect = 0.008
Identities = 17/18 (94%), Positives = 18/18 (100%), Gaps = 3/18 (16%)

 Query:      1 MVHLTPEEKSAVTALWGK 18
               MVHLTPEEKSAVTALWG+
 Sbjct:      1 MVHLTPEEKSAVTALWGQ 18
```



RAMACHANDRAN PLOT OF 2HHB:



Τα αμινοξέα που δεν στρέφουν την δευτεροταγή δομή καθώς δεν μπορούν να κινηθούν λόγο παρεμποδίσεων είναι: CGLY51, AGLY18, CGLY18, BGLY119, DGLY119, BGLY46 και τέλος το DGLY46.

Παρ όλα αυτά γνωρίζουμε ότι η γλυκίνη είναι το αμινοξύ που δεν έχει πλευρική ομάδα, και αρά δεν προκαλεί παρεμποδίσεις σε άλλα αμινοξέα, και έτσι βρίσκεται σε στροφές μιας πρωτεΐνης.