SWISS-MODEL Workspace

Workunit: P000001
Title:CS697 HW2 1B

Model Details: Batch.1

model pic

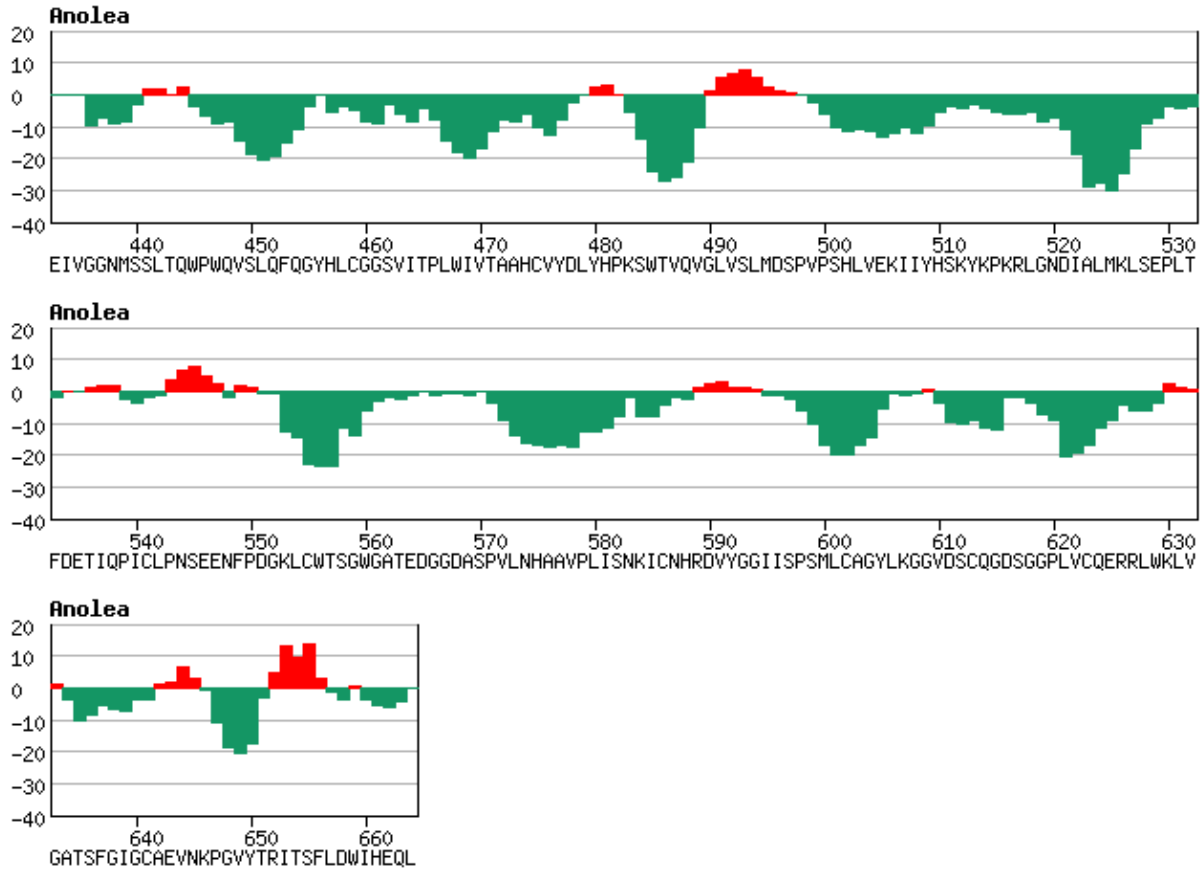
Target:	
modelled residue range:	217 to 448
based on template	1ekbB (2.30 A)
Sequence Identity [%]:	43.644
Evalue:	0

Alignment

```
TARGET    217     IVGGNMSS LTQWPWQVSL QFQGYHLCGG SVITPLWIVT AAHCVYDLY-
1ekbB     16      ivggsdsr egawpwvval yfddqqvcga slvsrdwlvs aahcvygrnm

TARGET                sss       sssss sss ssssss sss  sssss   hhh
1ekbB                 sss       sssss sss ssssss sss  sssss   hhh


TARGET    264   HPKSWTVQVG LVS---LMDS PVPSHLVEKI IYHSKYKPKR LGNDIALMKL
1ekbB     60    epskwkavlg lhmasnltsp qietrlidqi vinphynkrr knndiammhl

TARGET             ssssss               ssssssss sss            ssssss
1ekbB              ssssss   sss         ssssssss sss            ssssss


TARGET    311   SEPLTFDETI QPICLPNSEE NFPDGKLCWT SGWGATEDGG DASPVLNHAA
1ekbB     109   emkvnytdyi qpiclpeenq vfppgricsi agwgaliyqg stadvlqead

TARGET          s                        sssss ss ssss  s sss  sssss
1ekbB           s                        sssss ss ssss  s ssssssssss


TARGET    361   VPLISNKICN HRDVYGGIIS PSMLCAGYLK GGVDSCQGDS GGPLVCQERR
1ekbB     160   vpllsnekcq qqm-peynit enmvcagyea ggvdscqgds ggplmcqenn

TARGET          ssss hhhhh hh          ssssss               ssssssss
1ekbB           ssss hhhhh hh          ssssss               ssssssss
```

```
TARGET    411   LWKLVGATSF GIGCAEVNKP GVYTRITSFL DWIHEQLE
1ekbB     206   rwllagvtsf gyqcalpnrp gvyarvprft ewiqsflh-

TARGET          ssssssssss             ssssss   h hhhhh
1ekbB           ssssssssss             ssssss   h hhhhh
```

Anolea



Modelling log

```
3.70 (SP3)
Loading Template: 1ekbB.pdb
Loading Raw Sequence
Renumber target sequence starting from  (217)
Loading Alignment: ./NXXX.align.submit.fasta
Removing HET groups from template structure
Refining Raw Sequence Alignment
ProModII: doing simple assignment of backbone
ProModII: adding blocking groups
Adding Missing Sidechains
AddPolar H
BuildDeletetedLoopsModel
Trying Ligating with anchor residues LEU 262 and PRO 265
```

```
Number of Ligations found: 26
ACCEPTING loop   21: clash=   0 FF=        -88.7 PP= -1.00
Trying Ligating with anchor residues VAL 275 and MET 278
Trying Ligating with anchor residues LEU 274 and MET 278
Trying Ligating with anchor residues LEU 274 and ASP 279
Number of Ligations found: 79
ACCEPTING loop   11: clash=   0 FF=        960.1 PP=  0.00
Building CSP loop with anchor residues ASP 373 and GLY 376
Number of Ligations found: 1
ACCEPTING loop    0: clash=   0 FF=        818.8 PP= -5.00
Optimizing Sidechains
Adding Hydrogens
Optimizing loops and OXT (nb = 12)
Final Total Energy:       -5518.449 KJ/mol
Dumping Sequence Alignment
```

Model Details: Batch.2

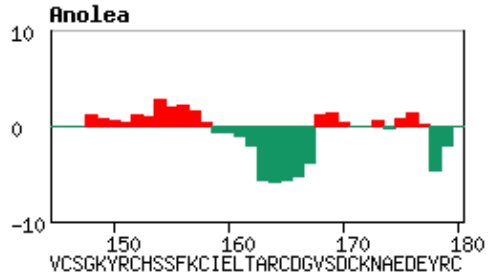
model pic

Target:	
modelled residue range:	73 to 108
based on template	3dprE (3.50 A)
Sequence Identity [%]:	39.474
Evalue:	1.5E-09

Alignment

```
TARGET    73      C-SGKYRC HS-SFKCIEL TARCDGVSDC KNAEDEYRCV
3dprE     3       criheisc gahstqcipv swrcdgendc dsgedeencg n

TARGET
3dprE
```

Anolea



Modelling log

```
3.70 (SP3)
Loading Template: 3dprE.pdb
Loading Raw Sequence
Renumber target sequence starting from  (73)
Loading Alignment: ./NXXX.align.submit.fasta
Removing HET groups from template structure
Refining Raw Sequence Alignment
ProModII: doing simple assignment of backbone
ProModII: adding blocking groups
Adding Missing Sidechains
AddPolar H
BuildDeletetedLoopsModel
Trying Ligating with anchor residues CYS 73 and LYS 76
Number of Ligations found: 7
ACCEPTING loop    0: clash=   0 FF=        136.6 PP=  0.00
connectivity problem (C-N > 3.0A) at residue: 5
Trying Ligating with anchor residues SER 74 and TYR 77
Trying Ligating with anchor residues CYS 73 and TYR 77
Number of Ligations found: 102
ACCEPTING loop   72: clash=   0 FF=        350.5 PP=-14.00
connectivity problem (C-N > 3.0A) at residue: 6
Trying Ligating with anchor residues GLY 75 and ARG 78
Number of Ligations found: 3
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues SER 74 and ARG 78
Number of Ligations found: 25
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues SER 74 and CYS 79
Number of Ligations found: 208
ACCEPTING loop  182: clash=   0 FF=         35.5 PP=  1.00
Trying Ligating with anchor residues HIS 80 and PHE 83
Number of Ligations found: 10
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues CYS 79 and PHE 83
Number of Ligations found: 1
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues CYS 79 and LYS 84
Number of Ligations found: 56
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues ARG 78 and LYS 84
Number of Ligations found: 125
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues TYR 77 and LYS 84
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues TYR 77 and CYS 85
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues LYS 76 and CYS 85
Number of Ligations found: 500
ACCEPTING loop  374: clash=   0 FF=       -388.8 PP= -1.00
Optimizing Sidechains
Adding Hydrogens
Optimizing loops and OXT (nb = 13)
Final Total Energy:        -623.585 KJ/mol
Dumping Sequence Alignment
```

Model Details: Batch.3

model pic

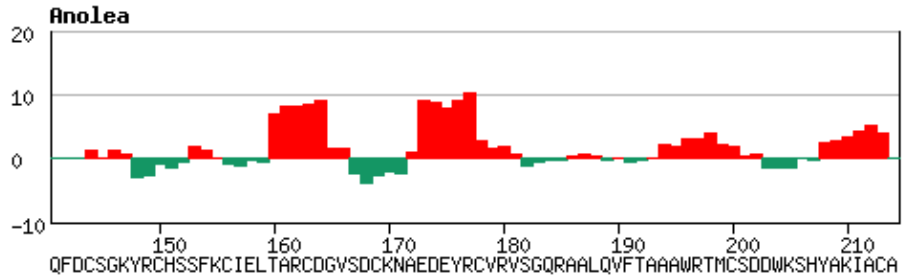
Target:	
modelled residue range:	71 to 144
based on template	1n7dA (3.70 A)
Sequence Identity [%]:	24.051
Evalue:	2.7E-11

Alignment

```
1n7dA     44    svtcksgdfs cggnrcipqf wrcdgqvdcn gsdeqgcppk tcsqdefrch

1n7dA

1n7dA     97    dgrqfvcdsd rdcldgsdea scpvltcgpa sfqcnsstci pqlwacdndp

1n7dA

TARGET    71                              FDC-S GKYRCHSSFK CIELTARCDG
1n7dA     151   dcedgsdewp qrcrglyvfq gds--spcsa fefhclsg-e cihsswrcdg

TARGET
1n7dA

TARGET    95    VSDCKNAEDE YRCVRV--SG QRAA--LQVF TAAAWRTMCS DDWKSHYAKI
1n7dA     198   gpdckdksde encavatcrp defqcsdgnc ihgsrqcdre ydckdmsdev

TARGET                              sss        sss
1n7dA                               sss        sss

TARGET    141   ACAQ ----- ---------- ---------- ---------- ----------
1n7dA     248   gcvnvtlceg pnkfkchsge citldkvcnm ardcrdwsde pikecgtnec

TARGET
1n7dA

TARGET          ---------- ---------- ---------- ---------- ----------
1n7dA     298   ldnnggcshv cndlkigyec lcpdgfqlva qrrcedidec qdpdtcsqlc

TARGET
1n7dA
```

```
TARGET          ---------- ---------- ---------- ---------- ----------
1n7dA     348   vnleggykcq ceegfqldph tkackavgsi aylfftnrhe rkmtldrsey

TARGET
1n7dA                                                       sss    ss


TARGET          ---------- ---------- ---------- ---------- ----------
1n7dA     399   tslipnlrnv valdtevasn riywsdlsqr micstqldra hgssydtvis

TARGET
1n7dA           s             sss   s ssss         sssss


TARGET          ---------- ---------- ---------- ---------- ----------
1n7dA     450   rdipdglavd wihsniywtd svlgtvsvad tkgvkrktlf reqgskprai

TARGET
1n7dA                                                             ss


TARGET          ---------- ---------- ---------- ---------- ----------
1n7dA     502   vvdpvhgfmy wtdwgtpaki kkgglngvdi yslvteniqw pngitldlls

TARGET
1n7dA           s     ssss ss         sssss               s ss


TARGET          ---------- ---------- ---------- ---------- ----------
1n7dA     552   grlywvdskl hsissidvng gnrktilede krlahpfsla vfedkvfwtd

TARGET
1n7dA             ssssss    sssss        sss              s ss  sss


TARGET          ---------- ---------- ---------- ---------- ----------
1n7dA     602   iineaifsan rltgsdvnll aenllspedm vlfhqltqpr gvnwcerttl

TARGET
1n7dA


TARGET          ---------- ---------- ---------- ---------- --
1n7dA     652   snggcqylcl papqinphsp kftcacpdgm llardmrscl te

TARGET
1n7dA                                           sss    sss
```

Anolea



Modelling log

```
3.70 (SP3)
Loading Template: 1n7dA.pdb
Loading Raw Sequence
Renumber target sequence starting from  (71)
Loading Alignment: ./NXXX.align.submit.fasta
Removing HET groups from template structure
Refining Raw Sequence Alignment
ProModII: doing simple assignment of backbone
ProModII: adding blocking groups
Adding Missing Sidechains
AddPolar H
BuildDeletetedLoopsModel
Small Ligation (C-N <3.0A) ignored;
GROMOS will repair it at residue SER 5
Trying Ligating with anchor residues ARG 109 and GLY 112
Trying Ligating with anchor residues VAL 108 and GLY 112
Trying Ligating with anchor residues CYS 107 and GLY 112
Trying Ligating with anchor residues ARG 106 and GLY 112
Trying Ligating with anchor residues TYR 105 and GLY 112
Trying Ligating with anchor residues GLU 104 and GLY 112
Trying Ligating with anchor residues ASP 103 and GLY 112
Number of Ligations found: 91
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues GLU 102 and GLY 112
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
+++ Warning: Ligation Failed, SparePart will be inserted later
+++          It is usually the sign that the region is misaligned.
Trying Ligating with anchor residues ALA 116 and VAL 119
Trying Ligating with anchor residues ALA 115 and VAL 119
Number of Ligations found: 80
ACCEPTING loop   44: clash=   0 FF=       -127.6 PP= -3.00
Building CSP loop with anchor residues SER 82 and CYS 85
Building CSP loop with anchor residues SER 81 and CYS 85
Number of Ligations found: 24
ACCEPTING loop   21: clash=   0 FF=         76.2 PP=  0.00
Finding Spare-Part loop with anchor residues ASN 100 and SER 111
ACCEPTING loop   2 from 3FXN_  Clash=   2 FF=       -157.8 PP=10.56
BadPhi=   0 BadGX=   0 BadXP=   0 weakXP=   0 Score= 3.00  rms= 0.00
Optimizing Sidechains
Adding Hydrogens
Optimizing loops and OXT (nb = 9)
Final Total Energy:        1006.523 KJ/mol
Dumping Sequence Alignment
```

Model Details: Batch.4

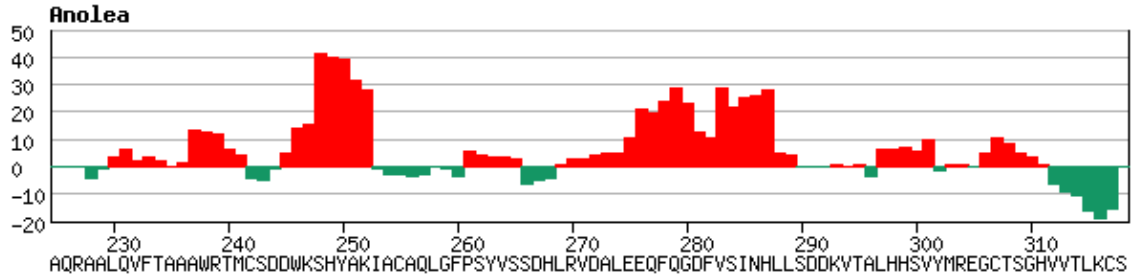
model pic

Target:	
modelled residue range:	113 to 206
based on template	1by2A (2.00 A)
Sequence Identity [%]:	14.737
Evalue:	2.6E-06

Alignment

```
TARGET    113                    QRA ALQVFTAAAW RTMCSDDWKS HYAKIACAQL
1by2A     0     avndgdmrla dggat--nqg rveifyrgqw gtvcdnlwdl tdasvvcral

TARGET                           sss ss sss  ss s sss         hhhhhhh
1by2A                 sssss      sss ssssss  ss s sss    h hhhhhhhhhh


TARGET    146   GFPSYVSSDH -LRVDALEEQ FQGDFVSINH LLSDDKVTAL HHSVYMREGC
1by2A     48    gfenatqalg raafgqgsgp imldevqctg --teasladc kslgwlksnc

TARGET              ssssss
1by2A               ssssss


TARGET    195   TSGHVVTLKC SA ---
1by2A     96    rherdagvvc tnettl

TARGET              sssssss s
1by2A               sssssss s
```

Anolea



Modelling log

```
3.70 (SP3)
Loading Template: 1by2A.pdb
Loading Raw Sequence
Renumber target sequence starting from  (113)
Loading Alignment: ./NXXX.align.submit.fasta
Removing HET groups from template structure
Refining Raw Sequence Alignment
ProModII: doing simple assignment of backbone
ProModII: adding blocking groups
Adding Missing Sidechains
AddPolar H
BuildDeletetedLoopsModel
Trying Ligating with anchor residues HIS 155 and VAL 158
Number of Ligations found: 6
ACCEPTING loop    2: clash=   0 FF=        -83.3 PP= -1.00
Building CSP loop with anchor residues HIS 174 and SER 177
Building CSP loop with anchor residues ASN 173 and SER 177
Number of Ligations found: 11
ACCEPTING loop    9: clash=   0 FF=        149.7 PP= -5.00
Optimizing Sidechains
Adding Hydrogens
Optimizing loops and OXT (nb = 8)
Final Total Energy:         913.840 KJ/mol
Dumping Sequence Alignment
```

Template Selection Log:

```
 - Start SMR-Pipeline in automated mode on BC2-cluster at Tue Mar 29 19:06:48 2011


 - Start BLAST for highly similar template structure identification
 - No suitable templates found!

 - Run HHSearch to detect remotely related template structures
 - Send 4 target-template alignments for modeling

 - @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
 -                                       *****************************************
 - building model based on 1ekbB (217-448) was successfull
 -              ******
 - building model based on 3dprE (73-108) was successfull
 -                    **************************************************************
 - building model based on 1z8gA (108-452) was not successfull go to next best template
 -              *************
 - building model based on 1n7dA (71-144) was successfull
 -                     ****************
 - building model based on 2oyaB (114-205) was not successfull go to next best template
 -                     *****************
 - building model based on 1by2A (113-206) was successfull
 - Workspace Pipeline parameter

   Cut-off parameters to model the target based on a BLAST target-template alignment
    Evalue :                                     0.0001
    Minimum Template size (aa) for ranking :     25
    Minimum Sequence identity :                  60

   Cut-off parameters to model the target based on a HHSearch target-template alignment
    Evalue :                                     0.0001
    Probability :                                50
    MAC :                                        0.3
```

```
  Parameters for model selection
   Minimal number of uncovered target
    residues after BLAST to run HHSEARCH :      50
   Minimal number of uncovered target
    residues to model an additional template :  25

- Finish SMR-Pipeline in automated mode on BC2-cluster at Tue Mar 29 19:38:41 2011
```

If you publish results using SWISS-MODEL, please cite the following papers:

- Arnold K., Bordoli L., Kopp J., and Schwede T. (2006). The SWISS-MODEL Workspace: A web-based environment for protein structure homology modelling. Bioinformatics, 22,195-201.
- Schwede T, Kopp J, Guex N, and Peitsch MC (2003) SWISS-MODEL: an automated protein homology-modeling server. Nucleic Acids Research 31: 3381-3385.
- Guex, N. and Peitsch, M. C. (1997) SWISS-MODEL and the Swiss-PdbViewer: An environment for comparative protein modelling. Electrophoresis 18: 2714-2723.