Workunit: P000002
Title:CDS3264

Model Details: Batch.1

Target:

modelled residue range:	88 to 708
based on template	3orgC (3.50 A)
Sequence Identity [%]:	83.736
Evalue:	0

Alignment

```
TARGET   88      SLMYLLRL VCFLTLLGVT AALFIFAVDL AVHGLEELRM KISRLAGRFA
3orgC    88      slmyllrl vcfltllgvt aalfifavdl avhgleelrm kisrlagrfa

TARGET           hhhhhh hhhhhhhhhh hhhhhhhhhh hhhhhhhhhh hhhh    hhh
3orgC            hhhhhh hhhhhhhhhh hhhhhhhhhh hhhhhhhhhh hhhh    hhh


TARGET   136     GYILYVVSGV ALCLLSTFWC AVLSTEAEGS GLPQMKSILS GFYDKMRSAL
3orgC    136     gyilyvvsgv alcllstfwc avlsteaegs glpqmksils gfydkmrsal

TARGET           hhhhhhhhhh hhhhhhhhhh hhh        hhhhhhhh   hh    hh
3orgC            hhhhhhhhhh hhhhhhhhhh hhh        hhhhhhhh   hh    hh


TARGET   186     ELRVLFAKAL GLICAIGGGL PVGWEGPNVH IACIIAHQFY RLGVFKELCT
3orgC    186     elrvlfakal glicaigggl pvgwegpnvh iaciiahqfy rlgvfkelct

TARGET             hhhhhhhh hhhhhhh        hhhhhh hhhhhhhhhh       hhh
3orgC              hhhhhhhh hhhhhhh        hhhhhh hhhhhhhhhh       hhh


TARGET   236     DRALRLQTLA AACAVGLASS FGAPLGGVLY SIETIASFYL VQAFWKGVLS
3orgC    236     dralrlqtla aacavglass fgaplggvly sietiasfyl vqafwkgvls

TARGET             hhhhhhhh hhhhhhhhhh   hhhhhhh hh         hhhhhhhhh
3orgC              hhhhhhhh hhhhhhhhhh   hhhhhhh hh         hhhhhhhhh
```

```
TARGET    286    ALSGAIVYEL LYTTPLVEAF EGTNFDASDV SRTQTLLYAI LGALMGVLGA
3orgC     286    alsgaivyel ---------- --------dv srtqtllyai lgalmgvlga

TARGET           hhhhhhhh                             hhhhh hhhhhhhhhh
3orgC            hhhhhhhh                             hhhhh hhhhhhhhhh


TARGET    336    LFIRCVRSIY ELRMRHYPGT NRYFLVGVVA LFASALQYPF RLFALDPRAT
3orgC     336    lfircvrsiy elrmrhypgt nryflvgvva lfasalqypf ------prat

TARGET           hhhhhhhh   hhh        hhhhhhhh hhhhhh              hh
3orgC            hhhhhhhh   hhh        hhhhhhhh hhhhhh              hh


TARGET    386    INDLFKAVPL YQTDHFGWTE LILMPIIKFI LVALSIGLPL PAGVFVPSFL
3orgC     386    indlfkav-- --------te lilmpiikfi lvalsiglpl pagvfvpsfl

TARGET           hhhhh  hh hhh        hhhhhhhh hhhhhh        hhhhhh
3orgC            hhhhh              hhhhhhhh hhhhhh        hhhhhh


TARGET    436    IGAGFGRLYG ELMRVVFGNA IVPGSYAVVG AAAFTAGVTR ALSCAVIIFE
3orgC     436    igagfgrlyg elmrvvfgna ivpgsyavvg aaaftagvtr alscaviife

TARGET           hhhhhhhhh hhhhh        hhhhhhh hhhhhhhhh    hhhhhhhh
3orgC            hhhhhhhhh    hhh        hhhhhhh hhhhhhhhh    hhhhhhhh


TARGET    486    VTGQIRHLVP VLISVLLAVI VGNAFNRSLY ETLVLMKHLP YMPILRRDRS
3orgC     486    vtgqirhlvp vlisvllavi vgnafnrsly etlvlmkhlp ympilrrdrs

TARGET                   hh hhhhhhhhhh hhhhh    hh hhhhhhh       sss
3orgC                    hh hhhhhhhhhh h    h    hh hhhhhh        sss


TARGET    536    PEMTAREIMH PIEGEPHLFP DSEPQHIKGI LEKFPNRLVF PVIDANGYLL
3orgC     536    pemtareimh piegephlfp dsepqhikgi lekfpnrlvf pvidangy--

TARGET              ssshhh                 hhhhhhh hhh    sss ss     sss
3orgC               ssshhh                 hhhhhh hhh    sss ss


TARGET    586    GAISRKEIVD RLQHVLEDVP EPIAGHRTLV LLDAADLSEN IEGLVDETPS
3orgC     584    ---------- ---------- ---------- llgaisrkei vdrl------

TARGET                   sss            sss      sssssshhhh hhhhhhhhhh
3orgC                                            sssshhhh h


TARGET    636    GEHSSKGKRT ATVLEPTSSL VVPCDVSPIV VTSYSLVRQL HFLFVMLMPS
3orgC     598    ---------- -------qhv vvpcdvspiv vtsyslvrql hflfvmlmps

TARGET           hh         hhhhhhhhhh h          sss sss    hhhhhh   s
3orgC                                       ss sss sss    hhhhh    s


TARGET    686    MIYVTERGKL VGIVEREDVA YGY -
3orgC     686    miyvtergkl vgiveredva ygysn

TARGET           ssssssssss ssssss  ss s
3orgC            ssssss  ss ssssss  ss s
```

Model Quality Estimation

Modelling log

```
3.70 (SP3)
Loading Template: 3orgC.pdb
Loading Raw Sequence
Renumber target sequence starting from  (88)
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
connectivity problem (C-N > 3.0A) at residue: 570
Trying Ligating with anchor residues SER 654 and VAL 657
Trying Ligating with anchor residues SER 653 and VAL 657
Trying Ligating with anchor residues SER 653 and PRO 658
Trying Ligating with anchor residues THR 652 and PRO 658
Trying Ligating with anchor residues PRO 651 and PRO 658
Trying Ligating with anchor residues GLU 650 and PRO 658
Trying Ligating with anchor residues LEU 649 and PRO 658
Trying Ligating with anchor residues VAL 648 and PRO 658
+++ Warning: Ligation Failed, SparePart will be inserted later
+++         It is usually the sign that the region is misaligned.
Building CSP loop with anchor residues PHE 375 and PRO 382
Number of Ligations found: 500
ACCEPTING loop  204: clash=   0 FF=       -222.0 PP= -2.00
Finding Spare-Part loop with anchor residues LEU 295 and ASP 314
ACCEPTING loop  10 from 1KPTA  Clash=   4 FF=        696.7 PP=1470.12
BadPhi=   1 BadGX=   0 BadXP=   0 weakXP=   0 Score= 7.00  rms= 0.00
Finding Spare-Part loop with anchor residues VAL 393 and THR 404
ACCEPTING loop 138 from 2AK3B  Clash=   4 FF=        328.1 PP=1470.44
BadPhi=   0 BadGX=   0 BadXP=   0 weakXP=   0 Score= 6.00  rms= 0.00
Finding Spare-Part loop with anchor residues TYR 583 and LEU 616
Sorry, no loop could be found in the database
Finding Spare-Part loop with anchor residues GLY 582 and LEU 616
ACCEPTING loop   3 from 1PAZ_  Clash=   4 FF=        773.5 PP=1480.19
BadPhi=   4 BadGX=   0 BadXP=   1 weakXP=   2 Score=11.00  rms= 0.00
Finding Spare-Part loop with anchor residues LEU 629 and VAL 657
connectivity problem --> including residue VAL 571
Finding Spare-Part loop with anchor residues LEU 629 and PRO 658
ACCEPTING loop  33 from 2HPDA  Clash=   4 FF=       1049.8 PP=1491.07
BadPhi=   1 BadGX=   0 BadXP=   0 weakXP=   0 Score= 7.00  rms= 0.00
Optimizing Sidechains
Adding Hydrogens
Optimizing loops and OXT (nb = 91)
Final Total Energy:       22033.709 KJ/mol
Dumping Sequence Alignment
```

Template Selection Log:

```
 - Start SMR-Pipeline in automated mode on BC2-cluster at Wed May 25 20:23:14 2011


- Start BLAST for highly similar template structure identification
- Blast template search was successfull, number of templates selected for modeling:  1
- Still uncovered regions of the target sequence detected, run: HHSEARCH
- Run HHSearch to detect remotely related template structures
- Send 1 target-template alignments for modeling

- @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
-           ****************************************************************
- building model based on 3orgC (88-708) 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 Wed May 25 21:14:45 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.