Workunit: P000001
Title:Full

1 632

Model Details: Batch.1

Target:

modelled residue range: 3 to 516

based on template 3orgC (3.50 A)

Sequence Identity [%]: 93.191

Evalue: 0

Alignment

```
TARGET    3      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    51     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    101    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    151    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    201   ALSGAIVYEL LYTTPLVEAF EGTNFDASDV SRTQTLLYAI LGALMGVLGA
3orgC     286   alsgaivyel ---------- --------dv srtqtllyai lgalmgvlga

TARGET          hhhhhhhh                              hhhhh hhhhhhhhhh
3orgC           hhhhhhhh                              hhhhh hhhhhhhhhh


TARGET    251   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    301   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    351   IGAGFGRLYG ELMRVVFGNA IVPGSYAVVG AAAFTAGVTR ALSCAVIIFE
3orgC     436   igagfgrlyg elmrvvfgna ivpgsyavvg aaaftagvtr alscaviife

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


TARGET    401   VTGQIRHLVP VLISVLLAVI VGNAFNRSLY ETLVLMKHLP YMPILRRDRS
3orgC     486   vtgqirhlvp vlisvllavi vgnafnrsly etlvlmkhlp ympilrrdrs

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


TARGET    451   PEMTAREIMH PIEGEPHLFP DSEPQHIKGI LEKFPNRLVF PVIDANGYLL
3orgC     536   pemtareimh piegephlfp dsepqhikgi lekfpnrlvf pvidangyll

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


TARGET    501   GAISRKEIVD RLQHVL --- ---------- ---------- ----------
3orgC     586   gaisrkeivd rlqhvvvpcd vspivvtsys lvrqlhflfv mlmpsmiyvt

TARGET          sssshhhhhh hh
3orgC           sssshhhhh              sssss s ss   hhhhh h    ssssss


TARGET          ---------- ----------
3orgC     691   ergklvgive redvaygysn

TARGET
3orgC           s  sssssss s  sss
```

Model Quality Estimation

Modelling log

```
3.70 (SP3)
Loading Template: 3orgC.pdb
Loading Raw Sequence
Renumber target sequence starting from  (3)
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
Building CSP loop with anchor residues PHE 290 and PRO 297
Number of Ligations found: 500
ACCEPTING loop  204: clash=   0 FF=        -222.2 PP= -2.00
Finding Spare-Part loop with anchor residues LEU 210 and ASP 229
ACCEPTING loop  10 from 1KPTA  Clash=   4 FF=         696.7 PP=1092.21
BadPhi=   1 BadGX=   0 BadXP=   0 weakXP=   0 Score= 7.00  rms= 0.00
Finding Spare-Part loop with anchor residues VAL 308 and THR 319
ACCEPTING loop 138 from 2AK3B  Clash=   4 FF=         328.1 PP=1092.52
BadPhi=   0 BadGX=   0 BadXP=   0 weakXP=   0 Score= 6.00  rms= 0.00
Optimizing Sidechains
Adding Hydrogens
Optimizing loops and OXT (nb = 36)
Final Total Energy:      -13376.023 KJ/mol
Dumping Sequence Alignment
```

Model Details: Batch.2

Target:	
modelled residue range:	563 to 625
based on template	3orgC (3.50 A)
Sequence Identity [%]:	87.302
Evalue:	1.69308e-23

Alignment

```
3orgC     88    slmyllrlvc fltllgvtaa lfifavdlav hgleelrmki srlagrfagy


3orgC            hhhhhhhh hhhhhhhhhh hhhhhhhhhh hhhhhhhhhh hh    hhhhh


3orgC     138   ilyvvsgval cllstfwcav lsteaegsgl pqmksilsgf ydkmrsalel
```

```
3orgC            hhhhhhhhh hhhhhhhhhh h         h hhhhhhh    hh    hh


3orgC      188   rvlfakalgl icaiggglpv gwegpnvhia ciiahqfyrl gvfkelctdr

3orgC            hhhhhhhhh hhhhh       hhhhhhhh hhhhhhhh       hhh


3orgC      238   alrlqtlaaa cavglassfg aplggvlysi etiasfylvq afwkgvlsal

3orgC            hhhhhhhhh hhhhhhhh    hhhhhhhhh         h hhhhhhhhhh


3orgC      288   sgaivyeldv srtqtllyai lgalmgvlga lfircvrsiy elrmrhypgt

3orgC            hhhhh        hhhhh hhhhhhhhhh hhhhhhhhh    hhh


3orgC      356   nryflvgvva lfasalqypf pratindlfk avtelilmpi ikfilvalsi

3orgC             hhhhhhhh hhhhhh      hhhhhhh      hhhh hhhhhhhhhh


3orgC      422   glplpagvfv psfligagfg rlygelmrvv fgnaivpgsy avvgaaafta

3orgC                      hh hhhhhhhhhh hhhh   hhh     hhh hhhhhhhhhh


3orgC      472   gvtralscav iifevtgqir hlvpvlisvl lavivgnafn rslyetlvlm

3orgC            hhh   hhhh hhhh        hhhhhhhh hhhhh    h     hhhhhhhh


3orgC      522   khlpympilr rdrspemtar eimhpiegep hlfpdsepqh ikgilekfpn

3orgC            h      sss       sssh hh                hhh hhhhhhh


TARGET     563                                 VLEPTSS LVVPCDVSPI VVTSYSLVRQ
3orgC      572   rlvfpvidan gyllgaisrk e--ivdrlqh vvvpcdvspi vvtsyslvrq

TARGET                                       hhh          s ssss
3orgC             sssss       ssssshh h  hh           s ssss sss


TARGET     590   LHFLFVMLMP SMIYVTERGK LVGIVEREDV AYGYSN
3orgC      675   lhflfvmlmp smiyvtergk lvgiveredv aygysn-
```

4

```
TARGET          hhhhhh      sssssss  s sssssss
3orgC           hhhhh       sssssss  s sssssss  s ss
```

Model Quality Estimation

Modelling log

```
3.70 (SP3)
Loading Template: 3orgC.pdb
Loading Raw Sequence
Renumber target sequence starting from  (563)
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: 10
Trying Ligating with anchor residues SER 569 and VAL 572
Trying Ligating with anchor residues SER 568 and VAL 572
Trying Ligating with anchor residues SER 568 and PRO 573
Trying Ligating with anchor residues THR 567 and PRO 573
Number of Ligations found: 88
ACCEPTING loop    0: clash=   0 FF=         -22.6 PP= -2.00
Optimizing Sidechains
Adding Hydrogens
Optimizing loops and OXT (nb = 7)
Final Total Energy:       -1329.866 KJ/mol
Dumping Sequence Alignment
```

Template Selection Log:

```
 - Start SMR-Pipeline in automated mode on BC2-cluster at Thu May 19 14:11:38 2011


 - Start BLAST for highly similar template structure identification
 - Blast template search was successfull, number of templates selected for modeling:  2; entering modeling mo

 - Send 2 target-template alignments for modeling

 - @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
 - ****************************************************************
 - building model based on 3orgC (3-516) was successfull
 -                                                    ********
 - building model based on 3orgC (563-625) 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 Thu May 19 14:12:43 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.