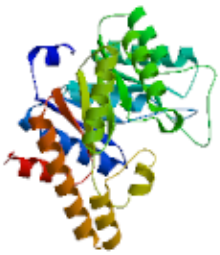
SWISS-MODEL Workspace

Workunit: P000002 Title:P42898

Model Summary:



Model information:

Modelled residue range:	48 to 340
Based on template:	3aptA (1.85 A)
Sequence Identity [%]:	37.5
Evalue:	0

Quality information:

QMEAN Z-Score: -1.251

Quaternary structure information:

Template (3aptA): Unknown
Model: SINGLE CHAIN

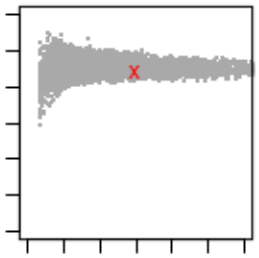
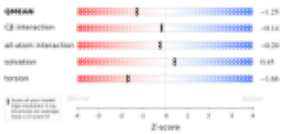
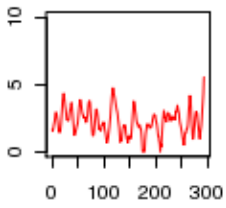
Ligand information:

Ligands in the template: FAD: 1.
Ligands in the model: none.

Global Model Quality Estimation:

QMEAN4 global scores:

Local scores:

QMEANscore4:	Estimated absolute model quality:	Score components:	Coloring by residue error:	Residue error plot:
0.696				

Z-Score: -1.251

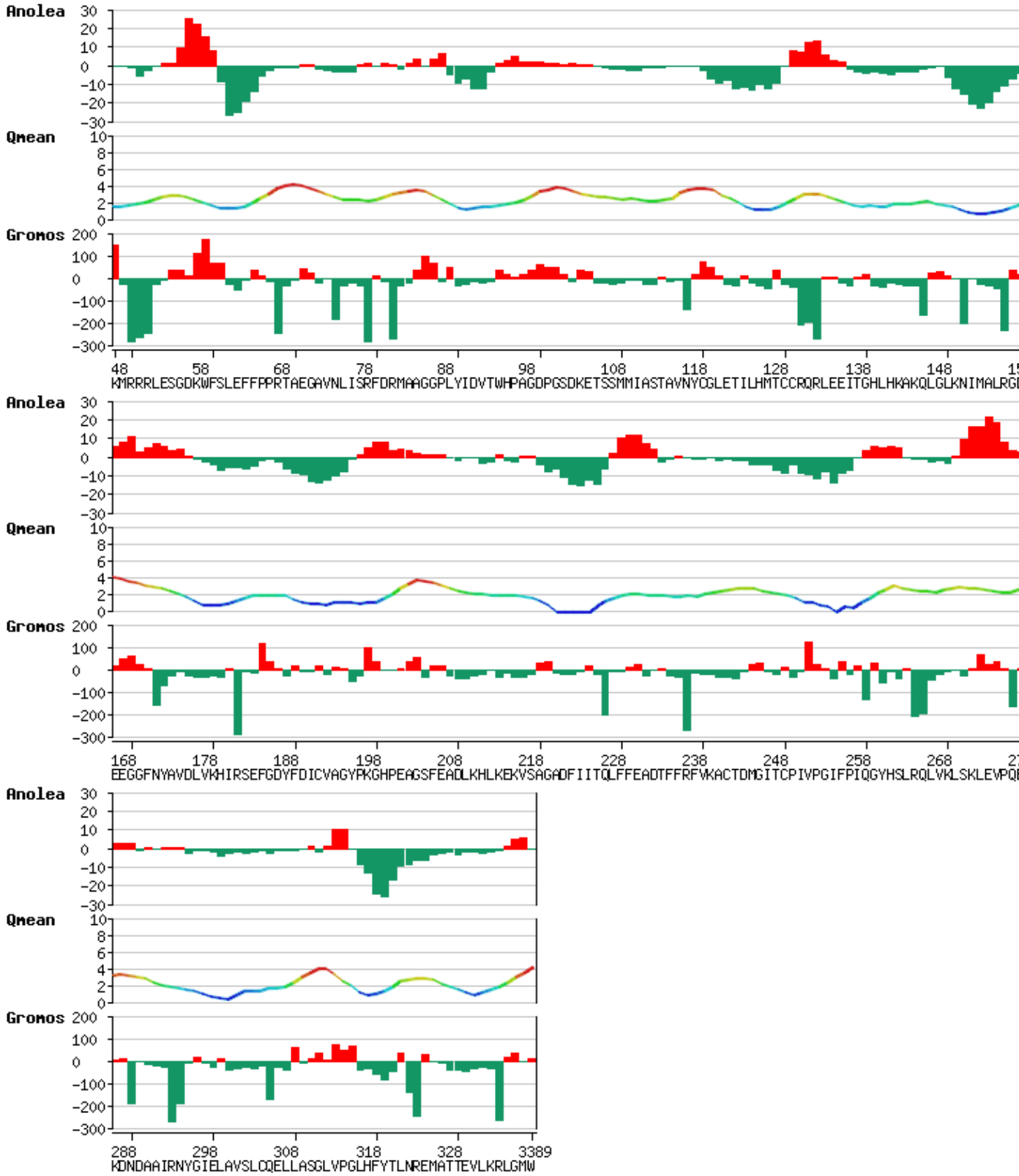
QMEAN4 global scores:

The QMEAN4 score is a composite score consisting of a linear combination of 4 statistical potential terms (estimated model reliability between 0-1). The pseudo-energies of the contributing terms are given below together with their Z-scores with respect to scores obtained for high-resolution experimental structures of similar size solved by X-ray crystallography:

Scoring function term	Raw score	Z-score
C_beta interaction energy	-128.52	-0.14
All-atom pairwise energy	-8569.81	-0.20
Solvation energy	-34.42	0.45
Torsion angle energy	-50.22	-1.66
QMEAN4 score	0.696	-1.25

If you publish results from QMEAN, please cite the following paper:
Benkert P, Biasini M, Schwede T. (2011). "Toward the estimation of the absolute quality of individual protein structure models." Bioinformatics, 27(3):343-50.

Local Model Quality Estimation:



Alignment:

```
TARGET    48       KMRRRLE -SGDKWFSLE FFPPRTAEGA VNLISRFDRM AAGGPLYIDV
3aptA     1     m--kirdllk arrgplfsfe ffppkdpege ealfrtleel kafrpafvsi
```

```
TARGET              hhhhh       sssss s     hhhh hhhhhhhhhh hh    ssss
3aptA               hhhhhh      sssss s     hhhh hhhhhhhhhh hh    ssss


TARGET    94    TWHPAGDPGS DKETSSMMIA STAVNYCGLE TILHMTCCRQ RLEEITGHLH
3aptA     49    tygamgst-- --rersvawa qriqs-lgln plahltvagq srkevaevlh

TARGET          s             hhhhhhh hhhhh        sssss     hhhhhhhhh
3aptA           s            hhhhhhhh hhhhh        sssss     hhhhhhhhh


TARGET    144   KAKQLGLKNI MALRGDPIGD Q--WEEEEGG FNYAVDLVKH IRSEFGDYFD
3aptA     94    rfvesgvenl lalrgdpprg ervfrphpeg fryaaelval irerygdrvs

TARGET          hhhh   sss sss                       hhhhhh hhhh     s
3aptA           hhhh   sss sss                       hhhhhh hhhh     s


TARGET    192   ICVAGYPKGH PEAGSFEADL KHLKEKVSAG ADFIITQLFF EADTFFRFVK
3aptA     144   vggaaypegh pesesleadl rhfkakveag ldfaitqlff nnahyfgfle

TARGET          sssss           hhhhh hhhhhhhh     sssss      hhhhhhhh
3aptA           sssss           hhhhh hhhhhhhh     sssss      hhhhhhhh


TARGET    242   ACTDMGITCP IVPGIFPIQG YHSLRQLVKL SKLEVPQEIK DVIEPIKDND
3aptA     194   rarragigip ilpgimpvts yrqlrrftev cgasipgpll aklerhqddp

TARGET          hhhhh    s sssss       hhhhhhhhh       hhhh hhhh     h
3aptA           hhhhh    s sssss       hhhhhhhhh       hhhh hh       h


TARGET    292   AAIRNYGIEL AVSLCQELLA SGLVPGLHFY TLNREMATTE VLKRLGMWT
3aptA     244   kavleigveh avrqvaelle ag-vegvhfy tlnkspatrm vlerlglrpa

TARGET          hhhhhhhhhh hhhhhhhhhh     ssssss s     hhhh hhhhh
3aptA           hhhhhhhhhh hhhhhhhhhh h   ssssss s     hhhh hhhhh
```

Modeling Log:

```
3.70 (SP3)
Loading Template: 3aptA.pdb
Loading Raw Sequence
Renumber target sequence starting from  (48)
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 GLU 54 and ASP 57
Trying Ligating with anchor residues GLU 54 and LYS 58
Number of Ligations found: 4
ACCEPTING loop    3: clash=   0 FF=        -35.6 PP= -3.00
Trying Ligating with anchor residues ASP 163 and GLU 166
Trying Ligating with anchor residues GLY 162 and GLU 166
Trying Ligating with anchor residues GLY 162 and GLU 167
```

```
Trying Ligating with anchor residues ILE 161 and GLU 167
Number of Ligations found: 10
ACCEPTING loop    7: clash=   0 FF=        300.5 PP=  0.00
Building CSP loop with anchor residues PRO 101 and GLU 106
Building CSP loop with anchor residues ASP 100 and GLU 106
Number of Ligations found: 184
all loops are bad; continuing CSP with larger segment
Building CSP loop with anchor residues GLY 99 and GLU 106
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
Building CSP loop with anchor residues ALA 98 and GLU 106
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
Building CSP loop with anchor residues PRO 97 and GLU 106
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
Building CSP loop with anchor residues HIS 96 and GLU 106
Number of Ligations found: 500
ACCEPTING loop  340: clash=   0 FF=        223.4 PP=  0.00
Building CSP loop with anchor residues ASN 118 and GLY 121
Number of Ligations found: 5
ACCEPTING loop    4: clash=   0 FF=        -71.6 PP= -4.00
Building CSP loop with anchor residues GLY 313 and PRO 316
Building CSP loop with anchor residues SER 312 and PRO 316
Number of Ligations found: 59
ACCEPTING loop   37: clash=   0 FF=        -61.3 PP=  2.00
Optimizing Sidechains
Adding Hydrogens
Optimizing loops and OXT (nb = 28)
Final Total Energy:       -7845.965 KJ/mol
Dumping Sequence Alignment
```

Template Selection Log:

```
 - Start SMR-Pipeline in automated mode on BC2-cluster at Mon Nov 14 04:46:13 2011


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

 - Run HHSearch to detect remotely related template structures
 - Send 1 target-template alignments for modeling

 - @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
 -       ************************************
 - building model based on 3aptA (48-340) 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 Mon Nov 14 05:32:59 2011
```

Sorry, we haven't found any oligomeric annotation for this template.
Either the complex was too large (>60 chains) or the structures was excluded for other reasons.
Please contact help@swissmodel.org for more information!

Ligand Modeling Log: Template's ligands section
Ligands in the template: FAD: 1.
Ligands in the template that will be assessed: FAD311.
Model's ligands section
FAD311
Not all the residues interacting with the ligand are completely conserved between model and template.
No RMSD calculation will be performed.
Given the properties calculated previously, the ligand A.FAD311 will not be included in the model.
FAD311: conservation:False, RMSD:False, included: False

No ligands were included in the model.

References: 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 modeling. 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 modeling. Electrophoresis 18: 2714-2723.

SWISS-MODEL is developed by the Protein Structure Bioinformatics group at the SIB - Swiss Institute of Bioinformatics & the Biozentrum University of Basel. © 2010.