

Workunit: P000003 Title:MT

1

656

Model Summary:



Model information:

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

Quaternary structure information:

Template (3aptA): Unknown
 Model: SINGLE CHAIN

Ligand information:

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

Quality information:

QMEAN Z-Score: -1.354

Global Model Quality Estimation:

QMEAN4 global scores:

QMEANscore4: Estimated absolute
 model quality:

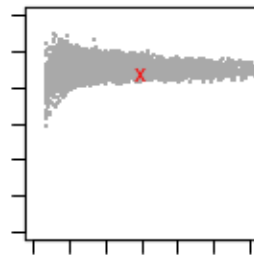
Score components:

Local scores:

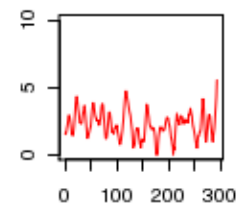
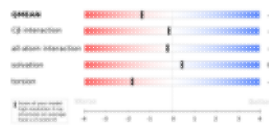
Coloring by residue
 error:

Residue error
 plot:

0.689



Z-Score: -1.354



QMEAN4 global scores:

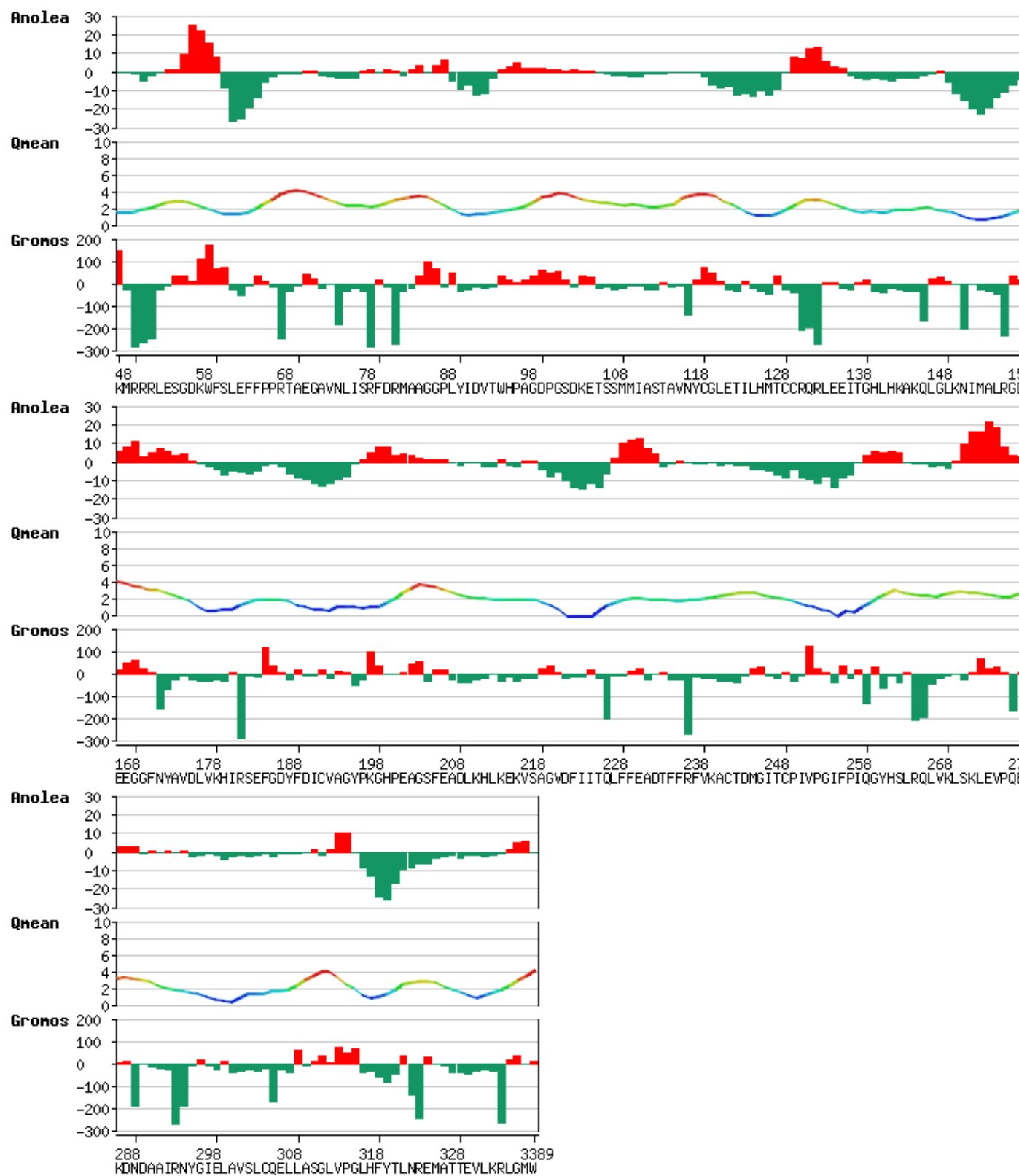
The QMEAN4 score is a composite score consisting of a linear combination of 4 statistical potential terms (estimated model reliability between 0-1). The pseudo-energies of the contributing terms are given below together with their Z-scores with respect to scores obtained for high-resolution experimental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

Scoring function term	Raw score	Z-score
C _β interaction energy	-130.22	-0.11
All-atom pairwise energy	-8609.01	-0.20
Solvation energy	-34.58	0.47
Torsion angle energy	-47.82	-1.79
QMEAN4 score	0.689	-1.35

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	KMRRRL	-SGDKWFSLE	FFPPRTAEGA	VNLISRFDRM	AAGGPLYIDV
3apta	1	m--kirdlik	arrgplfsfe	ffppkdpege	eafrtleel	kafrpafvsi

TARGET		hhhhh	sssss s	hhhh	hhhhhhhhhh	hh	ssss
3aptA		hhhhh	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	hhhhhhh	hhhhh	sssss	hhhhhhhhh

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

TARGET		hhhh	sss sss		hhhhh	hhhh	s
3aptA		hhhh	sss sss		hhhhh	hhhh	s

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

TARGET		sssss	hhhhh	hhhhhhh	sssss	hhhhhhh
3aptA		sssss	hhhhh	hhhhhhh	sssss	hhhhhhh

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

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

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

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

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

```

Template Selection Log:

- ```
- Start SMR-Pipeline in automated mode on BC2-cluster at Wed Nov 16 03:33:47 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

```

Value : 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

```

Value : 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 Nov 16 04:20:31 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](mailto: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.

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