SWISS-MODEL Workspace

Workunit: P000032 Title:My Pchem

Model Summary:

Model information:

Modelled residue range: 1 to 333

Based on template:

Quaternary structure information:

Quality information:

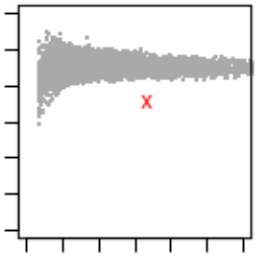
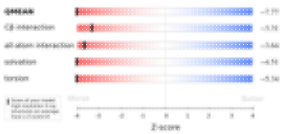
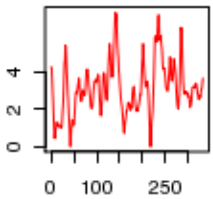
QMEAN Z-Score: -7.775

Ligand information:

Global Model Quality Estimation:

QMEAN4 global scores:

Local scores:

QMEANscore4:	Estimated absolute model quality:	Score components:	Coloring by residue error:	Residue error plot:
0.287				

Z-Score: -7.775

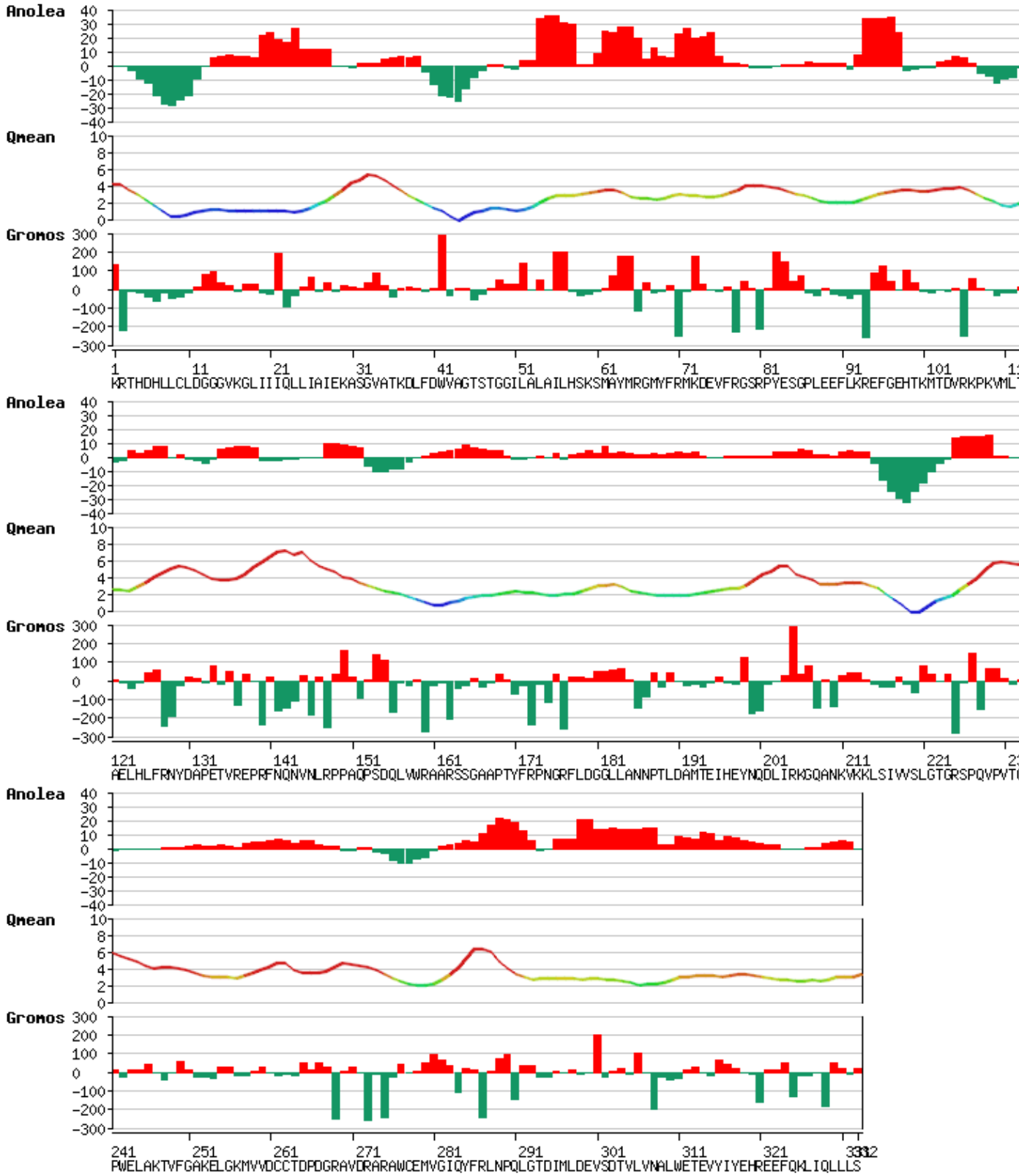
QMEAN4 global scores:

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	38.71	-3.31
All-atom pairwise energy	-522.39	-3.64
Solvation energy	11.80	-4.51
Torsion angle energy	17.72	-5.34
QMEAN4 score	0.287	-7.77

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    1       KRTHDHLL CLDGGGVKGL IIIQLLIAIE K-------AS GVATKDLFDW
1oxwA     25      lgexvtvl sidgggirgi ipatilefle gqlqexdnna darladyfdv
```

```
TARGET               ssss ssss   hhh hhhhhhhhhh                hhh ss
1oxwA                ssss ssss   hhh hhhhhhhhhh hhhhhh         hhh ss


TARGET    42    VAGTSTGGIL ALAILH---- ---SKSMAYM RGMYFRMKDE VFRGSR----
1oxwA     73    iggtstggll taxistpnen nrpfaaakei vpfyfehgpq ifnpsgqilg

TARGET          ssss hhhhh                        hhhhhhhhh h
1oxwA           ssss hhhhh hhhh sss    sss   hhh hhhhhhhhh h


TARGET    81    -PYESGPLEE FLKREFGEHT KMTDVRKPKV MLTGTLSDRQ PAELHLFRNY
1oxwA     123   pkydgkylxq vlqeklge-t rvhqaltevv issfdiktnk pviftksnla

TARGET               hhhhh hhhh     s ss     sss ssssss   s ssss
1oxwA                hhhhh hhhhhh   s ss     sss ssssss   s ssss


TARGET    130   DAPETVREPR FNQNVNLRPP AQPSDQLVWR AARSSGAAPT YFRPNG----
1oxwA     172   nspel----- ---------- ----dakxyd isystaaapt yfpphyfvtn

TARGET             sss   ss s    sss     sssssshh hhhhhh
1oxwA                                       ssshh hhhhhh         ssssss


TARGET    176   ---------R FLDGG--LLA NNPTLDAMTE IHEYNQDLIR KGQANKVKKL
1oxwA     203   tsngdeyefn lvdgavatva dpallsisva trlaqkdpaf asirslnykk

TARGET                   s ss           hhhhhhhh hhhh               s
1oxwA           s   ssssss ss  hh       hhhhhhhh hhhh               s


TARGET    215   SIVVSLGTGR SPQVPVTCVD VFRPSNPWEL AKTVFGAKEL GKMVVDCCTD
1oxwA     254   xlllslgtgt tsefdkty-- takeaatwta vhwxlviqkx tdaassyxtd

TARGET          ssssss                 hhhh    h hhhh   hhh hhhhhhh
1oxwA           sssssss                hh      h hhhh   hhh hhhhhhhhh


TARGET    265   ----PDGRAV DRARAWCEMV GIQYFRLNPQ LGTDIMLDEV SDTVLVNALW
1oxwA     301   yylstafqal dsknnylrv- -----qenal tgtttexdda seanxellvq

TARGET                         sssssh hh                    hhhhhhhhh
1oxwA           hhhhhhhhh      sssss                        hhhhhhhhh


TARGET    311   ETEVYIYEH- -------REE FQKLIQLLLS P --------
1oxwA     345   vgenllkkpv sednpetyee alkrfaklls drkklranka

TARGET          hhhhhh              h hhhhhhhhhh h
1oxwA           hhhhhh sss      ssshh hhhhhhhhhh hhhhhhh
```

Modeling Log:

```
3.70 (SP3)
Loading Template: 1oxwA.pdb
Loading Raw Sequence
```

```
Loading Alignment: ./user.align.submit.fasta.FF
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 LYS 29 and GLY 32
Trying Ligating with anchor residues LYS 29 and VAL 33
Number of Ligations found: 4
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues LYS 29 and ALA 34
Number of Ligations found: 177
ACCEPTING loop   68: clash=   0 FF=        148.5 PP= -3.00
Trying Ligating with anchor residues LEU 56 and LYS 59
Trying Ligating with anchor residues LEU 56 and SER 60
Number of Ligations found: 3
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues LEU 56 and MET 61
Number of Ligations found: 109
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues ILE 55 and MET 61
Number of Ligations found: 267
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues ILE 55 and ALA 62
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues ILE 55 and TYR 63
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues ALA 54 and TYR 63
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues ALA 54 and MET 64
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 SER 79 and TYR 82
Trying Ligating with anchor residues GLY 78 and TYR 82
Number of Ligations found: 1
all loops are bad; continuing CSP with larger segment
Trying Ligating with anchor residues GLY 78 and GLU 83
Number of Ligations found: 125
ACCEPTING loop   70: clash=   0 FF=       -241.5 PP=  2.00
Trying Ligating with anchor residues PRO 173 and ARG 176
Number of Ligations found: 5
ACCEPTING loop    3: clash=   0 FF=       -119.6 PP= -2.00
Trying Ligating with anchor residues GLY 180 and LEU 183
Number of Ligations found: 3
ACCEPTING loop    2: clash=   0 FF=         47.8 PP=  0.00
Trying Ligating with anchor residues THR 263 and ASP 266
Trying Ligating with anchor residues CYS 262 and ASP 266
Number of Ligations found: 7
ACCEPTING loop    6: clash=   0 FF=         68.9 PP= -1.00
Trying Ligating with anchor residues GLU 318 and GLU 321
Number of Ligations found: 2
ACCEPTING loop    1: clash=   0 FF=        164.0 PP=  0.00
Building CSP loop with anchor residues GLY 96 and THR 99
Number of Ligations found: 4
all loops are bad; continuing CSP with larger segment
Building CSP loop with anchor residues PHE 95 and THR 99
Number of Ligations found: 21
ACCEPTING loop    8: clash=   0 FF=         64.4 PP= -2.00
Building CSP loop with anchor residues CYS 232 and VAL 235
Building CSP loop with anchor residues THR 231 and VAL 235
Number of Ligations found: 11
```

```
all loops are bad; continuing CSP with larger segment
Building CSP loop with anchor residues VAL 230 and VAL 235
Number of Ligations found: 500
ACCEPTING loop   28: clash=   0 FF=         88.2 PP=  0.00
Building CSP loop with anchor residues VAL 280 and LEU 287
Building CSP loop with anchor residues MET 279 and LEU 287
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
Building CSP loop with anchor residues MET 279 and ASN 288
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
Building CSP loop with anchor residues MET 279 and PRO 289
Number of Ligations found: 500
all loops are bad; continuing CSP with larger segment
+++ Warning: CSP Loop Insertion Failed, will use SparePart later
Finding Spare-Part loop with anchor residues ALA 52 and TYR 63
ACCEPTING loop  24 from 3EST_  Clash=   4 FF=        602.4 PP=95.16
BadPhi=   0 BadGX=   0 BadXP=   0 weakXP=   0 Score= 6.00  rms= 0.00
Finding Spare-Part loop with anchor residues THR 134 and ASP 154
Sorry, no loop could be found in the database
Finding Spare-Part loop with anchor residues GLU 133 and ASP 154
Sorry, no loop could be found in the database
Finding Spare-Part loop with anchor residues PRO 132 and ASP 154
ACCEPTING loop   4 from 2FB4L  Clash=   5 FF=       -648.7 PP=97.04
BadPhi=   4 BadGX=   0 BadXP=   2 weakXP=   3 Score=13.25  rms= 0.00
Finding Spare-Part loop with anchor residues GLU 278 and PRO 289
ACCEPTING loop  74 from 1LFAA  Clash=   4 FF=        150.4 PP=94.89
BadPhi=   0 BadGX=   0 BadXP=   0 weakXP=   0 Score= 6.00  rms= 0.00
Optimizing Sidechains
Adding Hydrogens
Optimizing loops and OXT (nb = 58)
Final Total Energy:       -4490.163 KJ/mol
Dumping Sequence Alignment
```

Template Selection Log:

Ligand Modeling Log:

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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