

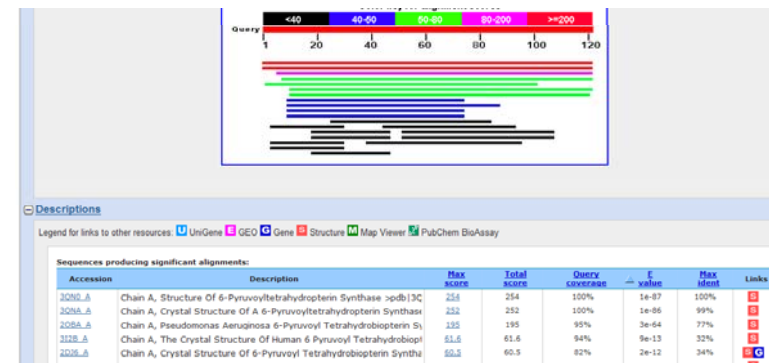
Protein 3D structure prediction

SWISS-MODEL: <http://swissmodel.expasy.org/>

Find 3D template

BlastP: using pdb database

Jpred



UNIVERSITY OF DUNDEE

Jpred3
Incorporating Jnet

The Barton Group

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Match found in PDB

You might want to reconsider the accuracy and what you might gain from secondary structure prediction, if close sequence homologues exist in the structural database.

If you still want to carry out a Jpred prediction click [continue](#)

Hits found

PDB	Chain	Description	Blast E-value
3qn9	B	6-pyruvoyl tetrahydrobiopterin SY...	4e-70
3qn9	A	6-pyruvoyl tetrahydrobiopterin SY...	4e-70
3qn0	F	6-pyruvoyl tetrahydrobiopterin SY...	4e-70



[myWorkspace]

[login]

SwissModel Automatic Modelling Mode

Email:

Project Title:

Provide a protein sequence or a UniProt AC Code: 

Advanced options:

Use a specific template: 

PDB-ID:

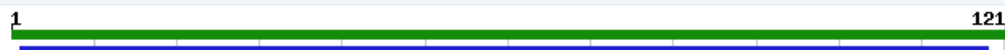
Chain:

or

Template file: 

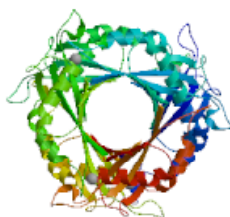

[\[myWorkspace \]](#)
[\[login \]](#)

Workunit: P000009 bPTPS - Overview



Print/Save this page as

Model Summary



Model information:

Modelled residue range: 2 to 119
Based on template: [3qn9A] (2.93 Å)
Remark: No search for template was performed.
Only user specified template was used for modelling.
Sequence Identity [%]: 100
Evalue: 3.98e-66

Quality information: [\[details\]](#)

QMEAN Z-Score: -0.82



Quaternary structure information: [\[details\]](#)

Template (3qn9): HEXAMER
Model: HEXAMER

Ligand information: [\[details\]](#)

Ligands in the template: ZN: 6.
Ligands in the model: ZN: 4

logs: [\[Templates\]](#) [\[Alignment\]](#) [\[Modelling\]](#)

display model: as [\[pdb\]](#) - as [\[DeepView project\]](#) - in [\[AstexViewer\]](#)

download model: as [\[pdb\]](#) - as [\[Deepview project\]](#) - as [\[text\]](#)

Global Model Quality Estimation [\[+/-\]](#)

QMEAN4 global scores:			Local scores	
QMEANscore4	Estimated absolute model quality	Score components	Coloring by residue error	Residue error plot
0.73		QMEAN: -0.82 CB interaction: -0.52 all atom interaction: 1.08 solvation: 0.05 hydrogen bond: -1.57	 [save jpg]	 [save png]

Structural alignment

ESPrpt: <http://esprpt.ibcp.fr/ESPrpt/ESPrpt/>

Execute ESPrpt: <http://esprpt.ibcp.fr/ESPrpt/cgi-bin/ESPrpt.cgi>

Upload aligned file (clustal format):
 template structure sequence
 model structure sequence

Upload secondary structure
 template structure

Click submit

To include model structure go to advanced

Assignment

Homology modelling with the most homologous bacterial protein

Structural alignment with ESPript

Evaluate similarity in 3D structure & secondary structure
run rasmol to show 3D pictures