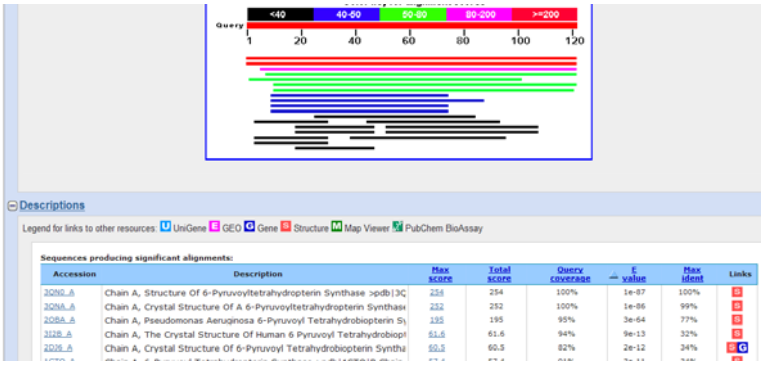
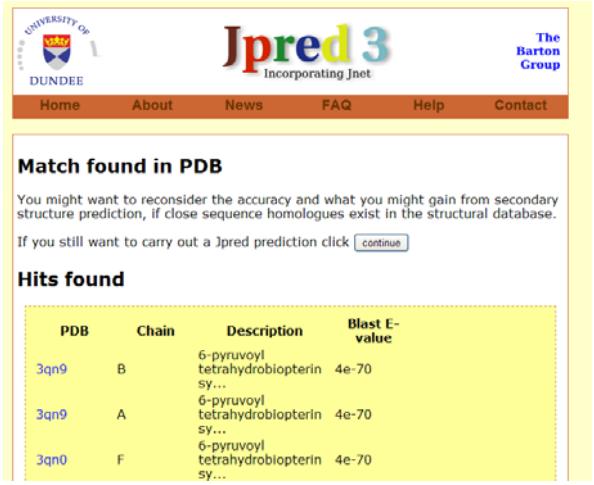
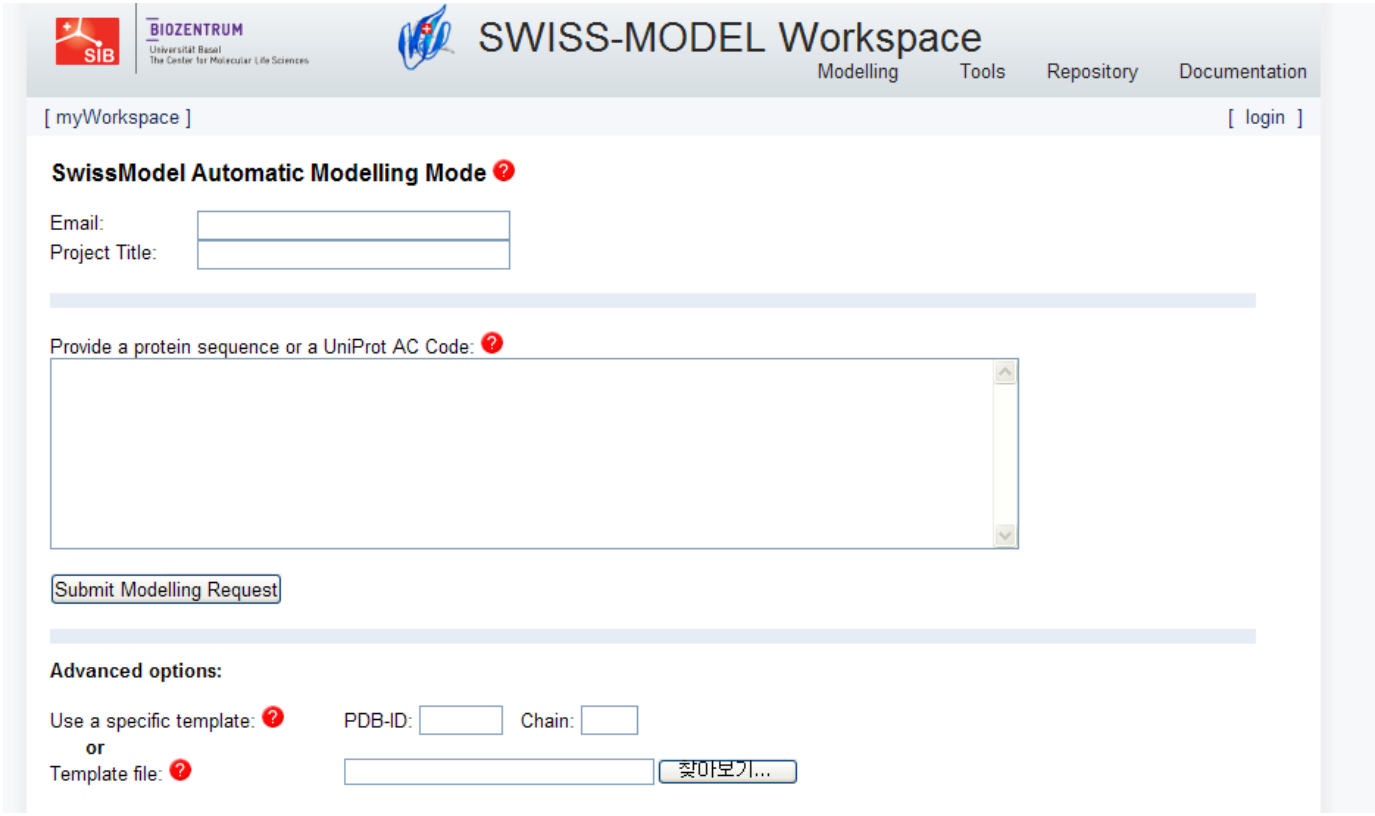
Protein 3D structure prediction

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

Find 3D template
BlastP: using pdb database
Jpred (http://www.compbio.dundee.ac.uk/www-jpred/index.html)



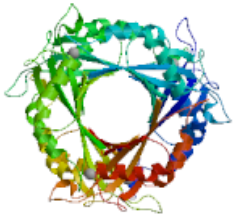



BIOZENTRUM
Universität Basel
The Center for Molecular Life Sciences
SIB
SWISS-MODEL Workspace
Modelling
Tools
Repository
Documentation
[myWorkspace]
[login]
SwissModel Automatic Modelling Mode
Email:
Project Title:
Provide a protein sequence or a UniProt AC Code:
Submit Modelling Request
Advanced options:
Use a specific template:
PDB-ID:
Chain:
or
Template file:
찾아보기...

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

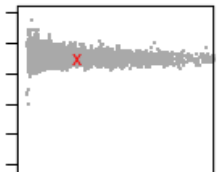
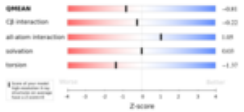
Quality information: [details]
QMEAN Z-Score: -0.82

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			[save jpg]	[save png]

Structural alignment

ESPript: http://espript.ibcp.fr/ESPript/ESPript/

Execute ESPript: http://espript.ibcp.fr/ESPript/cgi-bin/ESPript.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