SwissModel output options

SwissModel will return all results by email. Make sure, the email adress you provide in the request form is correct. The following options for the SwissModel results are available on the request pages:

File format:

❑   Short mode : will return only the final model as PDB-file

❑   Normal mode : will return the final model co-ordinates as PDB-file and the log-file tracing all actions taken by the server.

❑   SPDBV mode (default) : will return a SwissPDB viewer project file containing the final model co-ordinates and all templates superimposed.

   SwissPDB viewer [1,2] can be downloaded for free at: http://www.expasy.ch/spdbv/

Mail attachment:

SwissModel will return the final model co-ordinates as email attachment. If you linked the MIME type *chemical/pdb* to Swiss-PDB Viewer, you will be able to open the results directly by clicking on the attachment. If your mail program has difficulties receiving mail attachments, you may specify to receive the pdb-file as **plain ASCII** text. In this case, you have to save the incomming mail as a text file. Use any text editor to **remove all remaining mailheaders** from this file before loading it to your viewer. Valid lines in a PDB-file look like these:

```
HEADER     OXYGEN TRANSPORT                          14-SEP-94   1GDI      1GDI   2
COMPND     LEGHEMOGLOBIN (CARBON MONOXY)                                   1GDI   3
SOURCE     YELLOW LUPINE (LUPINUS LUTEUS L) ROOT NODULES                   1GDI   4
ATOM     1  N   GLY    1      52.779 -31.746  48.172  1.00 63.89          1GDI 327
ATOM     2  CA  GLY    1      52.019 -31.327  49.357  1.00 66.59          1GDI 328
ATOM     3  C   GLY    1      50.757 -30.516  49.051  1.00 65.69          1GDI 329
ATOM     4  O   GLY    1      49.642 -30.975  49.410  1.00 66.22          1GDI 330
```

WhatCheck report

A WhatCheck report [3] of the final model can be generated and sent in a seperate mail. This can help you to evaluate the quality of the model and identify regions of the model that might contain errors. The report generated by SwissModel is a subset of the original protein verification tools from the WHAT IF package. For further information see http://www.sander.embl-heidelberg.de/whatcheck/.

[1] Guex N and Peitsch MC (1999) Molecular modelling of proteins. Immunology News 6:132-134.
[2] Guex N, Diemand A and Peitsch MC (1999) Protein modelling for all. TiBS 24:364-367.
[3] Errors in protein structures. R.W.W. Hooft, G. Vriend, C. Sander, E.E. Abola, Nature (1996) 381, 272-272.

Viewing SwissModel results

SwissModel will return all results by email. For a typical SwissModel request you should receive the following answers:

❑ „Welcome message": is sent when the server starts working on this request; contains a unique process identifyer, e.g. **AAAa123456**

❑ „SwissModel News" (optional): about recent changes ...

❑ „Trace Log" (only *Normal* and *SPDBV mode*): Detailed log listing all actions taken by the modelling server.

❑ **„Modelling results"**: One or several mails containing the final model co-ordinates in PDB – format (*Short* or *normal mode*) or SPDBV-project file.

❑ „WhatCheck report" (optional): WhatCheck[4] report of the final model.

If you have problems opening the email attachment with the final model co-ordinates, use the „plain ASCII" option (see previous chapter: **SwissModel output options**).

For displaying and analysing SwissModel results, we recommend to use SwissPDB viewer [5,6], (SPDBV) which can be downloaded for free at: *http://www.expasy.ch/spdbv/.* If you are using a different viewer program, please use the *normal* or *short* output option and refer to the corresponding user manual. (Note: SPDBV project files will **not** be displayed correctly with RASMOL or chime.)

The following steps only summarize briefly how to display a model with spdbv. Please refer to the SPDBV user manual [7,8] for detailed instructions:

1. Load the model co-ordinate file from disk [File: Open PDB File]
2. Open the control panel [Window: Control Panel] to control the display properties of residues, chains and structures of the current layer.
3. Use the Layers Info [Window: Layers Info] to toggle the currently active layer and layer visibilty.
4. Open the Align Window [Window: Alignment] to check the alignment used during model building, especially the correct placemant of insertions / deletions.
5. Open the WhatCheck report [File: Open Text] to check the model for doubtful regions.

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[4] For further information about WhatCheck see *http://www.sander.embl-heidelberg.de/whatcheck/*
[5] Guex N and Peitsch MC (1999) Molecular modelling of proteins. Immunology News 6:132-134.
[6] Guex N, Diemand A and Peitsch MC (1999) Protein modelling for all. TiBS 24:364-367.
[7] Manual, tutorials and program updates are available at: http://www.expasy.ch/spdbv
[8] There is a detailled introduction and tutorial to SPDBV available at Gale Rhodes Website:
   http://www.usm.maine.edu/~rhodes/SPVTut/index.html