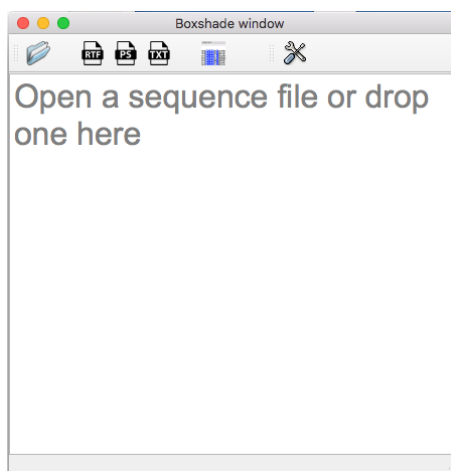


## RUNNING THE PROGRAM

When **pyBoxshade** first starts, it will create a preferences file, in *user/Library/Preferences* on Mac OSX, or in the *user* area of the registry if on Windows. This should be transparent to the user.

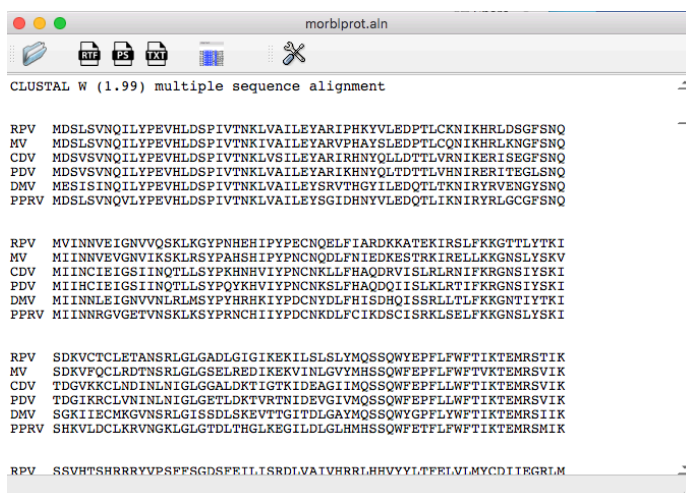
The main window looks like this:



You can drop files onto the window and the program will attempt to open them. Note that it currently only deals with one alignment at a time, so it will open the first file of a group if you drop multiple files.



(“Open”) opens a multiple sequence alignment file. This will be displayed in the main window, to allow the user to check the correct file has been imported, e.g.



The other options from this window are:



make RTF file using current parameters (program will ask for the name of the file to save using the normal dialogs)



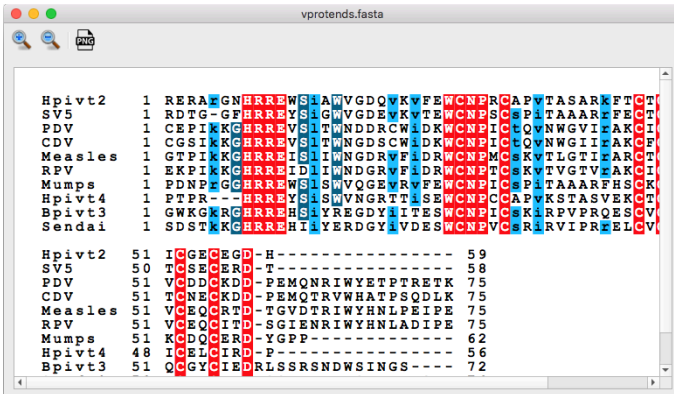
make PS file using current parameters (program will ask for the name of the file to save using the normal dialogs)



create a text file using the current parameters (program will ask for the name of the file to save using the normal dialogs)



open a window to show an image drawn using the current parameters;

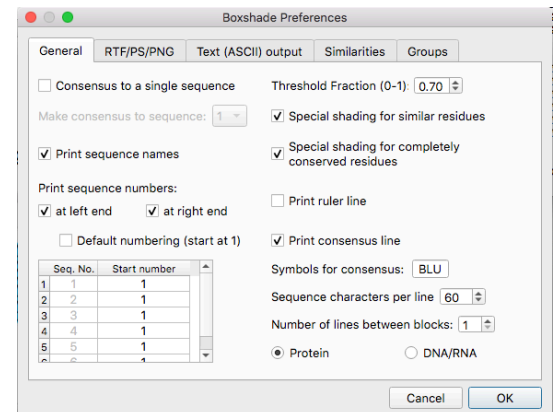


from this window the image may be saved by pressing the PNG icon (program will ask for the name of the file to save using the normal dialogs).

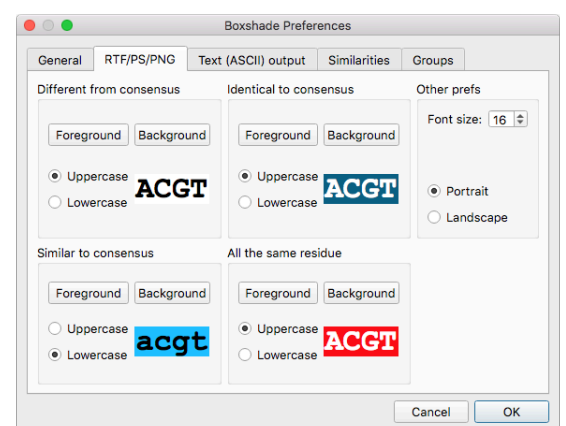


Open a dialog to adjust any of the program parameters. The Preferences dialog has a number of tabs:

1) General: This pane controls many parameters controlling what will be included in the image and what kind of consensus will be used.



2) RTF/PS/PNG : Foreground and background colours are set here, as also whether the amino acid/base will be shown in uppercase or lowercase for a particular type of conserved residue, font size, and Portrait/Landscape for PS files.



3) ASCII/Text: This is a very simple dialog that allows the user to set the character that will be used for amino acids/bases that are different to/identical to/similar to/globally conserved/ relative to the consensus sequence.

**Boxshade Preferences**

General RTF/PS/PNG Text (ASCII) output Similarities Groups

**Text (ASCII) output is only for comparison to a specific sequence.**

In the boxes below, enter the single character to be used to represent residues that are Different from, Identical to, or Similar to the consensus, or to be used when all sequences have the same residue (Conserved). Use upper or lowercase 'L' (L or l) to indicate the character itself or the lower case version of that character

Different: [ L ] Identical: [ . ] Similar: [ I ] Conserved: [ \* ]

Cancel OK

4) Sims: Table to allow the user to define which amino acids/bases will be considered similar to each amino acid/base in the consensus.

**Boxshade Preferences**

General RTF/PS/PNG Text (ASCII) output Similarities Groups

**Residues to be considered similar for shading purposes**

The "Sims" table allows one to set, for each amino acid (or nucleic acid), which residues are considered to be similar to it if it is the consensus residue. Each amino acid/base can have multiple amino acids/bases that are to be considered similar, or none, and amino acids/bases can appear multiple times on the "similar to" side. The relationship is one way, e.g. saying that H is similar to a consensus K does not make K similar to a consensus H.

	Amino Acid	Similar to:		Nucleic Acid	Similar to:
1	A	G	1	A	GR
2	C		2	C	TY
3	D	EN	3	G	
4	E	DQ	4	T	
5	F	YW	5	K	
6	G		6	M	
7	H	KR	7	R	
8	I	LM	8	S	
9	K	RH	9	W	
10	L	IM	10	Y	
11	M	IL	11	B	
12	N	EQ	12	D	
13	P	G	13	H	
14	Q		14	V	
15	R	KH			
16	S	T			
17	T	S			

Cancel OK

5) Grps: Table to allow the user to define which amino acids/bases will be considered similar when forming a "consensus by similarity" (see above).

**Boxshade Preferences**

General RTF/PS/PNG Text (ASCII) output Similarities Groups

**Residues to be considered as groups for shading purposes**

The "Groups" table defines groups of amino acids (or nucleic acids) which are to be considered similar when establishing a group consensus (e.g. all positive charged, all large hydrophobic, all purines). These relationships are multiway, e.g. making a group "LMFY" establishes relationships between all four amino acids.

	Amino Acid Groups		Nucleic Acid Groups
1	FYW	1	AGR
2	ILVM	2	CTY
3	DE	3	
4	GAP	4	
5	ST	5	
6	NQ	6	
7	RKH	7	
8		8	
9		9	
10		10	
11		11	
12		12	
13		13	

Cancel OK

## A note on fonts

The PostScript (PS) output expects Courier-Bold to be available on the system where the PS file is viewed; this font was chosen because it is a traditional PS font that is normally available as a PS or TrueType font on MacOSX and Windows. On Windows systems, if using Ghostscript or similar to view a PS file, a similar-looking font is used (Nimbus Mono). The image may look strange if no Courier (or substitute) font is available on your system (e.g systems set up using non-Roman scripts such as Chinese or Japanese).

The font used in the RTF files is Courier New by default. This is primarily historical, because it was assumed that the files would be opened with MS Word. An advantage of the RTF files, however, is that one can change the font just as with any word processed document; note that if the font used is not a monospaced font the alignment will no longer

be properly aligned.

The font used in the PNG pictures depends on the operating system. I tried to avoid any system dependence, but the fact remains that Courier on MacOSX looks a lot better than Courier New, while the reverse is true on Windows, so on those two platforms the better font is selected. On Linux, it is very hard to predict what fonts will be available. On a basic Ubuntu installation, you are likely to get the font Liberation Sans Mono, which is OK-ish. If you install the free MS-Core TrueType fonts, you will get Courier New, which is better.

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The people at the Qt Company who make the Qt application framework

Freepik at [www.flaticon.com](http://www.flaticon.com) for some of the icons I use