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Add your own data into the B-factor Field in pdb files

For your own data: this script that takes a pdb file and updates it with a two-column table (residue number vs whatever you'd like to plot). You run that and then colour the model according to b-factor in your favourite program.

Here's how it works:  
- generate a table with your data, no more than two decimal places.   
- it is important to normalise the numbers so that are smaller than 99.99, or in the range of +9.99 and -9.99 if using negative values.   
- do not include column titles, save as .txt  
- click selectPDB, choose the file you would like to modify  
- click on B-factors, choose your table  
- chain: which chain of the pdb file you would like to modify  
- ResPDB: name of the output file

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Additional feature. Does not change the B factors but shifts the residues number in the PDB file.   
- residue index shift: some pdb files don't have the same numbering as the protein sequence.

PDB can start with residue 1 which may be position 20 in the protein sequence. Very common for models.

This option takes a PDB file and shofts thw residue numbers inside by the “shift”.

For example, +19 will change 1 to 20.

start with amino acid 1. You can enter the shift between your table and pdf here so it gets the numbers right. If the pdb starts with 20 and your table starts with 1, enter -20.

Needs

1) source file name

2) destination file name

3) Chain ID – will use it irrespective of the tick box next to it. If the chain ID does not exist in the file, it is best to add it using “Add chain ID” feature

4) Offset is added to the existing residues number, if the chain ID matches.

All ATOM records are modified.

======Add chain ID ==========

The reason for this is that some models may come with no chain ID.

The assumption is that all ATOM records correspond to one chain.

Source, destination, and chain ID to set

All ATOM records are modified.

Can also be used to change chain ID, with a caveat that all ID will be changed.