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The use of the PLS-CADD set by X-ray crystallographers is now providing a number of new exciting areas for activity such as upgrading models of structures where clashes are observed with available data to be able to understand the problem and to propose a solution in a structure model, or to allow for automated calculation of clash functions in structures. An example of the application of the new functionality is shown in Figure 6.5. In this example, an automatically generated clash function is superimposed on a model structure generated using the crystal structure of the protein interleukin-2. The manual process for model building would have been to manually build the DNA sequence, perform NCA, and finally construct the final structure model. The proposed "automated" process is to allow for the use of the DNA structure to generate the clash function as the model. Figure 6.5 Demonstration of new functionality; clash function generated automatically from the DNA structure. The use of clash functions is another recent addition to the PLS-CADD structure building functionality. These are generated for clash analysis using the sequence that is deposited for the structure with those that are in the PDB that are based on the same sequence. Clash functions and potential clashes with observed data are now calculated to provide an assessment of the quality of the structure being built. Examples of this functionality are shown in Figure 6.6. Firstly, the initial structure models are assessed for clash with data in the PDB. As Clash functions can also be used to assess model quality, this is shown in the following example. A model of crambin is built using the sequence, the NCA is performed, and the clash function is calculated using the deposited sequence against the sequence that is present in the PDB. This is then used to assess the quality of the model which can be seen in the red line in the left hand image. In the example in the right hand image, the clash function is used to assess clashes with experimental data. Experimental data is supplied in the form of a data file that is easily uploaded. In this case, the structure of crambin is modelled for the high-resolution crystal structure at 1.8 Å. This is done by uploading the clash function for crambin produced by the automated clash function generation in PLS-CADD against the structure at 1.8 Å. The comparison of the clash function against the experimental data is shown in the right hand image. In this image, a clash function calculation is shown

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(2008-10-10) DEMO (2008-10-10) PARKS: First of all, I would like to say, if there's any way I can help out with this demo, I'd love to. I am not a programmer, but I'd love to learn, especially if it helps out with what I'm doing. (2008-10-10) STUDY: I have the same problem. An empty file exported by MGL is very different from MGL my previous export. How can I fix this? COMPANY: I tried the latest stable release,.13, but it still use the old engine. (2008-10-10) OTW: I am sorry to hear about your problems. It sounds like something wrong with your installation. I'd recommend you try re-installing PLS-CADD and let us know what happens. (2008-10-11) FIX: I have successfully updated the interactive version. (2008-10-11) FIX: There is a link somewhere to previous versions, I can't remember it off hand, I'll see if I can dig it up. (2008-10-11) STUDY: I just tried the PLS-CADD 15 and it works fine. What about your old workspace, did you try to import? If your workspace is something like (2008-10-11) WEB: OK, I've figured out what's going on. There was an updated version of PLS-CADD developed separately. The Interactive version does not work well. I've sent you a patch for the non-interactive version. (2008-10-11) FIX: I was able to fix your workspace issue by reverting a few of the files you sent me back in late September. I have a new version of these files for you to test. Let me know if you find anything else. (2008-10-11) SOLUTION: I have tested your new workspace version and it works fine for me. (2008-10-11) SOLUTION: All I can say is there's something wrong with your installation. I'll try to help if I can find out what. (2008-10-11) FIX 6d1f23a050

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