CONTACT README

Complex III is a homodimer where each monomer is composed of 11 chains.

For each of the 11 chains from a monomer, we study the residues involved in contacting with residues from the remaining 21 chains from the dimer.

There is a script (**ChainX\_2bc1\_contact.pl**) for each of the 11 chains (where X goes from A to K). The imput file for all these scripts is **modified\_2bc1.txt**, which is a pdb-like file obtained from 1be3.pdb2 (pdb for the homodimer bc1 complex). These scripts give two output files: **ChainX\_Detailed\_2bc1\_Results.txt** and **ChainX\_Contact\_2bc1\_Set.txt**. The first of these files gives details about the atoms involved in the contacts, and the second one give the chain X residues involved in contact, ordered according to the primary structure of chain X.

The code **atoms\_contacting.pl** gives the number of atoms interacting with each chain X residue as well as the number of different residues interacting with each chain X residue. The imput file is **ChainX\_Detailed\_2bc1\_Results.txt** and a file name **temp.txt** that can obtained from **ChainX\_Contact\_2bc1.Set.txt** with minor modifications. The results provided for this script are shown in the terminal and can be copied and pasted in **ChainX\_Contact\_2bc1\_Set.txt**.