Multidock Manual Supplement

Graham R. Smith, Gidon Moont, and Michael J. E. Sternberg

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Biomolecular Modelling Laboratory
Imperial Cancer Research Fund
Lincoln's Inn Fields, P.O. Box 123
London, WC2A 3PX
England

Atom Names and Order

Problems can be caused by the **ordering of atoms** within a residue in a pdb file. Multidock expects N CA C O (CB etc...). This is the most common ordering found in the PDB, but there are many exceptions and irregularities and neither multidock nor preprocess-pdb.perl are capable of fully reordering a pdb file by themselves. Also, pdb files produced by Molecular Dynamics programs commonly have a different atom ordering: N (H) CA (CB etc...) C O. Problems have also been caused by atom names, e.g. the δ-carbon in ILE should be called CD1 not just CD. Errors in atom ordering typically produce error messages like "problem equivalencing atoms in same residue".

Output Contains only the Interface

The output pdb file from multidock will not contain any atoms further from the interface than cut_jface. This makes it difficult to splice the output back into the pdb input file. We provide the perl script **multidock.perl** to help with this but do not guarantee it to run: you may need to modify it

for your own pdb file. It may be better to avoid the necessity of splicing back the output file by **increasing cut_jface** to include the whole of both components, if this is possible without exceeding the maximum number of atoms or residues allowed (though the N-termini nitrogens in each chain may still be deleted). It is also possible to increase the other cutoffs slightly.

Example of a control parameters file:

An appropriate params.dat reflecting these changes would then be:

```
imobile_mol=1
mobile_mol=2
nterm_neutral=1
nterm_neutral=2
temp= 298.0
cut_jface= 50.0
cut_iface= 12.0
cut_atom_nb= 12.0
cut_res_nb=17.0
cut_lface=17.0
ftol = 0.0001
dielectric= 4.0
eatmax= 2.5
emax=0.4
#atom_params_on
#file_output_off
#screen_output_off
define_disulphides
DISUL  CYX E  22  CYX E 157
DISUL  CYX E  42  CYX E  58
DISUL  CYX E 136  CYX E 201
DISUL  CYX E 168  CYX E 182
DISUL  CYX E 191  CYX E 220
DISUL  CYX I   3  CYX I  20
DISUL  CYX I  10  CYX I  22
DISUL  CYX I  16  CYX I  27
```

The disulphide information at the end should obviously be changed to the correct values for your protein.