

BINDING AFFINITY PREDICTION of PROTEIN-LIGAND (BAPPL) server

README FILE  
METHOD 2

A SAMPLE PDB FILE IS SHOWN HERE

THE FILE HAS BEEN TRUNCATED TO  
HIGHLIGHT THE MAIN FORMAT FEATURES

```
000000000100000000020000000003000000000400000000050000
123456789012345678901234567890123456789012345678901234
ATOM      1  N      PRO      1      27.687  39.749   6.133
ATOM      2  H2     PRO      1      26.845  39.527   5.607
ATOM      3  H3     PRO      1      27.701  40.768   6.052
.
.
.
ATOM     29  NE2    GLN      2      29.788  36.842  -2.103
ATOM     30  HE21  GLN      2      30.228  36.885  -3.003
ATOM     31  HE22  GLN      2      28.925  37.332  -1.868
.
.
.
ATOM    1568  C      PHE     99      23.968  34.664  -9.752
ATOM    1569  O      PHE     99      23.695  35.887  -9.764
ATOM    1570  OXT    PHE     99      23.666  33.948 -10.733
ATOM    1571  N      PRO    100      21.136  35.166 -10.482
ATOM    1572  H2     PRO    100      20.836  34.681  -9.641
ATOM    1573  H3     PRO    100      22.135  34.952 -10.605
.
.
.
ATOM    3136  HD2    PHE    198      23.588  40.185   7.863
ATOM    3137  C      PHE    198      25.733  41.419   4.747
ATOM    3138  O      PHE    198      26.823  41.261   4.144
ATOM    3139  OXT    PHE    198      25.713  41.819   5.928
ATOM    3140  O8     DRG    199       2.583  28.101   3.356
ATOM    3141  C7     DRG    199       2.773  27.608   2.263
ATOM    3142  O9     DRG    199       2.172  28.050   1.304
ATOM    3143  C6     DRG    199       3.866  26.571   2.062
ATOM    3144  H15    DRG    199       3.546  25.910   1.254
.
.
.
```

## FORMAT DESCRIPTION

COLUMNS	DATA TYPE	DEFINITION
1 - 4	Record Name	"ATOM"
5 - 11	Integer	Atom number
12	Blank space	
13 - 16	Atom	Atom name
17	Blank space	
18 - 20	Residue name	Residue name
21	Blank space	
22 - 26	Integer	Residue number
27	Blank space	
28 - 38	Float	Orthogonal coordinates for x in Å
39 - 46	Float	Orthogonal coordinates for y in Å
47 - 54	Float	Orthogonal coordinates for z in Å

## SOME IMPORTANT INSTRUCTIONS

1. The Atom number should increase in serial order starting with '1'.
2. The Residue number should start with '1' and should increment serially with every next residue.
3. There should be no "TER" records separating two protein chains or a protein chain from the ligand.
4. Atom names with four characters like HE21, HE22 etc. should be represented as such and not like 1HE2, 2HE2 etc.
5. The protein chain should not be specified by any separate variable like 'A' 'B' etc.
6. The chain termination of a protein should be indicated by "OXT" record in the Atom name column.
7. The ligand / drug should be specified by "DRG" in the Residue name record and should be present as the last residue of the protein-ligand complex file.