

BINDING AFFINITY PREDICTION of PROTEIN-LIGAND complex containing ZINC
BAPPL-Z server

README FILE

A SAMPLE PDB FILE IS SHOWN HERE

THE FILE HAS BEEN TRUNCATED TO
HIGHLIGHT THE MAIN FORMAT FEATURES

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000000000100000000020000000003000000000400000000050000000006000000000700000000
123456789012345678901234567890123456789012345678901234567890123456789012345678
ATOM      1  N      PRO      1      27.687  39.749   6.133 -0.2020   1.8750   0.1700
ATOM      2  H2     PRO      1      26.845  39.527   5.607  0.3120   0.6000   0.0157
ATOM      3  H3     PRO      1      27.701  40.768   6.052  0.3120   0.6000   0.0157
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ATOM     29  NE2    GLN      2      29.788  36.842  -2.103 -0.9407   1.8240   0.1700
ATOM     30  HE21   GLN      2      30.228  36.885  -3.003  0.4251   0.6000   0.0157
ATOM     31  HE22   GLN      2      28.925  37.332  -1.868  0.4251   0.6000   0.0157
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ATOM    1568  C      PHE     99      23.968  34.664  -9.752  0.7660   1.9080   0.0860
ATOM    1569  O      PHE     99      23.695  35.887  -9.764 -0.8026   1.6612   0.2100
ATOM    1570  OXT    PHE     99      23.666  33.948 -10.733 -0.8026   1.6612   0.2100
ATOM    1571  N      PRO    100      21.136  35.166 -10.482 -0.2020   1.8750   0.1700
ATOM    1572  H2     PRO    100      20.836  34.681  -9.641  0.3120   0.6000   0.0157
ATOM    1573  H3     PRO    100      22.135  34.952 -10.605  0.3120   0.6000   0.0157
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ATOM    3136  HD2    PHE    198      23.588  40.185   7.863  0.1408   1.4590   0.0150
ATOM    3137  C      PHE    198      25.733  41.419   4.747  0.7660   1.9080   0.0860
ATOM    3138  O      PHE    198      26.823  41.261   4.144 -0.8026   1.6612   0.2100
ATOM    3139  OXT    PHE    198      25.713  41.819   5.928 -0.8026   1.6612   0.2100
ATOM    3140  Zn      ZN2    199      21.623  31.917   2.976  1.3726   1.9500   0.2500
ATOM    3141  O8      DRG    200       2.583  28.101   3.356 -0.7851   1.6612   0.2100
ATOM    3142  C7      DRG    200       2.773  27.608   2.263  0.7886   1.9080   0.0860
ATOM    3143  O9      DRG    200       2.172  28.050   1.304 -0.7851   1.6612   0.2100
ATOM    3144  C6      DRG    200       3.866  26.571   2.062 -0.0834   1.9080   0.1094
ATOM    3145  H15     DRG    200       3.546  25.910   1.254  0.0142   1.4870   0.0157
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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
55 - 62	Float	Partial atomic charges
63 - 70	Float	van der Waals parameter (R*)
71 - 78	Float	van der Waals parameter (ϵ)

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 or the zinc ion.
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.
8. The zinc ion should have "Zn" as its atom type and "ZN2" as its residue name.
9. The PDB file should contain the partial atomic charges and van der Waals parameters for each atom in the format described.