

# Complex PDB documents using the Bioclipse ChildResourceCreator



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## Keywords

Bioclipse, Biojava, Cdk, Pdb, Jmol

## Abstract

Some time ago I blogged about the ChildResourceCreator extension point in Bioclipse and hinted as using that for PDB files. which contain 3D molecular models, sequences and bibliographic information. Using the new extension point, Bioclipse now treats PDB files as complex documents, creating child resources for the 3D molecular model (using the CDK plugin), and a sequence resource (using the BioJava plugin).

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Some time ago I blogged about the [ChildResourceCreator extension point in Bioclipse](#) and hinted as using that for [PDB files](#), which contain 3D molecular models, sequences and bibliographic information. Using the new extension point, [Bioclipse](#) now treats PDB files as complex documents, creating child resources for the 3D molecular model (using the [CDK](#) plugin), and a sequence resource (using the [BioJava](#) plugin).

The screenshot displays the Bioclipse application window. The **BioResource Navigator** on the left shows a tree structure with a 'test' folder containing several files, including '1SPX.pdb'. The central panel displays the PDB header for '1SPX.pdb', which is a glucose dehydrogenase from *Caenorhabditis elegans*. The header includes fields for title, compound, source, and keywords. The **Jmol View** on the right shows a 3D ribbon model of the protein structure. The **Sequence View** at the bottom displays the amino acid sequence of the protein, with residues numbered from 1 to 200.

**PDB Header:**

```

HEADER      OXIDOREDUCTASE
TITLE       CRYSTAL STRUCTURE OF GLUCOSE DEHYDROGENASE FROM CAENORHABDITIS ELEGANS
TITLE       2 CAENORHABDITIS ELEGANS
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: SHORT-CHAIN REDUCTASE;
COMPND      3 CHAIN: A;
COMPND      4 SYNONYM: GLUCOSE DEHYDROGENASE;
COMPND      5 EC: 1.1.1.1.47;
COMPND      6 ENGINEERED: YES
SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: CAENORHABDITIS ELEGANS;
SOURCE      3 GENE: D1054.8;
SOURCE      4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE      5 EXPRESSION_SYSTEM_COMMON_NAME: BL21;
SOURCE      6 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE      7 EXPRESSION_SYSTEM_VECTOR: PET28a(+);
SOURCE      8 EXPRESSION_SYSTEM_PLASMID: pET28a(+);
KEYWDS      PARALLEL BETA-SHEET OF SEVEN STRANDS;
KEYWDS      2 THREE ALPHA-HELICES ON EACH SIDE OF THE BETA-SHEET;
KEYWDS      3 ALPHA-HELIX ON TOP OF BETA-SHEET;
KEYWDS      4 PROTEIN STRUCTURE INITIALLY DETERMINED BY X-RAY DIFFRACTION;
EXPDTA      X-RAY DIFFRACTION
  
```

**Sequence View:**

```

M T R F A E K V A I I T G S S N G I G R A T A V L F A R E G A K V T I T G R H A E R L E E T R Q Q I
  5      10      15      20      25      30      35      40      45      50
L A A G V S E Q N V N S V V A D V T T D A G Q D E I L S T T L G K F G K L D I L V N N A G A A I P D
  55      60      65      70      75      80      85      90      95      100
S Q S K T G T A Q S I E S Y D A T L N L N L R S V I A L T K K A V P H L S S T K G E I V N I S S I A
  105     110     115     120     125     130     135     140     145     150
S G L H A T P D F P Y Y S I A K A A I D Q Y T R N T A I D L I Q H G I R V N S I S P G L V A T G F G
  155     160     165     170     175     180     185     190     195     200
G A M C N R E E T S K K E Y S T M A T M K E C Y R A G Y M C O R D L A E V I A E L A D R K T E C Y
  
```