48'th Annual Meeting of the Biophysical Society of Japan
at Tohoku University, on September 21, 2010

Tutorials for PDBj【1】

PDBj
Protein Data Bank Japan

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Institute for Protein Research,
Osaka University

http://www.protein.osaka-u.ac.jp/rcsfp/pi/

http://www.pdbj.org/

Tutorials【1】: How to view structures?

(1) Keyword Search → View Structure
→ Download Coordinates
→ Examine Several Information
→ Other Advanced Usages and Links

(2) Search by PDBID

(3) Search by Author Names

(4) Search by Sequence

(5) Advanced Search

Tutorials【1】: How to view structures?

(1) Keyword Search → View Structure
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Let's Search "アスパラギン合成酵素"
or "Asparagine Synthetase"
using the Keyword Search

Get Entry Data from browser, PDBj Mine

Access to *http://www.pdbj.org/*

Get Entry Data from our browser, PDBj Mine

(1) Keyword search in Japanese

Get Entry Data from our browser, PDBj Mine

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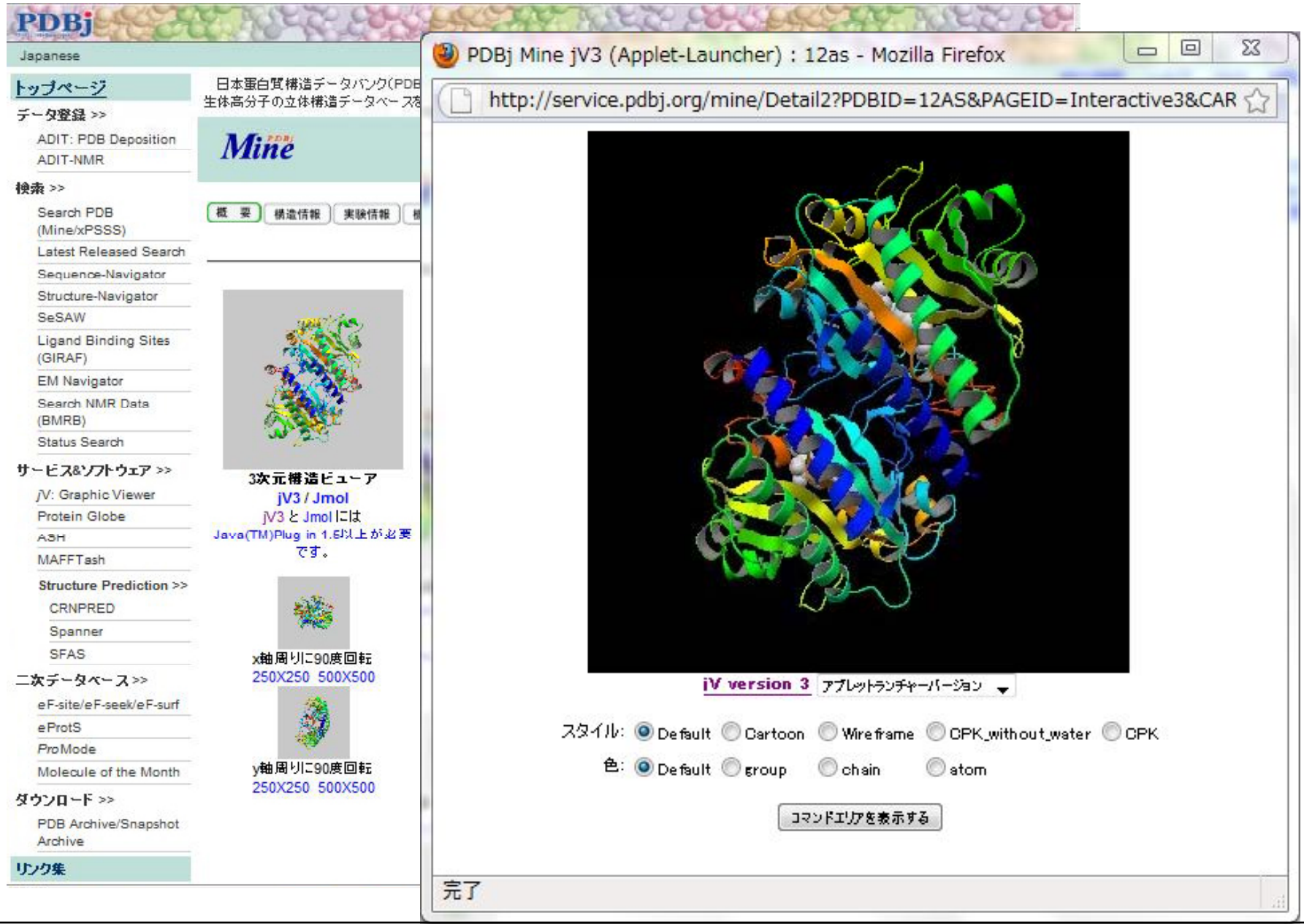
Get Entry Data from our browser, PDBj Mine

(1) Keyword search in Japanese



Graphic viewer: *j*V version 3.8

Access to *http://www.pdbj.org/jV/*

PDBjViewer (jV)

[Introduction | Basic Usage | Graphics Examples | Download & Install | Acknowledgment | jV wiki | PDBj Home]

Introduction

PDBjViewer (jV, for short) is a program to display molecular graphics of proteins and nucleic acids. jV supports the following features:

- jV can read and display PDBML files, the canonical XML format for the Protein Data Bank.
- Of course, jV can read and display the traditional PDB format files, too.
- RasMol-like usability.
- jV can process more than one molecules.
- jV can display polygons specified by XML. (XML Schema for polygons is available.)
- Multiple polygons can be processed simultaneously, and be superimposed onto molecular images.
- Animation can be realized. (Each frame of an animation is made of a single MODEL entity of the traditional PDB format file.)
- jV runs on the Java Runtime Environment (JRE) so that it can work as a stand-alone application as well as an applet.
- The graphics of jV is based on OpenGL (JOGL), thereby producing fairly beautiful pictures.

[Page top | Introduction | Basic Usage | Graphics Examples | Download & Install | Acknowledgment | jV wiki | PDBj Home]

Basic Usage

You can execute basic operations such as rotation and translation with mouse action. Major actions are described in the following table:

Action	Mouse Operation	
	Windows, Linux	Mac OS X
rotate around X (horizontal) axis rotate around Y (vertical) axis	left drag	drag
rotate around Z (anteroposterior) axis	Shift + right drag (move horizontally)	Shift + Command + drag (move horizontally)
translate along X axis (holizontally) translate along Y axis (vertically)	right drag	Command + drag
translate along Z axis (zoom in/out)	Shift + left drag	Shift + drag

Graphic viewer: *j*V version 3.8
Access to *jV wiki*

Log in

page | discussion | view source | history

Main Page

Welcome to jV wiki.

jV version 3 (formerly known as PDBjViewer) is a program to display molecular graphics of protein and nucleic acids. jV supports the following features:

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- jV runs on the Java Runtime Environment (JRE) so that it can work as a stand-alone application as well as an applet.
- The graphics of jV is based on OpenGL (JOGL), thereby producing fairly beautiful pictures.

The program 'jV' has been developed by Kengo Kinoshita (Graduate School of Information Sciences, Tohoku University) and Haruki Nakamura (Institute for Protein Research, Osaka Univeristy), with the support from JST-BIRD.

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- How to use
- Installation
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search

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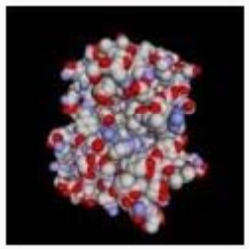
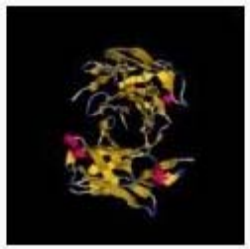
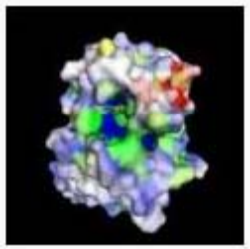
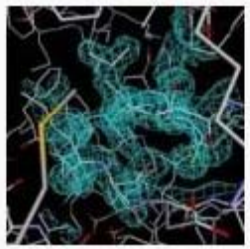
toolbox
- What links here
- Related changes
- Special pages
- Printable version
- Permanent link

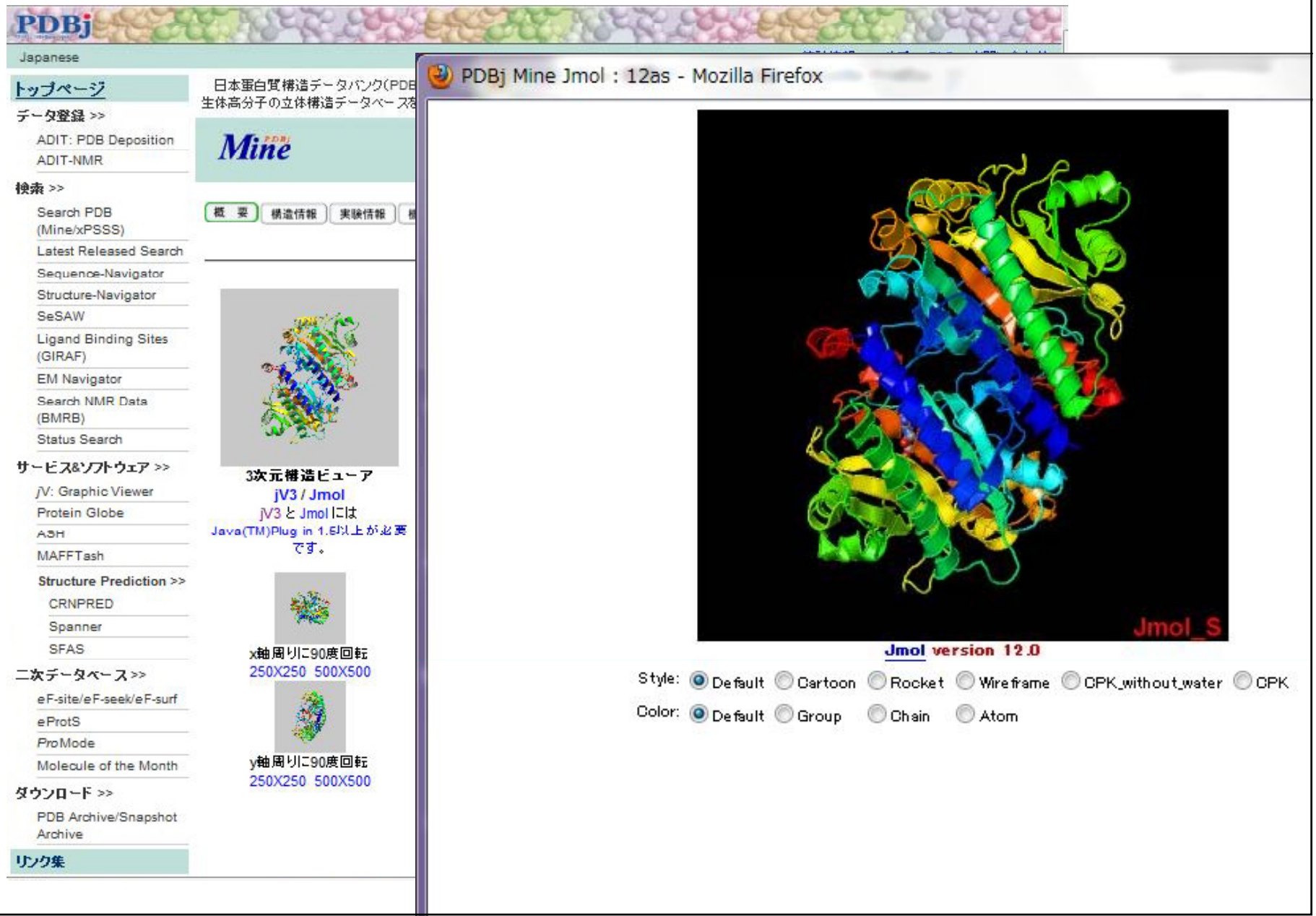





Get Entry Data from our browser, PDBj Mine

(1) Keyword search in Japanese

Get Entry Data from our browser, PDBj Mine

(1) Keyword search in Japanese

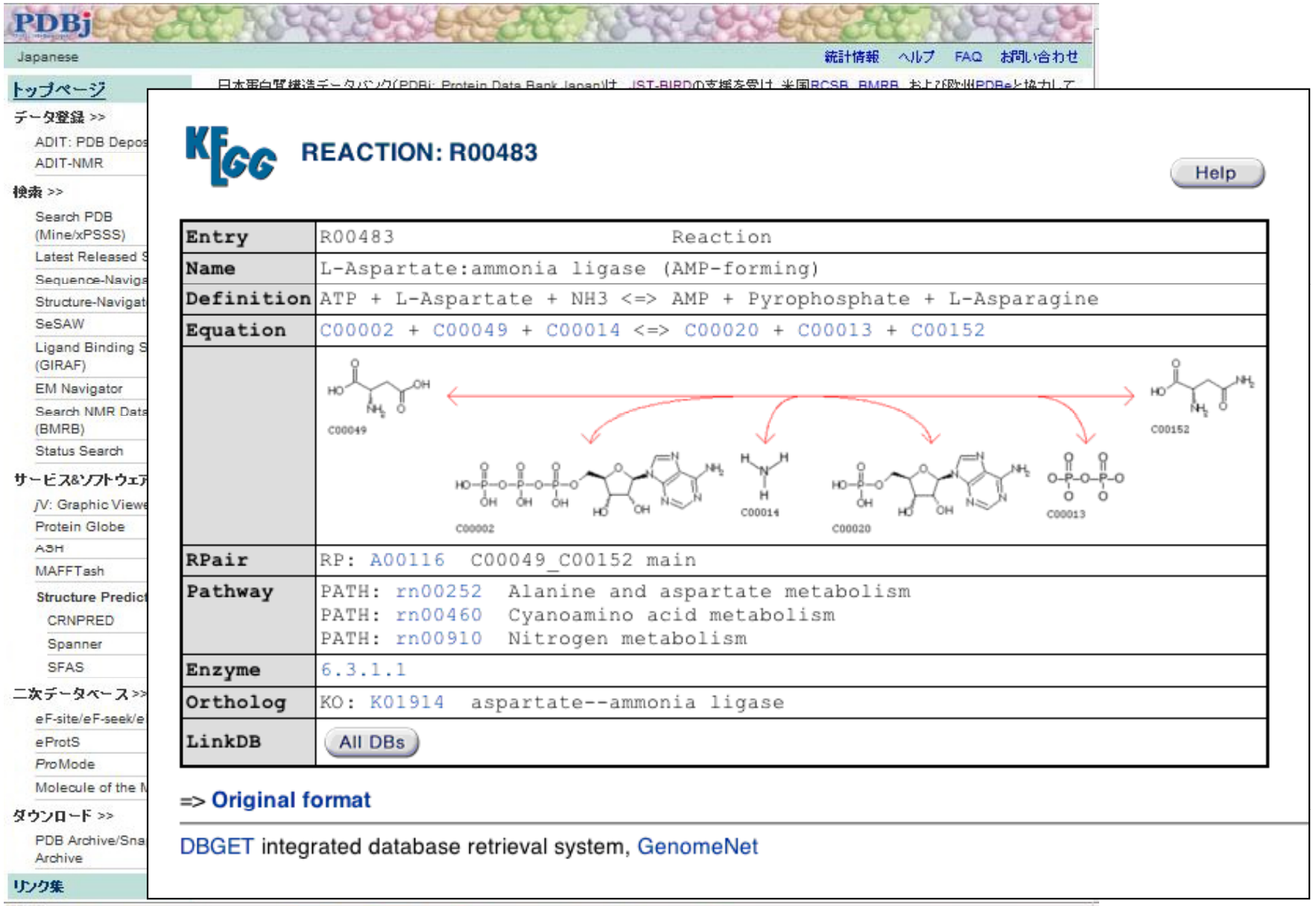


Get Entry Data from our browser, PDBj Mine

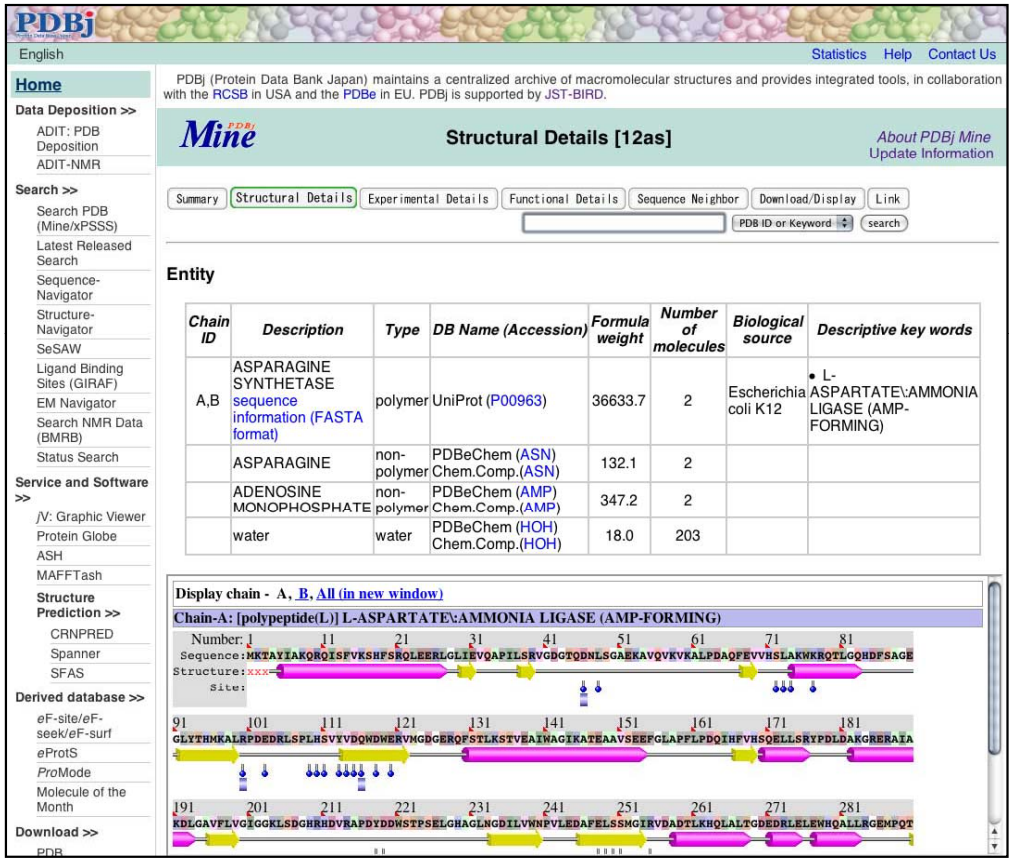
(1) Keyword search in Japanese

Get Entry Data from our browser, PDBj Mine

(1) Keyword search in Japanese



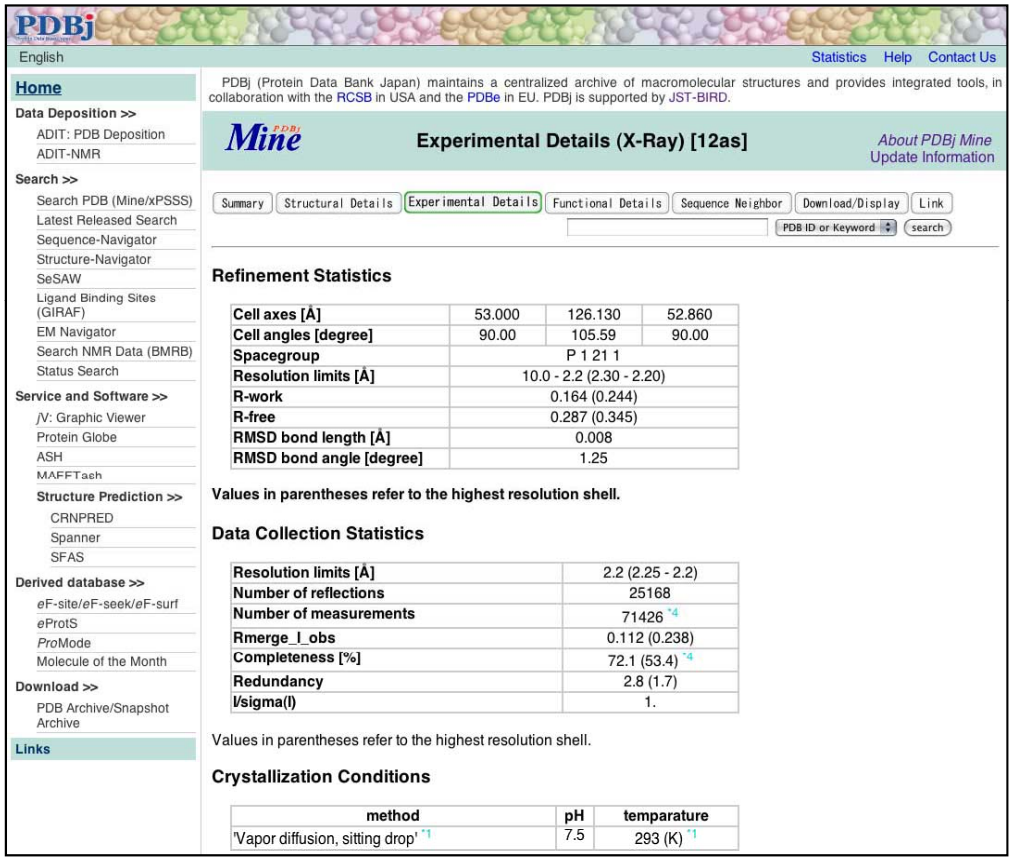
Several Information for each Entry: Structural Details



Details of the structure

- Name of the molecule(s)
- Molecular weight(s)
- Keywords
- Secondary structures, etc.

Several Information for each Entry: Experimental Details



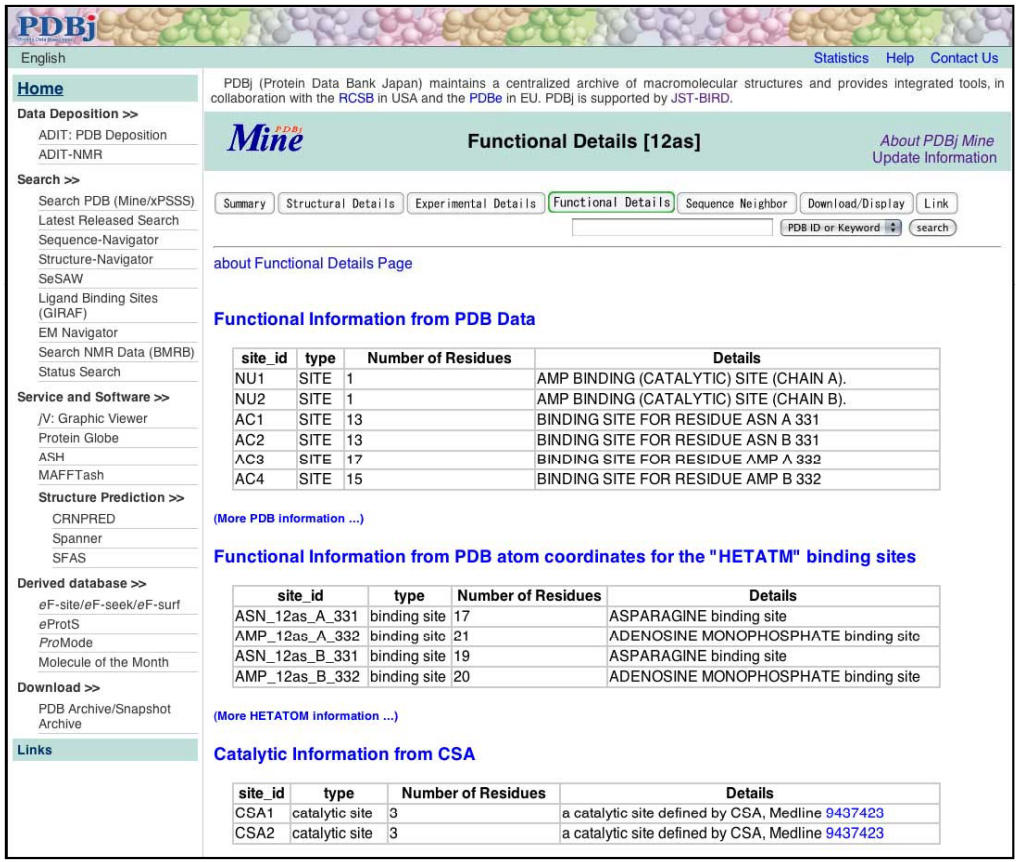
Details of the experiment

- Experimental method

(X-ray, NMR, EM, Neutron)

- Parameters for the crystal
- Crystallization conditions
- etc.

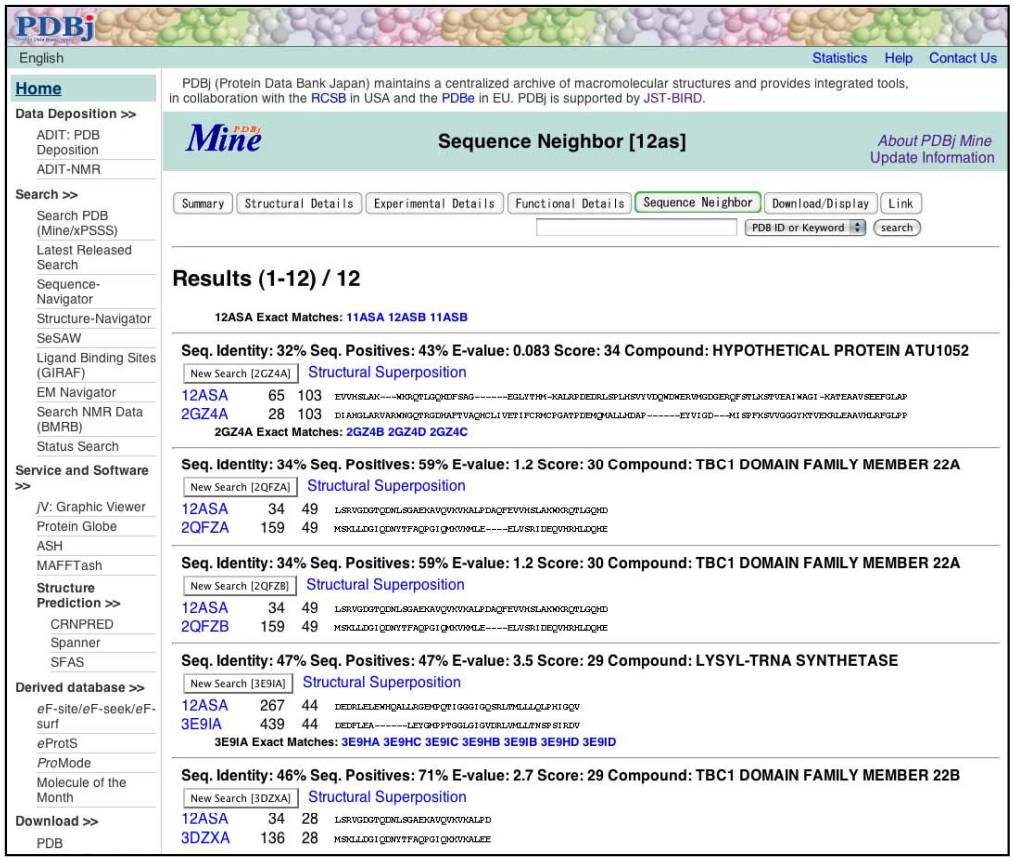
Several Information for each Entry: Functional Details



Details of the function

- Gene ontology information
- Ligand binding
- Functional site
- etc.

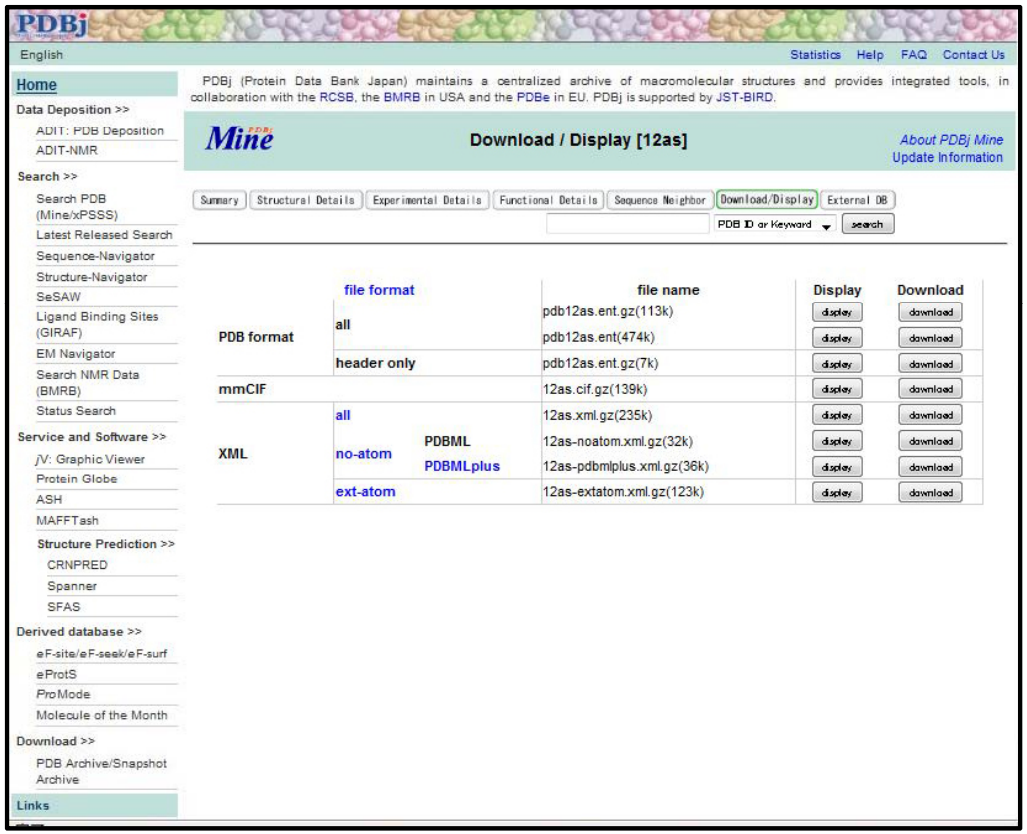
Several Information for each Entry: Sequence Neighbor



PDBID list of homologs

- Result of BLAST search
- Sequence Navigator is used.

Several Information for each Entry: Download/Display



Download or display of the archival data

- Conventional PDB format
- Conventional PDB header
- mmCIF
- PDBML/PDBMLplus
- PDBML without coordinates
- PDBML for only coordinates
- Structure factor

Data Formats of PDB data

- PDB (conventional and flat)
- PDB Exchange (mmCIF)
  - Mechanism for extension based on new demands
- PDBML
  - Derived from mmCIF
  - All entries converted to XML
  - Automatic translation from mmCIF data files and dictionaries
  - 3-styles of translation released

(Westbrook, Ito, Nakamura, Henrick, Berman (2005) Bioinformatics, 21, 988-992)

Example of PDBML for an atom coordinate.

```
ATOM      1  N   THR A   1      17.047  14.099   3.625  1.00 13.79
```

PDB-format

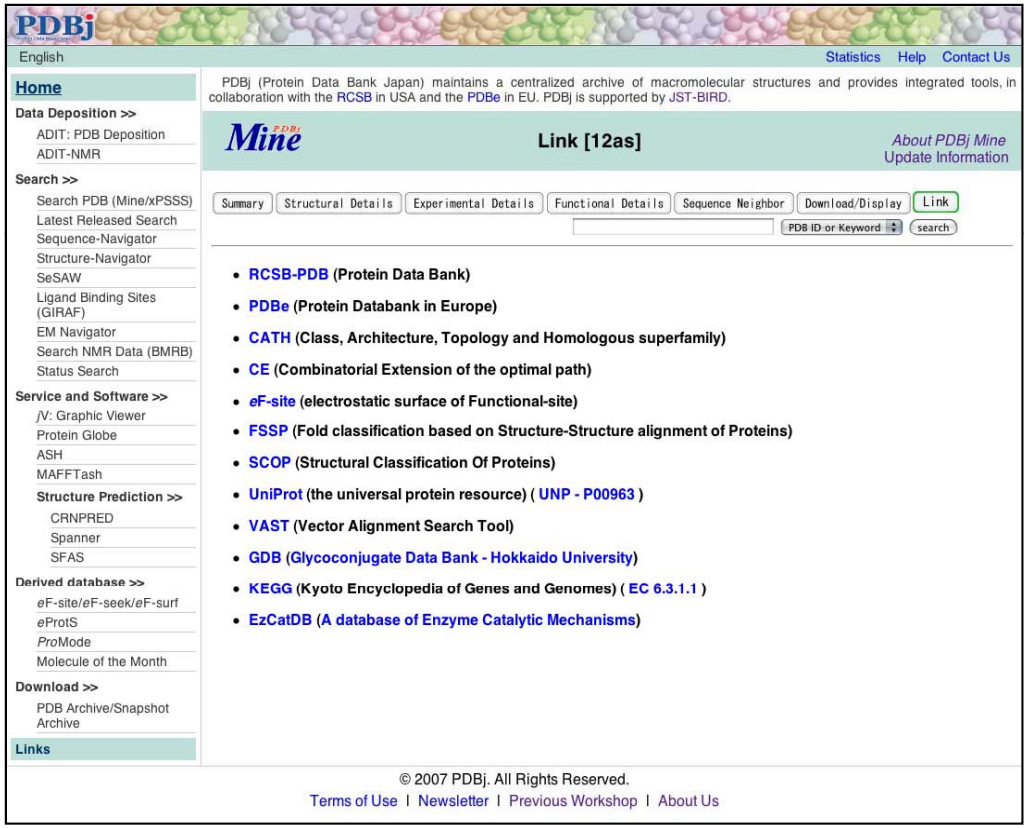
```
<PDBx:atom_siteCategory>
        <PDBx:atom_site id="1">
           <PDBx:group_PDB>ATOM</PDBx:group_PDB>
           <PDBx:type_symbol>N</PDBx:type_symbol>
           <PDBx:label_atom_id>N</PDBx:label_atom_id>
           <PDBx:label_comp_id>THR</PDBx:label_comp_id>
           <PDBx:label_asym_id>A</PDBx:label_asym_id>
           <PDBx:label_entity_id>1</PDBx:label_entity_id>
           <PDBx:label_seq_id>1</PDBx:label_seq_id>
           <PDBx:Cartn_x>17.047</PDBx:Cartn_x>
           <PDBx:Cartn_y>14.099</PDBx:Cartn_y>
           <PDBx:Cartn_z>3.625</PDBx:Cartn_z>
           <PDBx:occupancy>1.00</PDBx:occupancy>
           <PDBx:B_iso_or_equiv>13.79</PDBx:B_iso_or_equiv>
           <PDBx:auth_seq_id>1</PDBx:auth_seq_id>
           <PDBx:auth_comp_id>THR</PDBx:auth_comp_id>
           <PDBx:auth_asym_id>A</PDBx:auth_asym_id>
           <PDBx:auth_atom_id>N</PDBx:auth_atom_id>
           <PDBx:pdbx_PDB_model_num>1</PDBx:pdbx_PDB_model_num>
        </PDBx:atom_site>
```

Full-tag description

Separated file for coordinates

```
<atom_record id="1">ATOM 1 A A 1 1 ? . THR THR N N N 17.047 14.099 3.625 1.00 13.79</atom_record>
```

Several Information for each Entry: Link



Link to other databases

- RCSB-PDB, MSD-EBI
- CATH, SCOP, FSSP: folds
- UniProt: Sequences
- KEGG: Pathways
- EzCatDB: enzymes
- etc.

Tutorials【1】: How to view structures?

(1) Keyword Search → View Structure
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(2) Search by PDBID (PDBID: 12as)

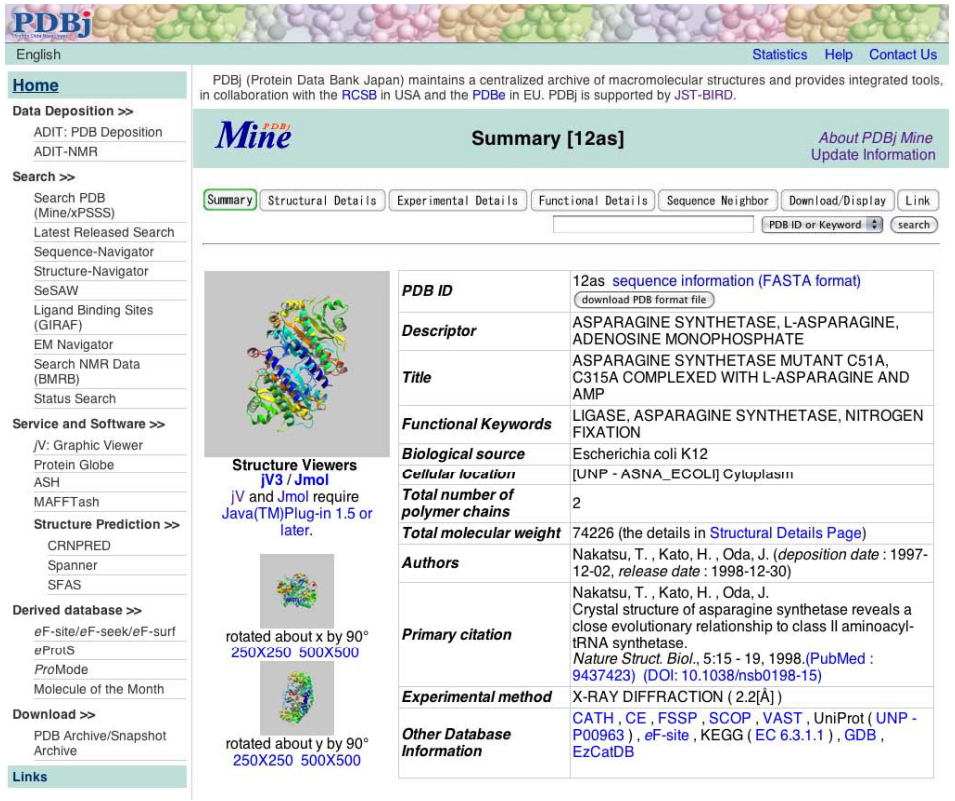
(3) Search by Author Names

(4) Search by Sequence

(5) Advanced Search

Get Entry Data from our browser, PDBj Mine

(2) PDBID search



PDBID (e.g. 12as) should be input in a box and GO → Summary for each PDBID is displayed.

Tutorials【1】: How to view structures?

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(2) Search by PDBID

(3) Search by Author Names (Oda, J.)

(4) Search by Sequence

(5) Advanced Search

Get Entry Data from our browser, PDBj Mine

(3) Search by Author Name

Get Entry Data from our browser, PDBj Mine

(3) Search by Author Name

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ADIT: PDB Deposition
ADIT-NMR
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Latest Released Search
Sequence-Navigator
Structure-Navigator
SeSAW
Ligand Binding Sites (GIRAF)
EM Navigator
Search NMR Data (BMRB)
Status Search
サービス&ソフトウェア >>
jV: Graphic Viewer
Protein Globe
ASH
MAFFTash
Structure Prediction >>
CRNPRED
Spanner
SFAS
二次データベース >>
eF-site/eF-seek/eF-surf
eProtS
ProMode
Molecule of the Month
ダウンロード >>
PDB Archive/Snapshot Archive
リンク集

日本蛋白質構造データバンク(PDBj: Protein Data Bank Japan)は、JST-BIRDの支援を受け、米国RCSB、BMRB、および欧州PDBeと協力して、生体高分子の立体構造データベースを国際的に統一化されたアーカイブとして運営するとともに、様々な解析ツールを提供しております。

Mine

検索結果ページ

日本語ページについて
PDBj Mineについて
更新情報

(PDB-IDをクリックすると、詳細情報をご覧いただけます)

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クエリ: Oda, J. PDB ID or Keyword 表示順: 一致件数

リセット 検索

2glt
分子名称 : GLUTATHIONE BIOSYNTHETIC LIGASE
タイトル : STRUCTURE OF ESCHERICHIA COLI GLUTATHIONE SYNTHETASE AT PH 6.0.
著者 : Matsuda, K., Yamaguchi, H., Kato, H., Nishioka, T., Katsube, Y., Oda, J.
実験手法 : X-RAY DIFFRACTION
登録日 : 1995-05-16
公開日 : 1995-07-31
ダウンロード

1gsh
分子名称 : GLUTATHIONE BIOSYNTHETIC LIGASE
タイトル : STRUCTURE OF ESCHERICHIA COLI GLUTATHIONE SYNTHETASE AT PH 7.5
著者 : Matsuda, K., Kato, H., Yamaguchi, H., Nishioka, T., Katsube, Y., Oda, J.
実験手法 : X-RAY DIFFRACTION
登録日 : 1995-05-16
公開日 : 1996-07-11
ダウンロード

1gsa
分子名称 : GLUTATHIONE SYNTHETASE, ADENOSINE-5"-DIPHOSPHATE, GLUTATHIONE
タイトル : STRUCTURE OF GLUTATHIONE SYNTHETASE COMPLEXED WITH ADP AND GLUTATHIONE
著者 : Hara, T., Kato, H., Nishioka, T., Katsube, Y., Oda, J.
実験手法 : X-RAY DIFFRACTION
登録日 : 1995-06-08
公開日 : 1996-06-20
ダウンロード

12as
分子名称 : ASPARAGINE SYNTHETASE, L-ASPARAGINE, ADENOSINE MONOPHOSPHATE
タイトル : ASPARAGINE SYNTHETASE MUTANT C51A, C315A COMPLEXED WITH L-ASPARAGINE AND AMP
著者 : Nakatsu, T., Kato, H., Oda, J.
実験手法 : X-RAY DIFFRACTION
登録日 : 1997-12-02

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(2) Search by PDBID

(3) Search by Author Names

(4) Search by Sequence (MKTAYIAKQRQISF)

(5) Advanced Search

Get Entry Data from our browser, PDBj Mine

(4) Search by Sequence

Get Entry Data from our browser, PDBj Mine

(4) Search by Sequence

Tutorials【1】: How to view structures?

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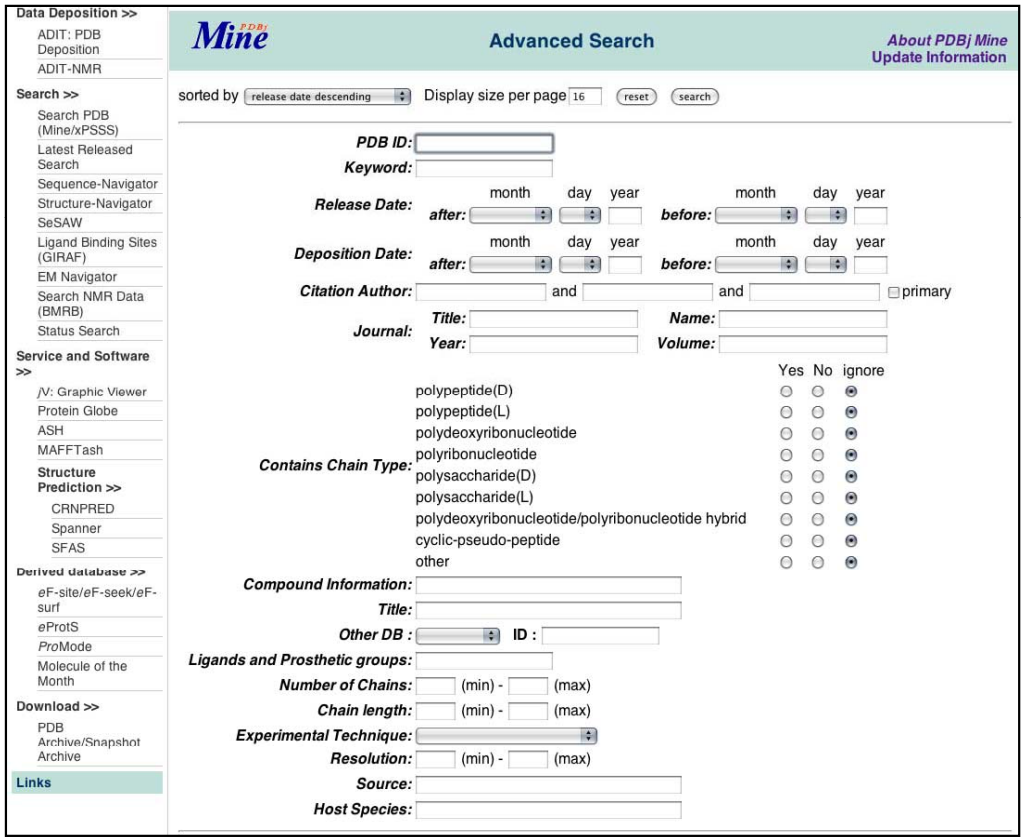
(5) Advanced Search

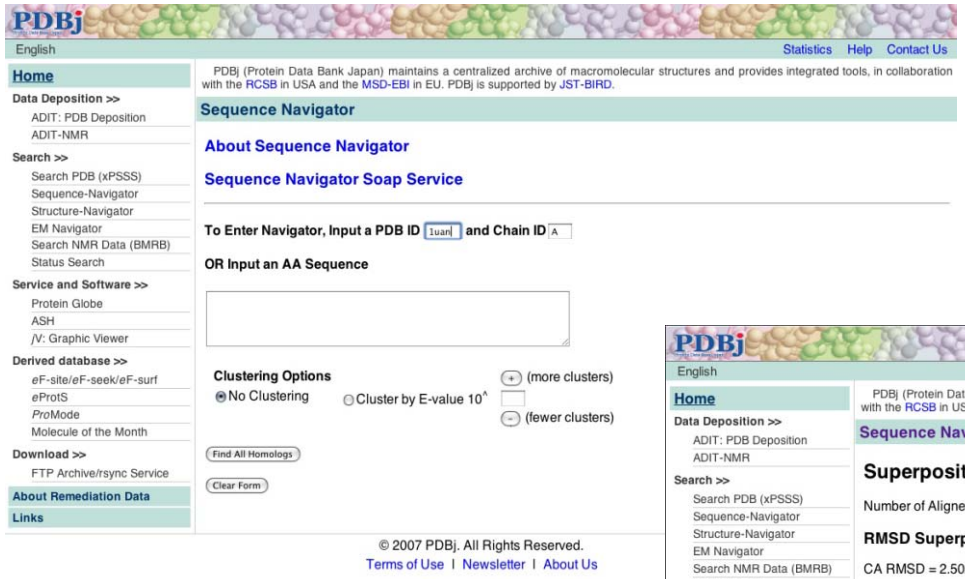
(5) Advanced Search
From "Advanced Search" on Top page

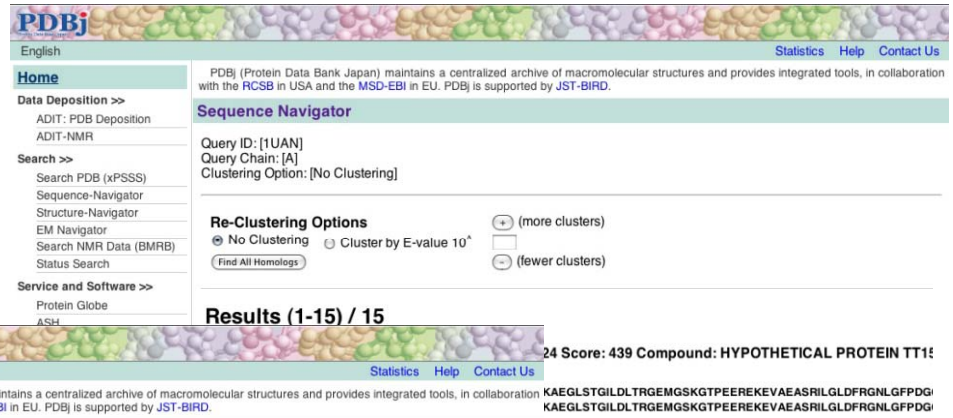


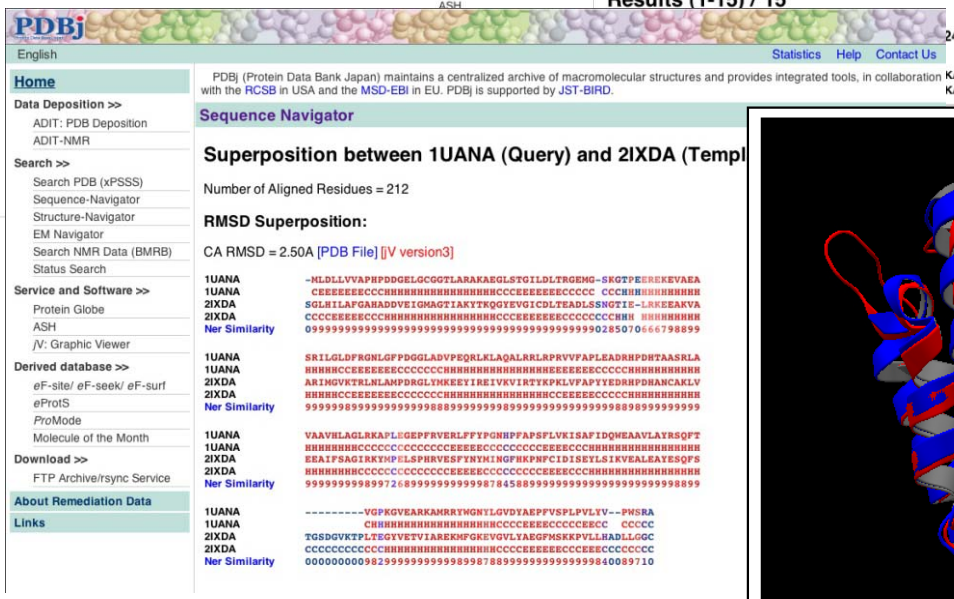
Search by many conditions

- Author names & Journal
- Experimental method
- Ligand name
- Residues
- Resolution
- Species
- etc.

Search of Similar Sequences: Sequence Navigator

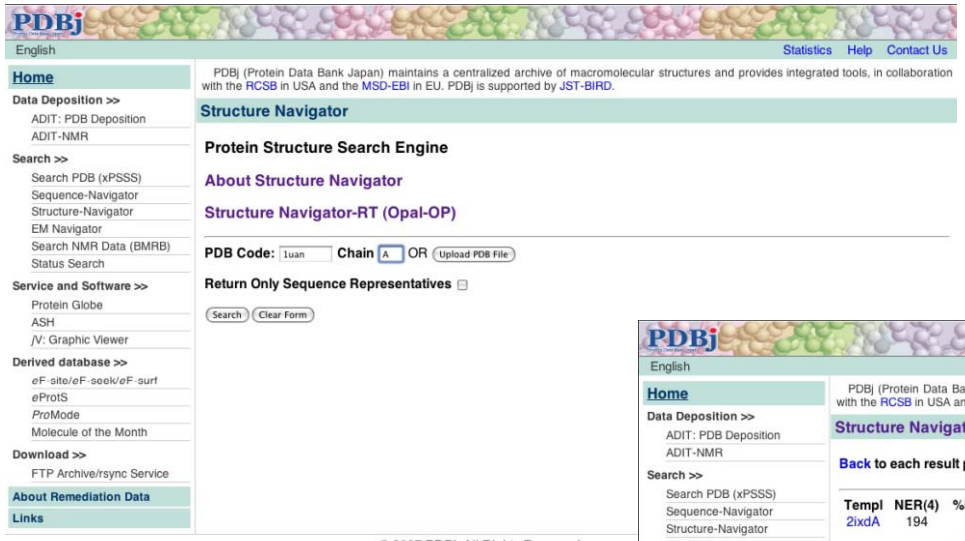


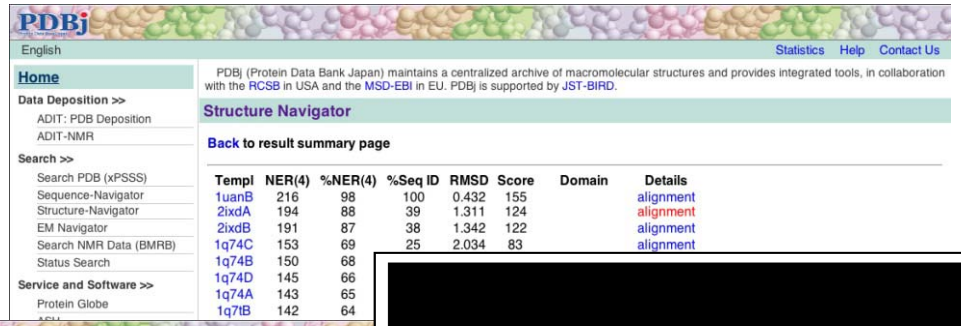


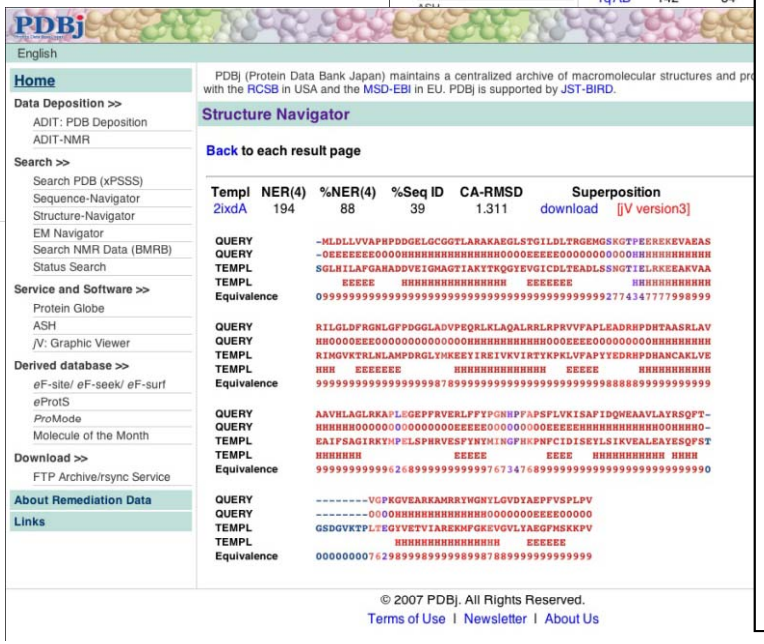


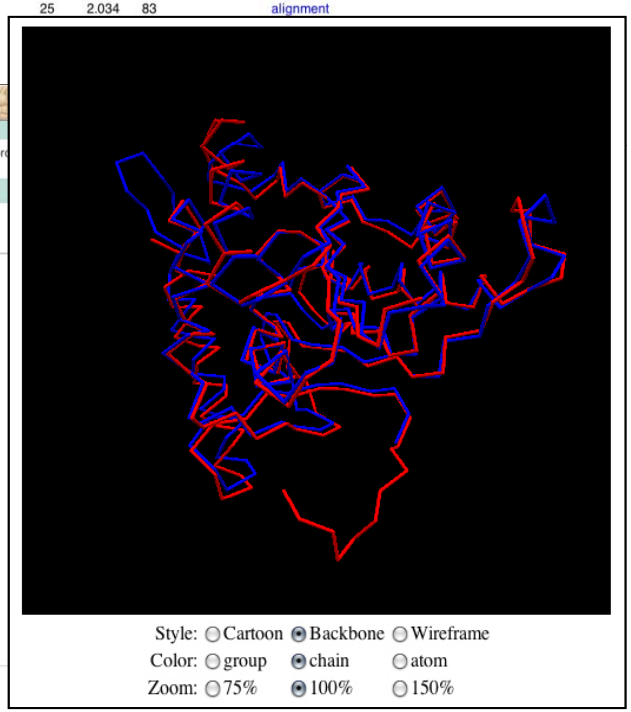
PDBID or amino-acid sequence should be input and "Find All Homologs" → List of hit PDBIDs is displayed.

Search of Similar Structures: Structure Navigator



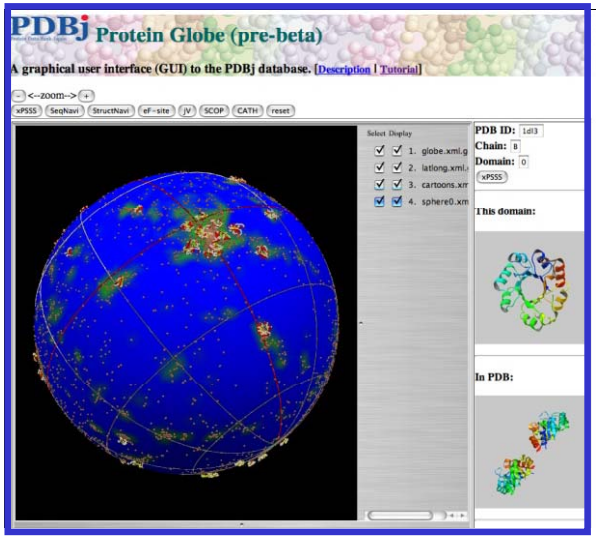




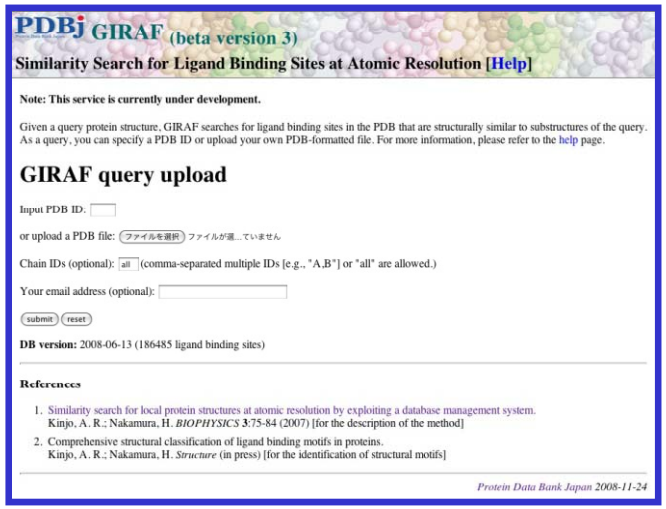


PDBID should be input and "Start Structure Navigator" → List of hit PDBIDs is displayed.

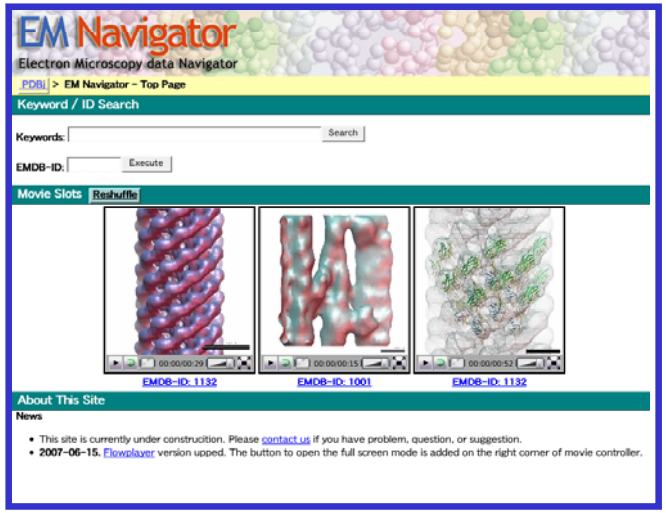
Development of other Databases and Services



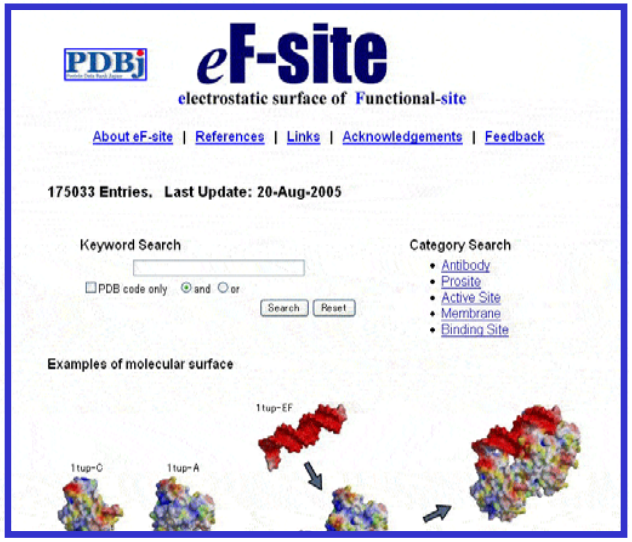
Protein Folds Browser, Protein Globe *(Kinjo & Standley)*



Ligand Binding Site Search, GIRAF *(Kinjo)*

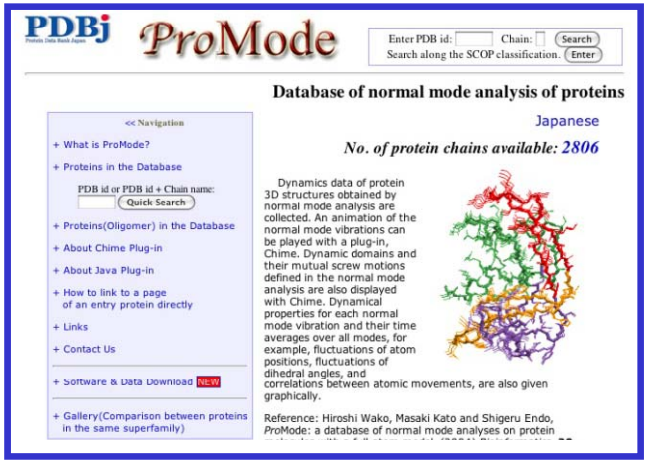


Electron Microscopy Navigator, EM-Navi *(Suzuki)*



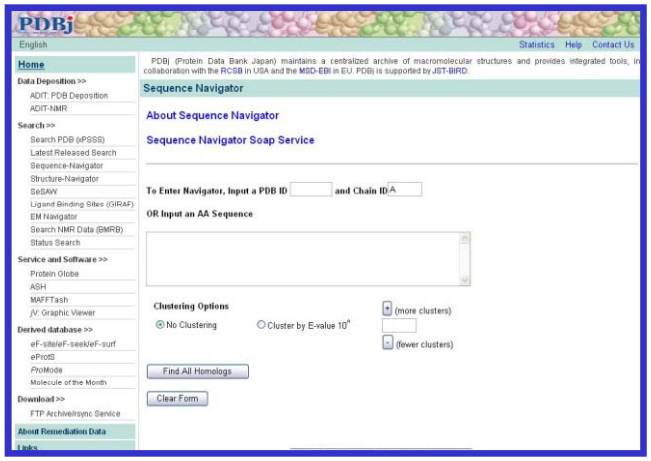
Protein Molecular Surface Database, *e*F-site *(Kinoshita & Nakamura)*

Search for Similar Surface, *e*F-seek *(Kinoshita & Nakamura)*



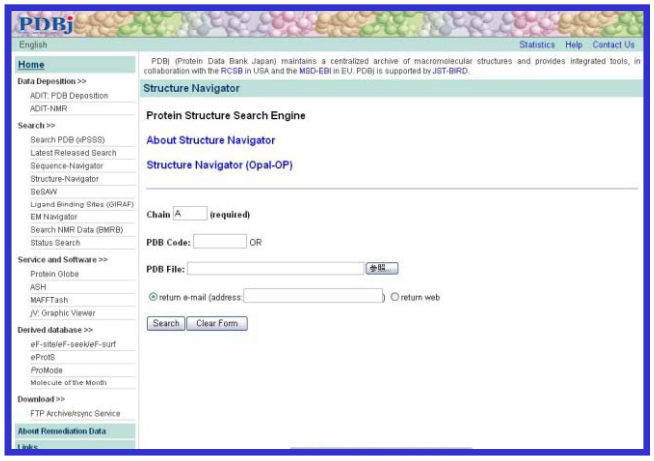
Protein Dynamics Database, *Pro*Mode *(Wako & Endo)*

Development of other Databases and Services



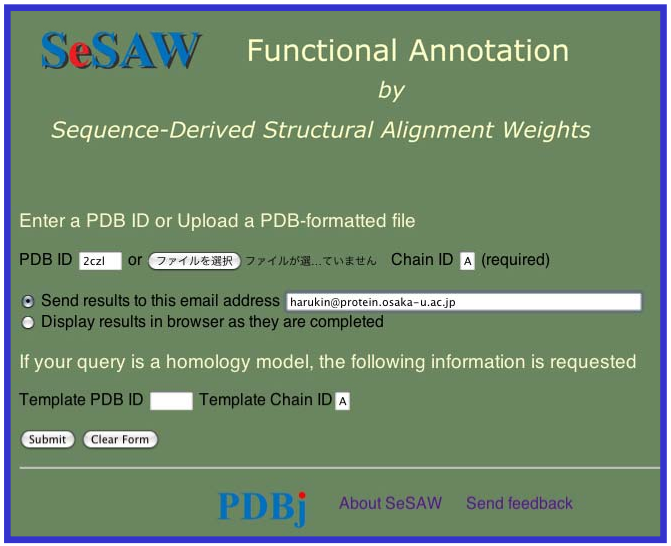
Homolog protein search,

Sequence Navigator
(Standley)

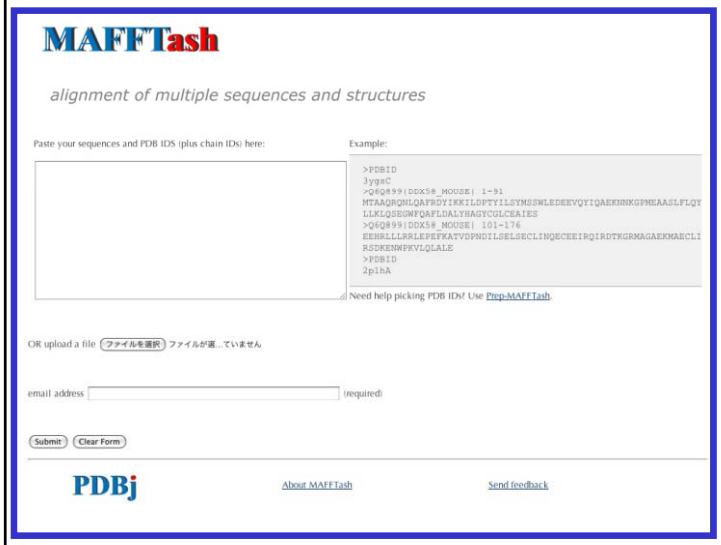


Similar fold search,

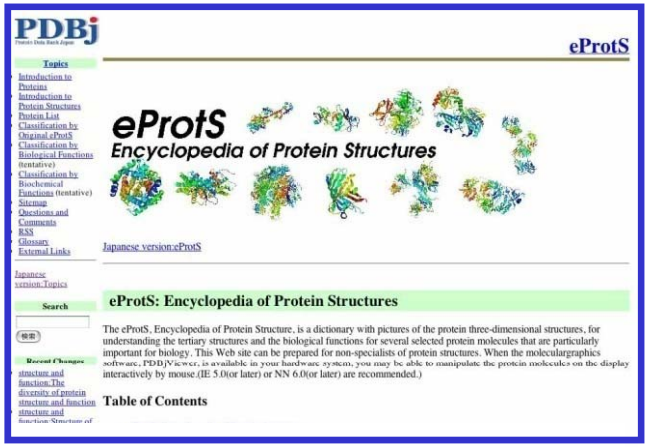
Structure Navigator
(Standley & Toh)



Function Annotation from Folds and Sequences, SeSAW *(Standley)*



Alignment of Sequence and Structures. MAFFTash
(Kato. Toh & Standley)

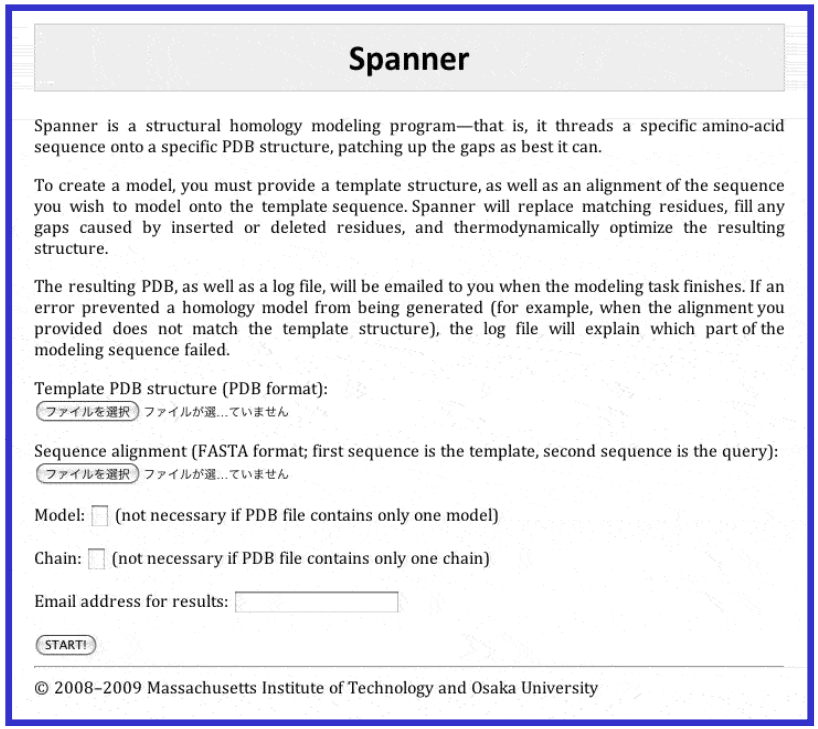


Encyclopedia of Protein Structures, eProtS
(Kinjyo, Kudo, & Ito)

Molecule of the Month, MoM
(Goodsell & Kudo)

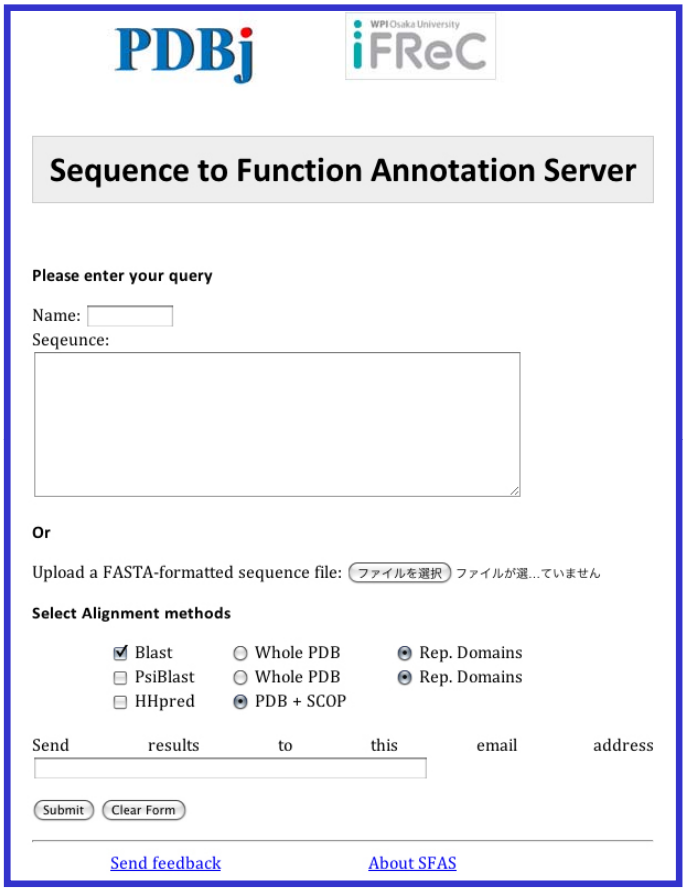
Development of other Databases and Services

http://www.pdbj.org/spanner/



Homology modeling service (Mieszko, Standley, Nakamura)

http://www.pdbj.org/sfas/



Function Annotation from Sequences, SFAS *(Standley)*

When you have any difficulties/troubles, please do not hesitate to ask us from: