

WEBLEM 7

Introduction of Structure Database

The Protein Data Bank (PDB) at Brookhaven National Laboratory (BNL), is a database containing experimentally determined three-dimensional structures of proteins, nucleic acids and other biological macromolecules (Abola et al., 1987, 1997; Bernstein et al., 1977).

The PDB has a 26-year history of service to a global community of researchers, educators and students in a wide variety of scientific disciplines.

The archives contain atomic coordinates, citations, primary and secondary structure information, crystallographic structure experimental data, as well as hyperlinks to many other scientific databases.

Scientists around the world contribute structures to the PDB and use it on a daily basis. The common interest shared by this community is a need to access information that can relate the biological functions of macromolecules to their three-dimensional structures.

RCSB PDB (Research Collaboratory for Structural Bioinformatics PDB) operates the US data center for the global PDB archive, and makes PDB data available at no charge to all data consumers without limitations on usage (Policies).

Observations:

The screenshot displays the RCSB PDB website interface. The top navigation bar includes links for Deposit, Search, Visualize, Analyze, Download, Learn, More, Documentation, and Careers. A 'MyPDB' button is located on the right. The left sidebar contains several filter categories:

- Refinements:** Includes a search bar for 'SCIENTIFIC NAME OF SOURCE ORGANISM' and a list of organisms with checkboxes (e.g., Homo sapiens, Rattus norvegicus, Mus musculus).
- TAXONOMY:** Includes a list of taxonomic groups with checkboxes (e.g., Eukaryota, Bacteria, other sequences, Riboviria).
- EXPERIMENTAL METHOD:** Includes a list of experimental methods with checkboxes (e.g., X-RAY DIFFRACTION, SOLUTION NMR, ELECTRON MICROSCOPY).
- POLYMER ENTITY TYPE:** Includes a list of entity types with checkboxes (e.g., Protein, DNA, RNA).

The main content area displays a list of protein structures. The first three structures shown are:

- 2DSP:** Structural Basis for the Inhibition of Insulin-like Growth Factors by IGF Binding Proteins. Released: 2006-08-22. Method: X-RAY DIFFRACTION 2.5 Å. Organisms: Homo sapiens. Macromolecule: Insulin-like growth factor IB (protein), Insulin-like growth factor-binding protein 4 (protein).
- 2DSQ:** Structural Basis for the Inhibition of Insulin-like Growth Factors by IGF Binding Proteins. Released: 2006-08-22. Method: X-RAY DIFFRACTION 2.8 Å. Organisms: Homo sapiens. Macromolecule: Insulin-like growth factor IB (protein), Insulin-like growth factor-binding protein 1 (protein), Insulin-like growth factor-binding protein 4 (protein).
- 6FEY:** Crystal structure of Drosophila neural ectodermal development factor Imp-L2 with Drosophila DILP5 insulin. Released: 2019-09-26. Method: X-RAY DIFFRACTION 3.48 Å. Organisms: Drosophila melanogaster. Macromolecule: Neuroectodermal development factor IMP-L2 (protein).

Fig1. Summary form in PDB Database

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Refinements

SCIENTIFIC NAME OF SOURCE ORGANISM

- ☐ Homo sapiens (5563)
- ☐ Rattus norvegicus (788)
- ☐ Mus musculus (611)
- ☐ Bos taurus (321)
- ☐ Gallus gallus (214)
- ☐ Sus scrofa (162)
- ☐ synthetic construct (155)
- ☐ Lama glama (75)
- ☐ Oryctolagus cuniculus (65)
- ☐ Escherichia coli (43)
- [More...](#)

TAXONOMY

- ☐ Eukaryota (7155)
- ☐ Bacteria (298)
- ☐ other sequences (156)
- ☐ Riboviria (123)
- ☐ Archaea (33)
- ☐ Duplodnaviria (30)
- ☐ Varidnaviria (8)
- ☐ unclassified sequences (8)

EXPERIMENTAL METHOD

- ☐ X-RAY DIFFRACTION (6431)
- ☐ SOLUTION NMR (591)
- ☐ ELECTRON MICROSCOPY (490)
- ☐ SOLID-STATE NMR (16)
- ☐ ELECTRON CRYSTALLOGRAPHY (14)
- ☐ POWDER DIFFRACTION (13)
- ☐ NEUTRON DIFFRACTION (6)
- ☐ SOLUTION SCATTERING (2)

POLYMER ENTITY TYPE

- ☐ Protein (7557)
- ☐ DNA (146)
- ☐ RNA (19)

Summary Gallery Compact Tabular Report Score Download Files All Selected

Displaying 1 to 25 of 7557 Structures Page 1 of 303 Previous Next

Display 25 per page

2DSP 2DSQ 6FEY 2WFV

2WFU 11GL 5L3N 5L3M

5L3L 2INS 1PID 1B2V

2KJI 1BOM 1HO0 5KQV

Fig2. Gallery form in PDB database

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Refinements

SCIENTIFIC NAME OF SOURCE ORGANISM

- ☐ Homo sapiens (5563)
- ☐ Rattus norvegicus (788)
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- ☐ Eukaryota (7155)
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EXPERIMENTAL METHOD

- ☐ X-RAY DIFFRACTION (6431)
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- ☐ Protein (7557)
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Summary Gallery Compact Tabular Report Score Download Files All Selected

Displaying 1 to 25 of 7557 Structures Page 1 of 303 Previous Next

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| ID | Title | Released |
|------|---|------------|
| 2DSP | Structural Basis for the Inhibition of Insulin-like Growth Factors by IGF Binding Proteins | 2006-08-22 |
| 2DSQ | Structural Basis for the Inhibition of Insulin-like Growth Factors by IGF Binding Proteins | 2006-08-22 |
| 6FEY | Crystal structure of Drosophila neural ectodermal development factor Imp-L2 with Drosophila DILP5 insulin | 2018-09-26 |
| 2WFV | Crystal structure of DILP5 variant C4 | 2010-05-26 |
| 2WFU | Crystal structure of DILP5 variant DB | 2010-05-26 |
| 11GL | SOLUTION STRUCTURE OF HUMAN INSULIN-LIKE GROWTH FACTOR II RELATIONSHIP TO RECEPTOR AND BINDING PROTEIN INTERACTIONS | 1995-02-14 |
| 5L3N | D11 bound [N29, S39_PQ3-IGF-II] | 2016-08-10 |
| 5L3M | D11 bound [S39_PQ3-IGF-II] | 2016-08-10 |
| 5L3L | D11 bound IGF-II | 2016-08-10 |
| 2INS | THE STRUCTURE OF DES-PHE B1 BOVINE INSULIN | 1982-08-05 |
| 1PID | BOVINE DESPENTAPEPTIDE INSULIN | 1996-12-07 |
| 1B2V | [D-ALA829]-DES(B27-B30)-INSULIN-B26-AMIDE A SUPERPOTENT SINGLE-REPLACEMENT INSULIN ANALOGUE, NMR, MINIMIZED AVERAGE STRUCTURE | 1995-05-18 |
| 2KJI | A divergent ins protein in c. elegans structurally resemble insulin and activates the human insulin receptor | 2009-06-16 |
| 1BOM | THREE-DIMENSIONAL STRUCTURE OF BOMBYXIN-II, AN INSULIN-RELATED BRAIN-SECRETORY PEPTIDE OF THE SILKMOTH BOMBYX MORI: COMPARISON WITH INSULIN AND RELAXIN | 1994-11-01 |
| 1HO0 | NEW B-CHAIN MUTANT OF BOVINE INSULIN | 2000-12-20 |
| 5KQV | Insulin receptor ectodomain construct comprising domains L1, CRL2, Frtil-1 and alphaCT peptide in complex with bovine insulin and FAS 83-14 (REVISED STRUCTURE) | 2017-07-19 |
| 7ELJ | Prion Derived Tetrapeptide Stabilizes Thermolabile Insulin via Conformational Trapping | 2021-04-28 |
| 4IDW | Polycrystalline T6 Bovine Insulin: Anisotropic Lattice Evolution and Novel Structure Refinement Strategy | 2013-06-05 |
| 3KR3 | Crystal structure of IGF-II antibody complex | 2010-06-16 |
| 1BON | THREE-DIMENSIONAL STRUCTURE OF BOMBYXIN-II, AN INSULIN-RELATED BRAIN-SECRETORY PEPTIDE OF THE SILKMOTH BOMBYX MORI: COMPARISON WITH INSULIN AND RELAXIN | 1995-01-26 |
| 1DPI | CONFORMATIONAL CHANGES IN CUBIC INSULIN CRYSTALS IN THE PH RANGE 7-11 | 1993-01-15 |
| 1BPH | CONFORMATIONAL CHANGES IN CUBIC INSULIN CRYSTALS IN THE PH RANGE 7-11 | 1993-01-15 |
| 1APH | CONFORMATIONAL CHANGES IN CUBIC INSULIN CRYSTALS IN THE PH RANGE 7-11 | 1993-01-15 |
| 6BNT | Crystal structure of AP2 mu1 adaptin C-terminal domain with IRS-1 peptide | 2018-11-21 |
| 1CPH | CONFORMATIONAL CHANGES IN CUBIC INSULIN CRYSTALS IN THE PH RANGE 7-11 | 1993-01-15 |

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Display 25 per page

Fig3. Compact form in PDB database

| ID | Title | Released |
|------|---|------------|
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| 2DSQ | Structural Basis for the Inhibition of Insulin-like Growth Factor | 2006-08-22 |
| 6FEY | Crystal structure of Drosophila neural ectodermal development | 2018-09-26 |
| 2WVF | Crystal structure of DILP5 variant C4 | 2010-05-26 |
| 2WFU | Crystal structure of DILP5 variant DB | 2010-05-26 |
| 1IGL | SOLUTION STRUCTURE OF HUMAN INSULIN-LIKE GROWTH FACTOR II RELATIONSHIP TO RECEPTOR AND BINDING PROTEIN INTERACTIONS | 1995-02-14 |
| 5L3N | D11 bound [N29, S39_PQJ-IGF-II] | 2016-08-10 |
| 5L3M | D11 bound [S39_PQJ-IGF-II] | 2016-08-10 |
| 5L3L | D11 bound IGF-II | 2016-08-10 |
| 2INS | THE STRUCTURE OF DES-PHE B1 BOVINE INSULIN | 1982-08-05 |
| 1PID | BOVINE DESPENTAPEPTIDE INSULIN | 1996-12-07 |
| 1B2V | [D-ALAB29;DES1827-830]-INSULIN-826-AMIDE A SUPERPOTENT SINGLE-REPLACEMENT INSULIN ANALOGUE, NMR, MINIMIZED AVERAGE STRUCTURE | 1999-05-18 |
| 2KJI | A divergent ins protein in c. elegans structurally resemble insulin and activates the human insulin receptor | 2009-06-16 |
| 1BOM | THREE-DIMENSIONAL STRUCTURE OF BOMBYXIN-II, AN INSULIN-RELATED BRAIN-SECRETORY PEPTIDE OF THE SILKMOTH BOMBYX MORI: COMPARISON WITH INSULIN AND RELAXIN | 1994-11-01 |
| 1H00 | NEW B-CHAIN MUTANT OF BOVINE INSULIN | 2000-12-20 |
| 5KQV | Insulin receptor ectodomain construct comprising domains L1,CR1,2, FcIII-1 and alphaCT peptide in complex with bovine insulin and FAB 83-14 (REVISED STRUCTURE) | 2017-07-19 |
| 7ELJ | Prion Derived Tetrapeptide Stabilizes Thermolabile Insulin via Conformational Trapping | 2021-04-28 |
| 4IDW | Polycrystalline T6 Bovine Insulin: Anisotropic Lattice Evolution and Novel Structure Refinement Strategy | 2013-06-05 |
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| 1BPH | CONFORMATIONAL CHANGES IN CUBIC INSULIN CRYSTALS IN THE PH RANGE 7-11 | 1993-01-15 |
| 1APH | CONFORMATIONAL CHANGES IN CUBIC INSULIN CRYSTALS IN THE PH RANGE 7-11 | 1993-01-15 |
| 6BNT | Crystal structure of AP2 mu1 adaptin C-terminal domain with IRS-1 peptide | 2018-11-21 |
| 1CPH | CONFORMATIONAL CHANGES IN CUBIC INSULIN CRYSTALS IN THE PH RANGE 7-11 | 1993-01-15 |

Fig4. Tabular Report form in PDB Database

| ID | Title | Released |
|------|---|------------|
| 2DSF | Structural Basis for the Inhibition of Insulin-like Growth Factor | 2006-08-22 |
| 2DSQ | Structural Basis for the Inhibition of Insulin-like Growth Factor | 2006-08-22 |
| 6FEY | Crystal structure of Drosophila neural ectodermal development | 2018-09-26 |
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| 1CPH | CONFORMATIONAL CHANGES IN CUBIC INSULIN CRYSTALS IN THE PH RANGE 7-11 | 1993-01-15 |

Fig5. Score form in PDB Database.

References:

1. Sussman, J. L., Lin, D., Jiang, J., Manning, N. O., Prilusky, J., Ritter, O., & Abola, E. E. (1998). Protein Data Bank (PDB): Database of Three-Dimensional Structural Information of Biological Macromolecules. Acta Crystallographica Section D Biological Crystallography, 54(6), 1078–1084. <https://doi.org/10.1107/s0907444498009378>
2. Bank, R. P. (n.d.). Homepage. Retrieved from <https://www.rcsb.org/>

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(URL: <https://www.rcsb.org/>)

Aim:

To study “Insulin” Query in Structure Database PDB.

Introduction:

The Protein Data Bank (PDB) at Brookhaven National Laboratory (BNL), is a database containing experimentally determined three-dimensional structures of proteins, nucleic acids and other biological macromolecules (Abola et al., 1987, 1997; Bernstein et al., 1977).

The PDB has a 26-year history of service to a global community of researchers, educators and students in a wide variety of scientific disciplines.

The archives contain atomic coordinates, citations, primary and secondary structure information, crystallographic structure experimental data, as well as hyperlinks to many other scientific databases.

Insulin is a medication used in the treatment and management of diabetes mellitus type-1 and sometimes diabetes mellitus type-2, both of which are significant risk factors for coronary artery disease, stroke, peripheral vascular disease, and a host of other vascular conditions. This activity reviews the indications, contraindications, activity, adverse events, and other key elements of Insulin therapy in the clinical setting related to the essential points needed by members of an interprofessional team managing the care of patients with diabetes and its related conditions and sequelae.

Methodology:

1. Open the Homepage of PDB.
2. Enter the Query “Insulin”
3. Open the Result page for the query
4. Interpret the results.

Observation:

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RCSB PDB 182949 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

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Developers: Join the RCSB PDB Team [Explore Open Positions](#) [Take the RCSB.org Survey](#)

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Search

Visualize

Analyze

Download

Learn

A Structural View of Biology

This resource is powered by the Protein Data Bank archive—information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

As a member of the wwPDB, the RCSB PDB curates and annotates PDB data.

The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

COVID-19 CORONAVIRUS Resources

October Molecule of the Month

Fifty Years of Open Access to PDB Structures

Latest Entries *As of Tue Oct 05 2021*

Features & Highlights

Take the RCSB.org User Survey

User Survey: Tell RCSB PDB About Your Interests

Please take this brief survey to be entered into a drawing for a set of PDB50 Structural Biology Playing Cards.

PDBx/mmCIF data files to include P1

News

Publications

Blucurator Milestone: >10,000 Depositions Processed

Congratulations to wwPDB's Dr. Sutapa Ghosh and Dr. Monica Sekharan on processing more than 10,000 PDB structures as of 10/12/2021

Fig1. Homepage of PDB Database

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Enter search terms or PDB ID(s). [Advanced Search](#) | [Browse Annotations](#) [Help](#)

Search **History** **Browse Annotations** **MyPDB**

QUERY: Full Text = "Insulin" [JSON](#) [MyPDB Login](#)

Advanced Search Query Builder [Help](#)

Refinements

SCIENTIFIC NAME OF SOURCE ORGANISM

☐ Homo sapiens (5563)

☐ Rattus norvegicus (798)

☐ Mus musculus (611)

☐ Bos taurus (321)

☐ Gallus gallus (214)

☐ Sus scrofa (162)

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☐ Archaea (33)

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☐ unclassified sequences (8)

EXPERIMENTAL METHOD

Summary **Gallery** **Compact** **Tabular Report** **Score** **Download Files** **All** **Selected**

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2DSP [Download File](#) [View File](#)

Structural Basis for the Inhibition of Insulin-like Growth Factors by IGF Binding Proteins

Sitar, T., Popowicz, G.M., Siwanowicz, I., Huber, R., Holak, T.A.

(2006) Proc Natl Acad Sci U S A 103: 13028-13033

Released 2006-08-22

Method X-RAY DIFFRACTION 2.5 Å

Organisms Homo sapiens

Macromolecule Insulin-like growth factor IB (protein)
Insulin-like growth factor-binding protein 4 (protein)

3D View

2DSQ [Download File](#) [View File](#)

Structural Basis for the Inhibition of Insulin-like Growth Factors by IGF Binding Proteins

Sitar, T., Popowicz, G.M., Siwanowicz, I., Huber, R., Holak, T.A.

(2006) Proc Natl Acad Sci U S A 103: 13028-13033

Released 2006-08-22

Method X-RAY DIFFRACTION 2.8 Å

Organisms Homo sapiens

Macromolecule Insulin-like growth factor IB (protein)

Fig2. Hitpage for query "Insulin"

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Enter search terms or PDB ID(s). Advanced Search | Browse Annotations Help

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Celebrating 50 YEARS OF Protein Data Bank

Structure Summary 3D View Annotations Experiment Sequence Genome Versions

2DSP

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Structural Basis for the Inhibition of Insulin-like Growth Factors by IGF Binding Proteins

Present annotations:

- Domain Annotation: SCOP Classification
- Domain Annotation: CATH
- Protein Family Annotation
- Gene Product Annotation

Domain Annotation: SCOP Classification SCOP Database (version: 2.0) Homepage

| Chains | Domain Info | Class | Fold | Superfamily | Family | Domain | Species |
|------------|-------------|--------------------------------|--|---|---|--|--|
| A [auth B] | d2dsp1 | Small proteins | Knottins (small inhibitors, toxins, lectins) | Growth factor receptor domain | Growth factor receptor domain | Insulin-like growth factor-binding protein 4, IGFBP4 | human (Homo sapiens) [Taxid: 9606] |
| B [auth I] | d2dsp1 | Small proteins | Insulin-like | Insulin-like | Insulin-like | Insulin-like growth factor | human (Homo sapiens) [Taxid: 9606] |

Domain Annotation: CATH CATH Database (version 4.2.0) Homepage

| Chain | Domain | Class | Architecture | Topology | Homology |
|------------|------------|--|---------------------------|---------------------------------|----------|
| A [auth B] | 4.10.40.20 | Few Secondary Structures | Irregular | Omega-AgatoxinV | |

Fig5. Annotations for my query Insulin

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Enter search terms or PDB ID(s). Advanced Search | Browse Annotations Help

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Structure Summary 3D View Annotations Experiment Sequence Genome Versions

2DSP

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Structural Basis for the Inhibition of Insulin-like Growth Factors by IGF Binding Proteins

X-RAY DIFFRACTION

Crystallization

Crystallization Experiments

| ID | Method | pH | Temperature | Details |
|----|-------------------------------|----|-------------|---|
| 1 | VAPOR DIFFUSION, SITTING DROP | 7 | 290 | 23% PEG 1500, 25mM Tris pH 7, VAPOR DIFFUSION, SITTING DROP, temperature 290K |

Crystal Properties

| Matthews coefficient | Solvent content |
|----------------------|-----------------|
| 2.18 | 43.46 |

Crystal Data

| Unit Cell | | Symmetry | |
|------------|-----------|-------------|--|
| Length (Å) | Angle (°) | Space Group | |
| a = 32.33 | α = 90 | P 1 2 1 1 | |
| b = 38.99 | β = 99.89 | | |
| c = 61.93 | γ = 90 | | |

Fig6. Experiment for my query Insulin



Fig7. Sequence for my query Insulin



Fig8. Genome for my query Insulin

The screenshot shows the RCSB PDB website interface. The search bar at the top contains the query: "QUERY: Full Text = 'Insulin' AND Scientific Name of the Source Organism = 'Homo sapiens'". Below the search bar, the 'Advanced Search Query Builder' is visible. In the 'Refinements' section, under 'SCIENTIFIC NAME OF SOURCE ORGANISM', the checkbox for 'Homo sapiens (5563)' is selected and highlighted with a red box. The search results display two entries: '2DSP' and '2DSQ', both titled 'Structural Basis for the Inhibition of Insulin-like Growth Factors by IGF Binding Proteins'. The '2DSP' entry is highlighted with a red box. The '2DSQ' entry is also visible below it. The 'Refinements' section also includes 'TAXONOMY' and 'EXPERIMENTAL METHOD' filters.

Fig11. Refinement filtering for homo sapiens for query Insulin

The screenshot shows the RCSB PDB website interface. The search bar at the top contains the query: "QUERY: Full Text = 'Insulin' AND (Scientific Name of the Source Organism = 'Homo sapiens' AND Parent Scientific Name (typically superkingdom or clade) = 'Eukaryota')". Below the search bar, the 'Advanced Search Query Builder' is visible. In the 'Refinements' section, under 'TAXONOMY', the checkbox for 'Eukaryota (5563)' is selected and highlighted with a red box. The search results display two entries: '2DSP' and '2DSQ', both titled 'Structural Basis for the Inhibition of Insulin-like Growth Factors by IGF Binding Proteins'. The '2DSP' entry is highlighted with a red box. The '2DSQ' entry is also visible below it. The 'Refinements' section also includes 'SCIENTIFIC NAME OF SOURCE ORGANISM' and 'EXPERIMENTAL METHOD' filters.

Fig12. Refinements filtering for Taxonomy Eukaryota.

Results:

| Sr. No | Refinements Filter | No. of structures |
|--------|--------------------|-------------------|
| 1 | Unfiltered | 7557 |
| 2 | Homo sapiens | 5563 |
| 3 | Taxonomy | 5563 |

Conclusion:

PDB is taken care of by RCSB(Research Collaboratory for Structural Bioinformatics PDB) . PDB Form is most use & Accepted formed. Every month they upload molecular structure. Its provides access to 3D structure data for large biological molecules (proteins, DNA & RNA). These are the molecules of life, found in all organisms on the planet.

References:

1. Mathieu C, Gillard P, Benhalima K. Insulin analogues in type 1 diabetes mellitus: getting better all the time. *Nat Rev Endocrinol*. 2017 Jul;13(7):385-399
2. Bank, R. P. (n.d.). Homepage. Retrieved from <https://www.rcsb.org/>
3. Retrieved from <https://www.rcsb.org/structure/2DSP>
4. Retrieved from <https://www.rcsb.org/3d-view/2DSP>
5. Retrieved from <https://www.rcsb.org/annotations/2dsp>
6. Retrieved from <https://www.rcsb.org/experimental/2DSP>
7. Retrieved from <https://www.rcsb.org/sequence/2DSP>
8. Retrieved from <https://www.rcsb.org/genome/2DSP>
9. Retrieved from <https://www.rcsb.org/versions/2DSP>