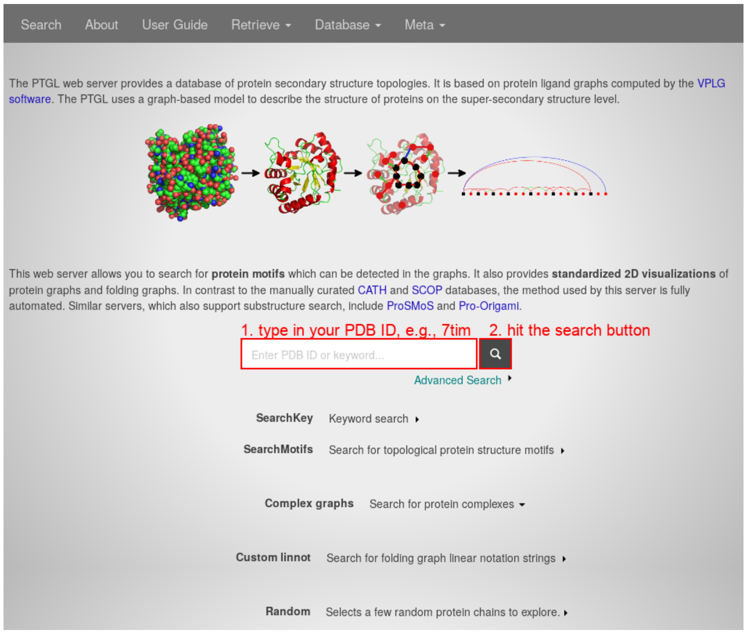
1: Protein and Folding Graph of a PDB ID

First, open the PTGL website under http://ptgl.uni-frankfurt.de. You will see this page:

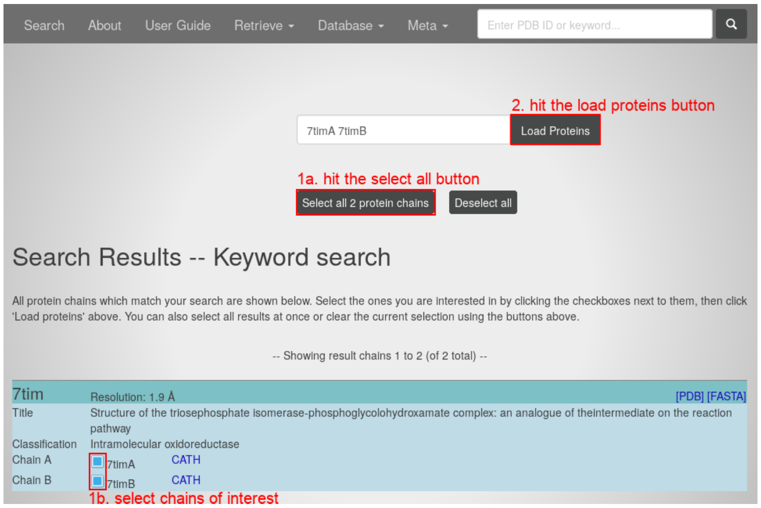


The PTGL web server provides a database of protein secondary structure topologies. It is based on protein ligand graphs computed by the VPLG software. The PTGL uses a graph-based model to describe the structure of proteins on the super-secondary structure level.

This web server allows you to search for **protein motifs** which can be detected in the graphs. It also provides **standardized 2D visualizations** of protein graphs and folding graphs. In contrast to the manually curated CATH and SCOP databases, the method used by this server is fully automated. Similar servers, which also support substructure search, include ProSMoS and Pro-Origami.

SearchKey	Keyword search
SearchMotifs	Search for topological protein structure motifs
Complex graphs	Search for protein complexes
Custom linnot	Search for folding graph linear notation strings
Random	Selects a few random protein chains to explore.

1. In the center search field, type in your PDB ID, e.g., 7tim.
2. Hit the search button. You will see a list of chains:



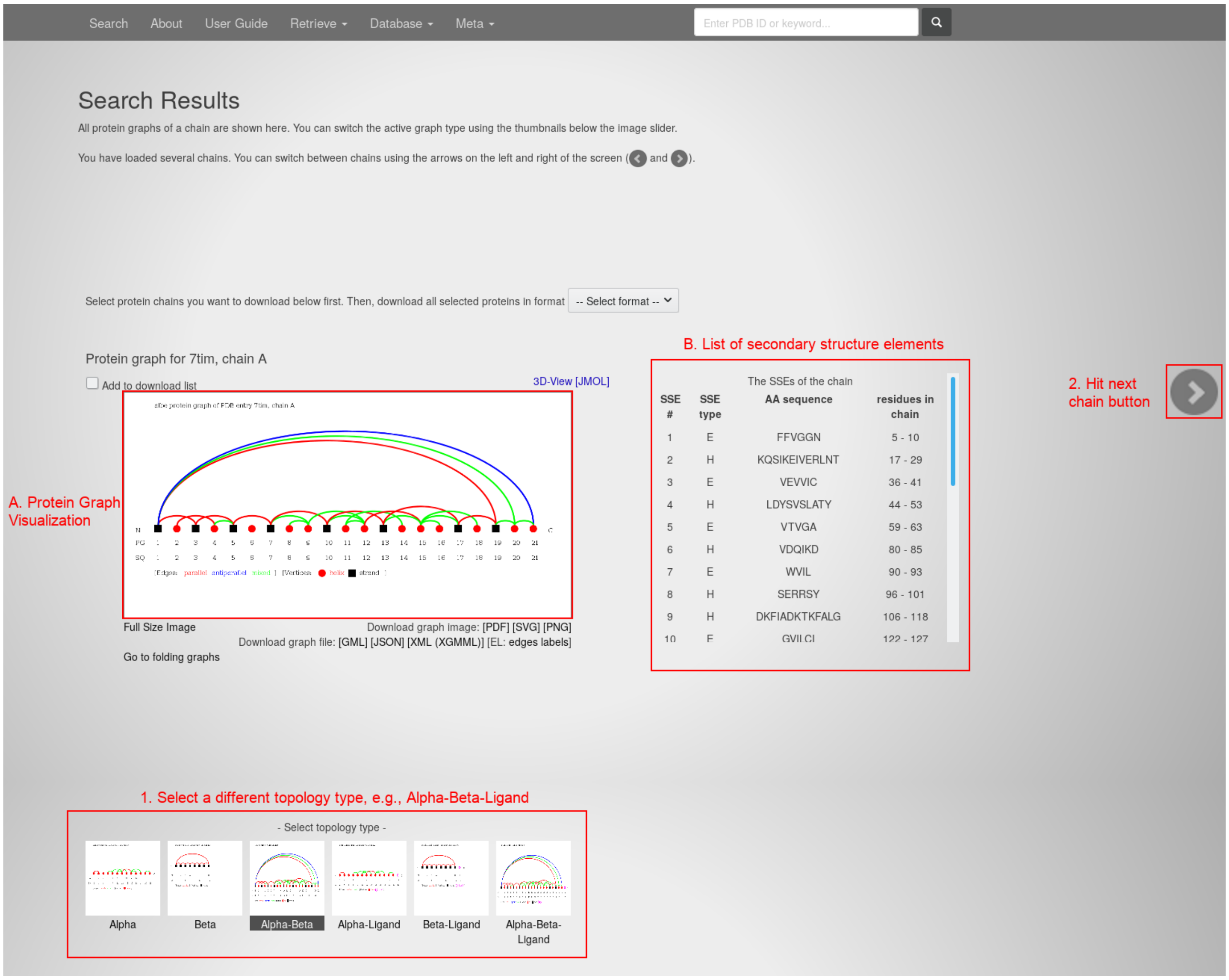
Search Results -- Keyword search

All protein chains which match your search are shown below. Select the ones you are interested in by clicking the checkboxes next to them, then click 'Load proteins' above. You can also select all results at once or clear the current selection using the buttons above.

-- Showing result chains 1 to 2 (of 2 total) --

7tim	Resolution: 1.9 Å	[PDB] [FASTA]
Title	Structure of the triosephosphate isomerase-phosphoglycolohydroxamate complex: an analogue of theintermediate on the reaction pathway	
Classification	Intramolecular oxidoreductase	
Chain A	☐ 7timA CATH	
Chain B	☐ 7timB CATH	

1. Either hit the select all protein chains button or select the chains of interest by their check boxes in the list at the bottom.
2. Hit the load proteins button. You will see the Protein Graph of the first selected chain:



Search Results

All protein graphs of a chain are shown here. You can switch the active graph type using the thumbnails below the image slider.

You have loaded several chains. You can switch between chains using the arrows on the left and right of the screen (and).

Select protein chains you want to download below first. Then, download all selected proteins in format -- Select format --

Protein graph for 7tim, chain A

☐ Add to download list

3D-View [JMOL]

Full Size Image

Download graph image: [PDF] [SVG] [PNG]

Download graph file: [GML] [JSON] [XML (XGMML)] [EL: edges labels]

Go to folding graphs

The SSEs of the chain

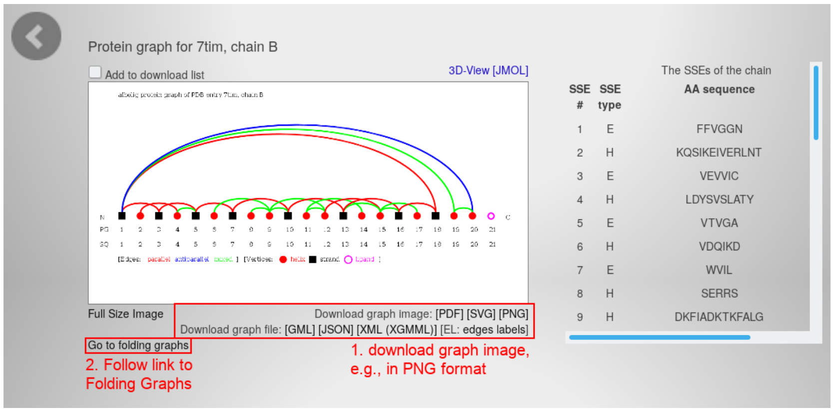
SSE #	SSE type	AA sequence	residues in chain
1	E	FFVGGN	5 - 10
2	H	KQSIKEIVERLNT	17 - 29
3	E	VEVVIC	36 - 41
4	H	LDYSVSLATY	44 - 53
5	E	VTVGA	59 - 63
6	H	VDQIKD	80 - 85
7	E	WVIL	90 - 93
8	H	SERRSY	96 - 101
9	H	DKFIADKTKFALG	106 - 118
10	E	GVILCI	122 - 127

The page contains:

- A. The Protein Graph Visualization in the center.
- B. The list of contained secondary structure elements on the right.

Now:

1. Select the alpha-beta-ligand topology type at the bottom. The image slides to the respective visualization.
2. Hit the next protein chain button in the center of the right edge. The page slides to the respective protein chain:



Protein graph for 7tim, chain B

☐ Add to download list

3D-View [JMOL]

Full Size Image

Download graph image: [PDF] [SVG] [PNG]

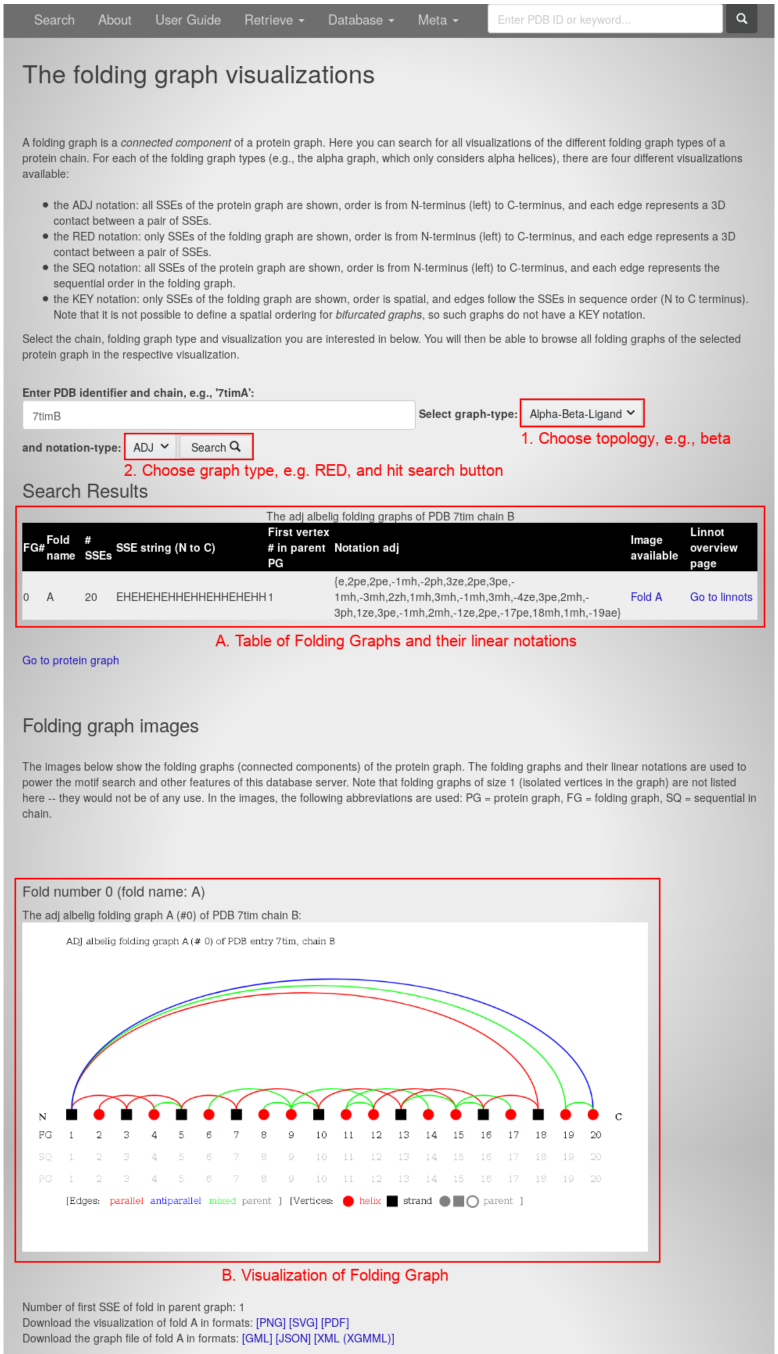
Download graph file: [GML] [JSON] [XML (XGMML)] [EL: edges labels]

Go to folding graphs

The SSEs of the chain

SSE #	SSE type	AA sequence
1	E	FFVGGN
2	H	KQSIKEIVERLNT
3	E	VEVVIC
4	H	LDYSVSLATY
5	E	VTVGA
6	H	VDQIKD
7	E	WVIL
8	H	SERRS
9	H	DKFIADKTKFALG

1. Download the graph visualization as PNG file with the link beneath the image.
2. Follow the link beneath the visualization on the left to open the Folding Graphs of this chain. You will see this page:



The folding graph visualizations

A folding graph is a *connected component* of a protein graph. Here you can search for all visualizations of the different folding graph types of a protein chain. For each of the folding graph types (e.g., the alpha graph, which only considers alpha helices), there are four different visualizations available:

- the ADJ notation: all SSEs of the protein graph are shown, order is from N-terminus (left) to C-terminus, and each edge represents a 3D contact between a pair of SSEs.
- the RED notation: only SSEs of the folding graph are shown, order is from N-terminus (left) to C-terminus, and each edge represents a 3D contact between a pair of SSEs.
- the SEQ notation: all SSEs of the protein graph are shown, order is from N-terminus (left) to C-terminus, and each edge represents the sequential order in the folding graph.
- the KEY notation: only SSEs of the folding graph are shown, order is spatial, and edges follow the SSEs in sequence order (N to C terminus). Note that it is not possible to define a spatial ordering for *bifurcated graphs*, so such graphs do not have a KEY notation.

Select the chain, folding graph type and visualization you are interested in below. You will then be able to browse all folding graphs of the selected protein graph in the respective visualization.

Enter PDB identifier and chain, e.g., '7timA': 7timB **Select graph-type:** Alpha-Beta-Ligand

1. Choose topology, e.g., beta

and notation-type: ADJ Search

2. Choose graph type, e.g. RED, and hit search button

Search Results

The adj albelig folding graphs of PDB 7tim chain B

FG#	Fold name	# SSEs	SSE string (N to C)	First vertex # in parent PG	Notation adj	Image available	Linnot overview page
0	A	20	EHEHEHEHHEHHEHHEHEHH	1	{e,2pe,2pe,-1mh,-2ph,3ze,2pe,3pe,-1mh,-3mh,2zh,1mh,3mh,-1mh,3mh,-4ze,3pe,2mh,-3ph,1ze,3pe,-1mh,2mh,-1ze,2pe,-17pe,18mh,1mh,-19ae}	Fold A	Go to linnots

A. Table of Folding Graphs and their linear notations

Go to protein graph

Folding graph images

The images below show the folding graphs (connected components) of the protein graph. The folding graphs and their linear notations are used to power the motif search and other features of this database server. Note that folding graphs of size 1 (isolated vertices in the graph) are not listed here -- they would not be of any use. In the images, the following abbreviations are used: PG = protein graph, FG = folding graph, SQ = sequential in chain.

Fold number 0 (fold name: A)

The adj albelig folding graph A (#0) of PDB 7tim chain B:

B. Visualization of Folding Graph

Number of first SSE of fold in parent graph: 1

Download the visualization of fold A in formats: [PNG] [SVG] [PDF]

Download the graph file of fold A in formats: [GML] [JSON] [XML (XGMML)]

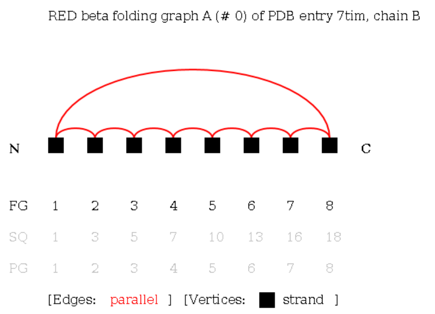
The page contains:

A. A table of all Folding Graphs for this Chain in the center. For each Folding Graphs it lists the Folding Graph number (FG#), fold name, number of secondary structure elements (#SSEs), the sequence of secondary structure elements from N- to C-terminus (SSE string), the vertex number of the first vertex in the parent Protein Graphs (PG), the linear notation, a link to the graph visualization and a link to the overview of the linear notations (linnot).

B. The Folding Graph visualization at the bottom.

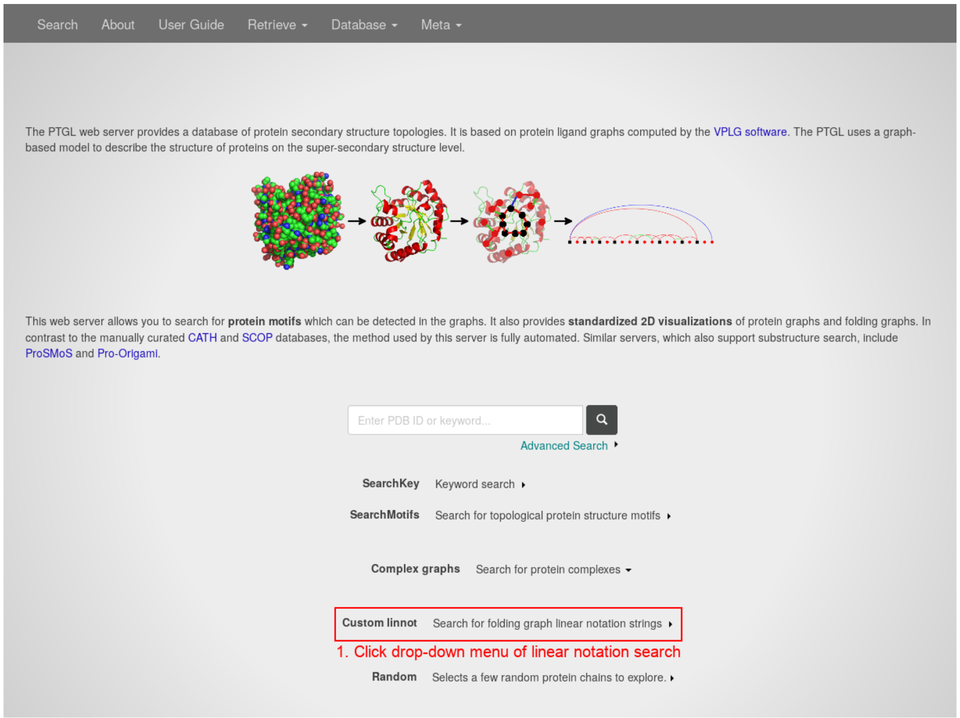
You can choose different Folding Graphs to be loaded above the table:

1. From the graph-type drop-down menu, choose the beta topology.
2. From the notation-type drop-down menu, choose the RED notation.
3. Hitting the search button you will see the page containing this graph visualization:



2: Search proteins exhibiting a structural topology by their linear notation

Open the PTGL website under http://ptgl.uni-frankfurt.de. You will see this page:



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SearchKey Keyword search

SearchMotifs Search for topological protein structure motifs

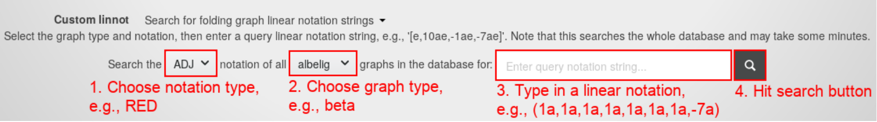
Complex graphs Search for protein complexes

Custom linnot Search for folding graph linear notation strings

1. Click drop-down menu of linear notation search

Random Selects a few random protein chains to explore.

1. Open the drop-down menu of the linear notation search by clicking anywhere on the respective line.



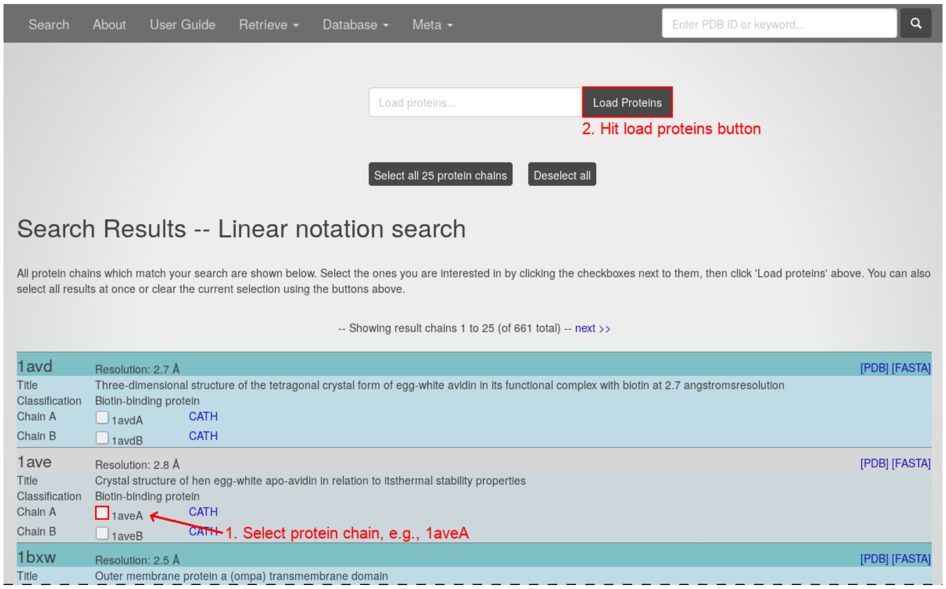
Custom linnot Search for folding graph linear notation strings

Select the graph type and notation, then enter a query linear notation string, e.g., '[e,10ae,-1ae,-7ae]'. Note that this searches the whole database and may take some minutes.

Search the ADJ notation of all albelig graphs in the database for: Enter query notation string...

1. Choose notation type, e.g., RED
2. Choose graph type, e.g., beta
3. Type in a linear notation, e.g., (1a,1a,1a,1a,1a,1a,1a,-7a)
4. Hit search button

1. In the notation-type drop-down menu, choose reduced (RED).
2. In the graph-type drop-down menu, choose beta.
3. Type '(1a,1a,1a,1a,1a,1a,1a,-7a)' in the search field.
4. Hit the search button.



2. Hit load proteins button

Search Results -- Linear notation search

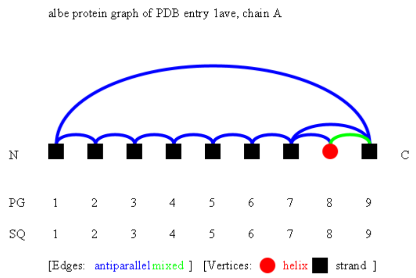
All protein chains which match your search are shown below. Select the ones you are interested in by clicking the checkboxes next to them, then click 'Load proteins' above. You can also select all results at once or clear the current selection using the buttons above.

-- Showing result chains 1 to 25 (of 661 total) -- next >>

1avd	Resolution: 2.7 Å	[PDB] [FASTA]
Title	Three-dimensional structure of the tetragonal crystal form of egg-white avidin in its functional complex with biotin at 2.7 angstromsresolution	
Classification	Biotin-binding protein	
Chain A	☐ 1avdA	CATH
Chain B	☐ 1avdB	CATH
1ave	Resolution: 2.8 Å	[PDB] [FASTA]
Title	Crystal structure of hen egg-white apo-avidin in relation to itsthermal stability properties	
Classification	Biotin-binding protein	
Chain A	☐ 1aveA	CATH
Chain B	☐ 1aveB	CATH
1bxw	Resolution: 2.5 Å	[PDB] [FASTA]
Title	Outer membrane protein a (ompa) transmembrane domain	

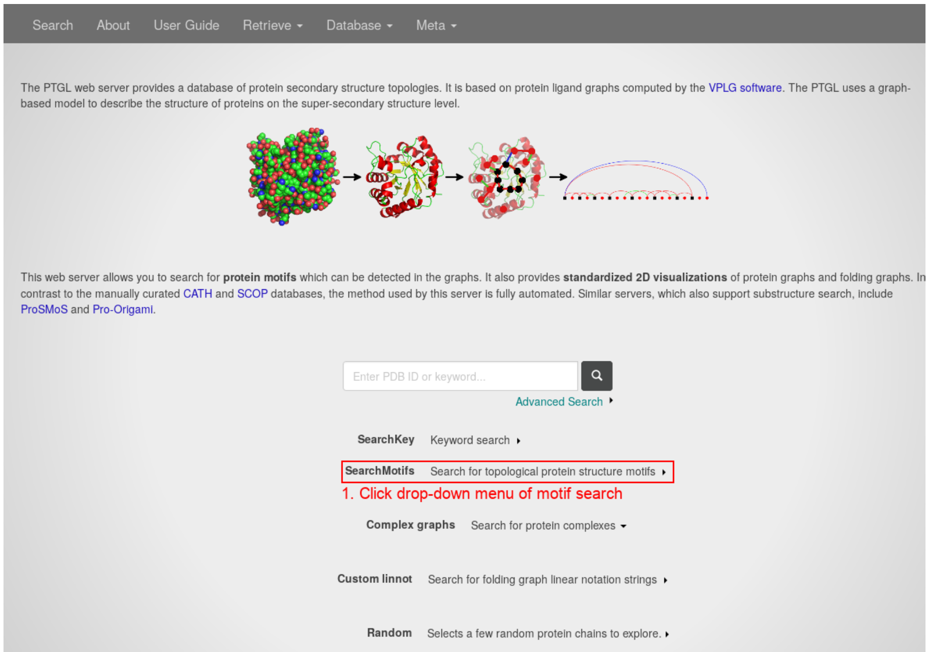
1. Select protein chain, e.g., 1aveA

1. Select the protein chain 1aveA by clicking the respective check box.
2. Hitting the load proteins button you will see the page containing this graph visualization:



3: Search structures containing a predefined motif

Open the PTGL website under http://ptgl.uni-frankfurt.de. You will see this page:



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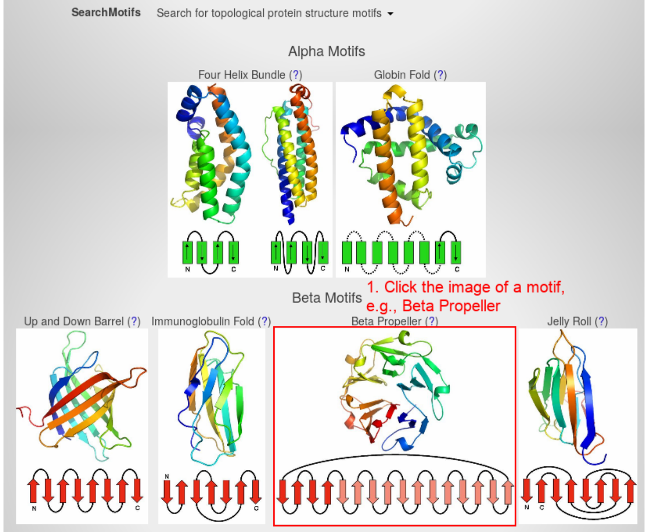
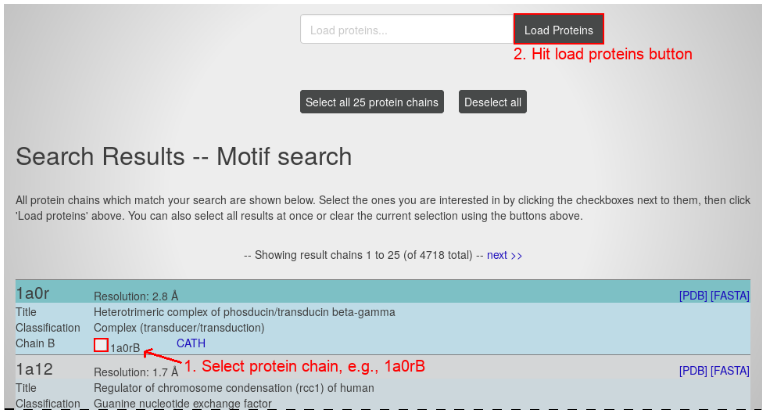
1. Click drop-down menu of motif search

1. Open the drop-down menu of the motif search by clicking anywhere on the respective line.



1. Click the image of a motif, e.g., Beta Propeller

1. Search for the beta propeller motif by clicking on the respective image.



2. Hit load proteins button

Search Results -- Motif search

All protein chains which match your search are shown below. Select the ones you are interested in by clicking the checkboxes next to them, then click 'Load proteins' above. You can also select all results at once or clear the current selection using the buttons above.

-- Showing result chains 1 to 25 (of 4718 total) -- next >>

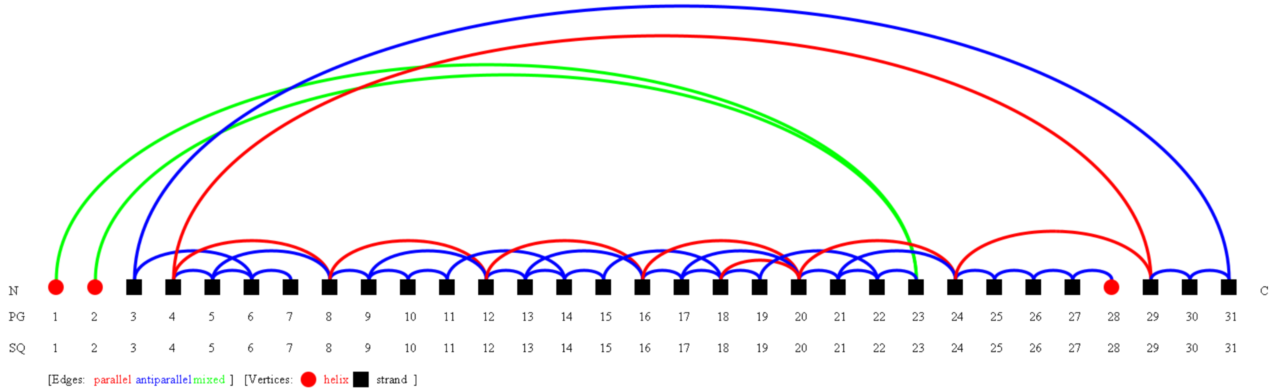
1a0r Resolution: 2.8 Å
Title Heterotrimeric complex of phosducin/transducin beta-gamma
Classification Complex (transducer/transduction)
Chain B ☐ 1a0rB

1. Select protein chain, e.g., 1a0rB

1a12 Resolution: 1.7 Å
Title Regulator of chromosome condensation (rcc1) of human
Classification Guanine nucleotide exchange factor

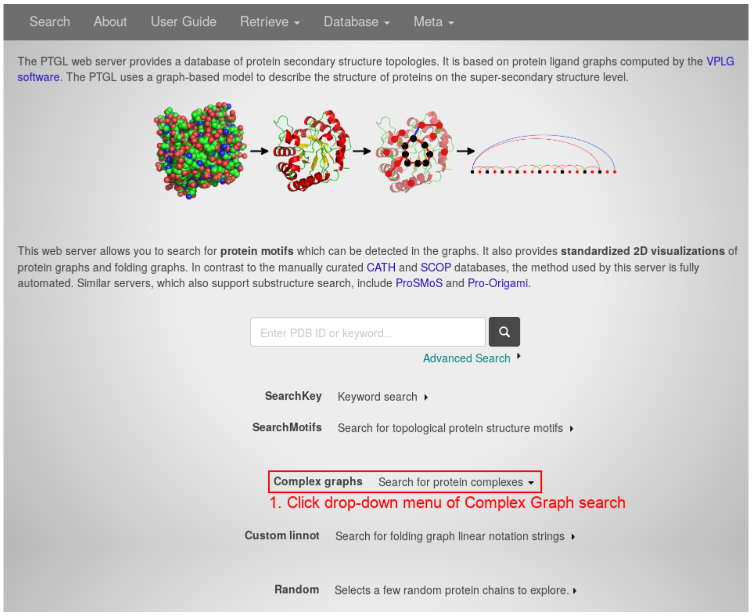
1. Select the protein chain 1a0rB by clicking the respective check box.
2. Hitting the load proteins button you will see the page containing this graph visualization:

albe protein graph of PDB entry 1a0r, chain B



4: Complex Graph of a PDB ID

Open the PTGL website under http://ptgl.uni-frankfurt.de. You will see this page:



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SearchKey Keyword search

SearchMotifs Search for topological protein structure motifs

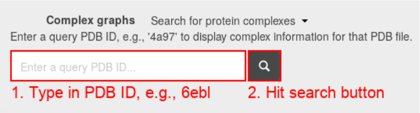
Complex graphs Search for protein complexes

1. Click drop-down menu of Complex Graph search

Custom linnot Search for folding graph linear notation strings

Random Selects a few random protein chains to explore.

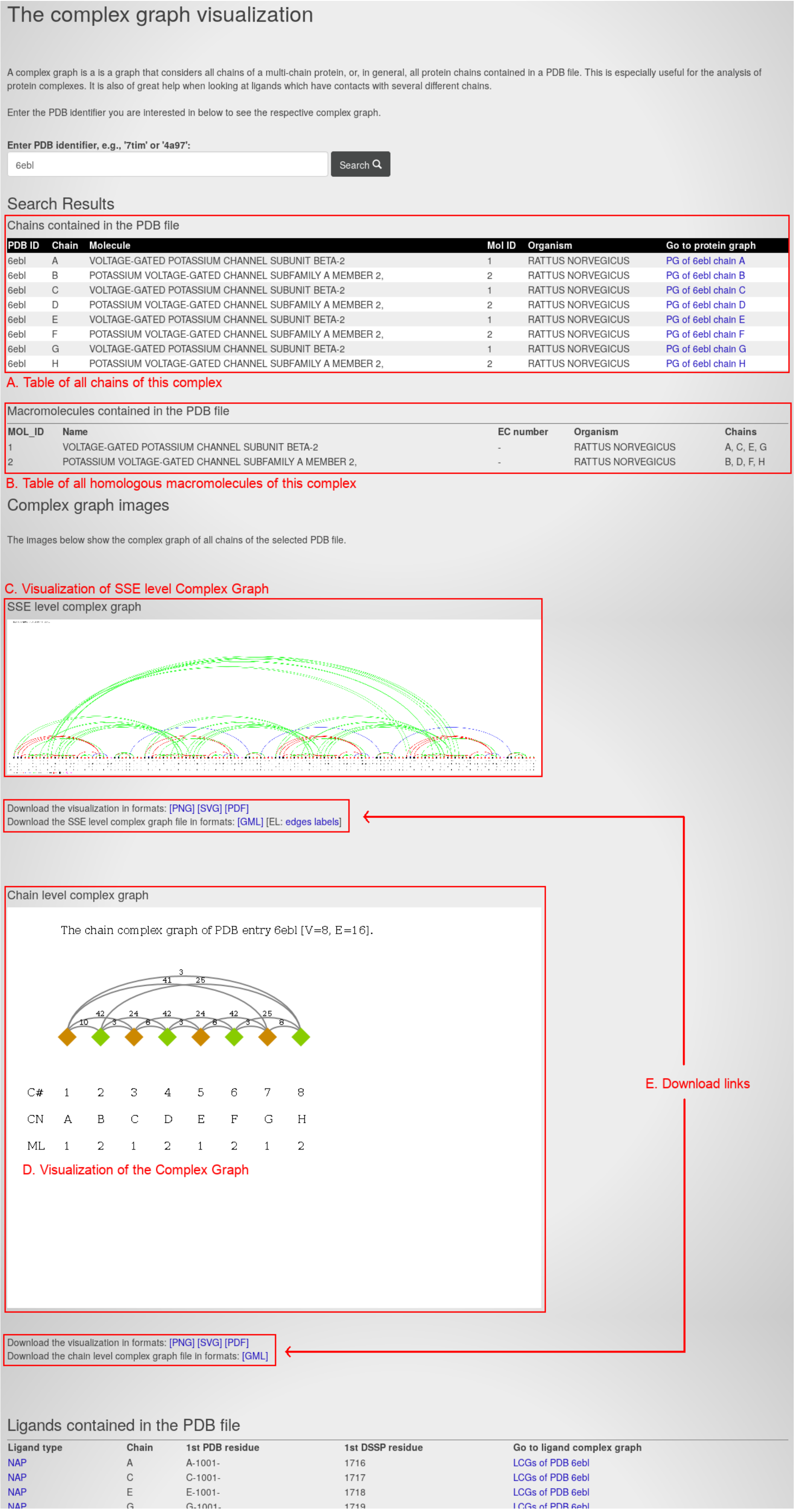
1. Open the drop-down menu of the Complex Graph search by clicking anywhere on the respective line.


Complex graphs Search for protein complexes

Enter a query PDB ID, e.g., '4a97' to display complex information for that PDB file.

1. Type in PDB ID, e.g., 6ebl
2. Hit search button

1. Type in the search field the PDB ID 6ebl.
2. Hitting the search button, you see this page:



The complex graph visualization

A complex graph is a is a graph that considers all chains of a multi-chain protein, or, in general, all protein chains contained in a PDB file. This is especially useful for the analysis of protein complexes. It is also of great help when looking at ligands which have contacts with several different chains.

Enter the PDB identifier you are interested in below to see the respective complex graph.

Enter PDB identifier, e.g., '7tim' or '4a97':

6ebl

Search Results

Chains contained in the PDB file

PDB ID	Chain	Molecule	Mol ID	Organism	Go to protein graph
6ebl	A	VOLTAGE-GATED POTASSIUM CHANNEL SUBUNIT BETA-2	1	RATTUS NORVEGICUS	PG of 6ebl chain A
6ebl	B	POTASSIUM VOLTAGE-GATED CHANNEL SUBFAMILY A MEMBER 2,	2	RATTUS NORVEGICUS	PG of 6ebl chain B
6ebl	C	VOLTAGE-GATED POTASSIUM CHANNEL SUBUNIT BETA-2	1	RATTUS NORVEGICUS	PG of 6ebl chain C
6ebl	D	POTASSIUM VOLTAGE-GATED CHANNEL SUBFAMILY A MEMBER 2,	2	RATTUS NORVEGICUS	PG of 6ebl chain D
6ebl	E	VOLTAGE-GATED POTASSIUM CHANNEL SUBUNIT BETA-2	1	RATTUS NORVEGICUS	PG of 6ebl chain E
6ebl	F	POTASSIUM VOLTAGE-GATED CHANNEL SUBFAMILY A MEMBER 2,	2	RATTUS NORVEGICUS	PG of 6ebl chain F
6ebl	G	VOLTAGE-GATED POTASSIUM CHANNEL SUBUNIT BETA-2	1	RATTUS NORVEGICUS	PG of 6ebl chain G
6ebl	H	POTASSIUM VOLTAGE-GATED CHANNEL SUBFAMILY A MEMBER 2,	2	RATTUS NORVEGICUS	PG of 6ebl chain H

A. Table of all chains of this complex

Macromolecules contained in the PDB file

MOL_ID	Name	EC number	Organism	Chains
1	VOLTAGE-GATED POTASSIUM CHANNEL SUBUNIT BETA-2	-	RATTUS NORVEGICUS	A, C, E, G
2	POTASSIUM VOLTAGE-GATED CHANNEL SUBFAMILY A MEMBER 2,	-	RATTUS NORVEGICUS	B, D, F, H

B. Table of all homologous macromolecules of this complex

Complex graph images

The images below show the complex graph of all chains of the selected PDB file.

C. Visualization of SSE level Complex Graph

SSE level complex graph

Download the visualization in formats: [PNG] [SVG] [PDF]
Download the SSE level complex graph file in formats: [GML] [EL: edges labels]

Chain level complex graph

The chain complex graph of PDB entry 6ebl [V=8, E=16].

C#	1	2	3	4	5	6	7	8
CN	A	B	C	D	E	F	G	H
ML	1	2	1	2	1	2	1	2

D. Visualization of the Complex Graph

E. Download links

Download the visualization in formats: [PNG] [SVG] [PDF]
Download the chain level complex graph file in formats: [GML]

Ligands contained in the PDB file

Ligand type	Chain	1st PDB residue	1st DSSP residue	Go to ligand complex graph
NAP	A	A-1001-	1716	LCGs of PDB 6ebl
NAP	C	C-1001-	1717	LCGs of PDB 6ebl
NAP	E	E-1001-	1718	LCGs of PDB 6ebl
NAP	G	G-1001-	1719	LCGs of PDB 6ebl

The page contains the following information:

A. A table of all chains of this complex. For each chain, it lists the PDB ID, Chain ID, Molecule name, Molecule (Mol) ID, source organism, and a link to the Protein Graph.
B. A table of all macromolecules of this complex. For each macromolecule, its lists the macromolecule ID (MOL_ID), the name, the enzyme class (EC) number, the source organism and the homologous chains.
C. The Visualization of the secondary structure-level Complex Graph. It corresponds to a Protein Graph extended by all secondary structure elements of the complex.
D. The Visualization of the Complex Graph.
E. The download links for the graphs and their visualization in different file types.