

PDBe and PDBe-KB webpages tutorial for ligand analysis and visualisation

1. PDBe entry pages

Introduction

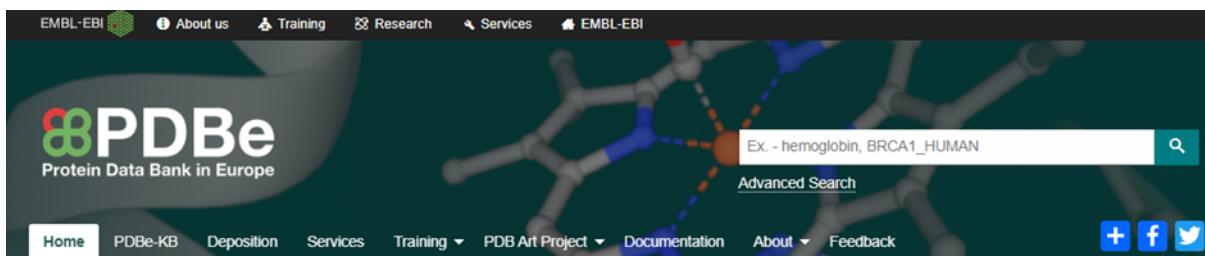
This tutorial demonstrates how to access ligand-related information from PDBe entry pages, examine PDB-ligand interactions, and evaluate ligand quality using wwPDB validation reports.

Example used: Imatinib

In this tutorial, all the tasks are marked in red.

Section 1: Navigating ligands on PDBe entry pages

- Go to [PDBe.org](http://www.ebi.ac.uk/pdbe/)
 - You should see the following header bar:



- Your search begins with the search bar at the top right.

- Type “**Imati**” into the search bar.
- Typing generates autocomplete results, grouped into different fields. The number next to each option tells you how many PDB entries are associated with it. **Click on the first option**.

The screenshot shows the PDBe website interface. At the top, there's a navigation bar with links to About us, Training, Research, Services, and EMBL-EBI. Below the header, the PDBe logo and "Protein Data Bank in Europe" text are visible. A search bar contains the query "imati". Below the search bar, a dropdown menu shows "Ligand STI : IMATINIB (28)". The main content area displays a molecular structure of Imatinib (STI) bound to a protein.

- This will lead you to the PDBe search page with all the PDB entries where Imatinib (PDB ligand ID: STI) is bound as shown in the image below

The screenshot shows the PDBe search results for "STI : IMATINIB". The left sidebar has a "Filter by" section with a red box around it. The main area shows a table of search results with columns for Entries, Macromolecules, Compounds, and Protein families. The first entry is highlighted: "6jol Crystal structure of PDGFRA in complex with imatinib by co-crystallization". To the right, there's a detailed view of the entry, including assembly information, source organism (Homo sapiens), and a 3D visualization of the protein-ligand complex.

- Using the **Filter by** option on the left side menu of this page, filter all the structures which are present in the humans

The screenshot shows the "Macromolecules" filter menu. Under "Organism name", the option "Homo sapiens (18)" is highlighted with a red box. Other options listed are Mus musculus (7), Gallus gallus (2), and synthetic construct (1).

- Navigate through all the results shown and find the PDB structure of PDGFRA in complex with imatinib
- Click on the **PDB ID** to view the PDBe entry page for that structure.

6jol Crystal structure of PDGFRA in complex with imatinib by co-crystallization

Liang L, Yan XE, Yun CH
To be published

Source organism: *Homo sapiens*

Assembly composition: protein only structure

Bound ligands: STI STI

Assembly name: Platelet-derived growth factor receptor alpha (Preferred) [search this complex](#)

PDBe complex ID: PDB-CPX-147663 (Preferred) [search this ID](#)

[3D Visualisation](#) [Download files](#)

X-ray diffraction
1.9Å resolution
Released: 25 Mar 2020
DOI: [10.2210/pdb6jol/pdb](#)
Model geometry
Fit model/data

- This will lead you to the PDBe entry page for that structure.

Section 2: Visualise ligand interactions

From a given PDBe entry page for that structure, the ligand interactions can be viewed from ‘Ligand and Environments’ section.

- Click on the ligand image to visualise the ligand interaction

PDBe > 6jol

Crystal structure of PDGFRA in complex with imatinib by co-crystallization
Source organism: *Homo sapiens*
Entry authors: Liang L, Yan XE, Yun CH

X-ray diffraction
1.9Å resolution
Released: 25 Mar 2020
DOI: [10.2210/pdb6jol/pdb](#)
Model geometry
Fit model/data

Quick links

- 6jol overview
- Citations
- Structure analysis
- Function and Biology
- Ligands and Environments
- Experiments and Validation

View

- Archive mmCIF file
- Updated mmCIF file
- PDB file
- PDB header
- Assembly composition XML
- FASTA (Entry)
- Summary report (PDF)
- Full report (PDF)
- Percentile plot (PNG)
- Percentile plot (SVG)
- 6jol @ RCSB
- 6jol @ PDBJ
- 6jol @ PDBSum
- 6jol @ Proteopedia

Function and Biology

Reaction catalysed: ATP + a [protein]-L-tyrosine = ADP + a [protein]-L-tyrosine phosphate

Biochemical function: ATP binding

Biological process: cell surface receptor protein tyrosine kinase signalling pathway

Cellular component: not assigned

Ligands and Environments

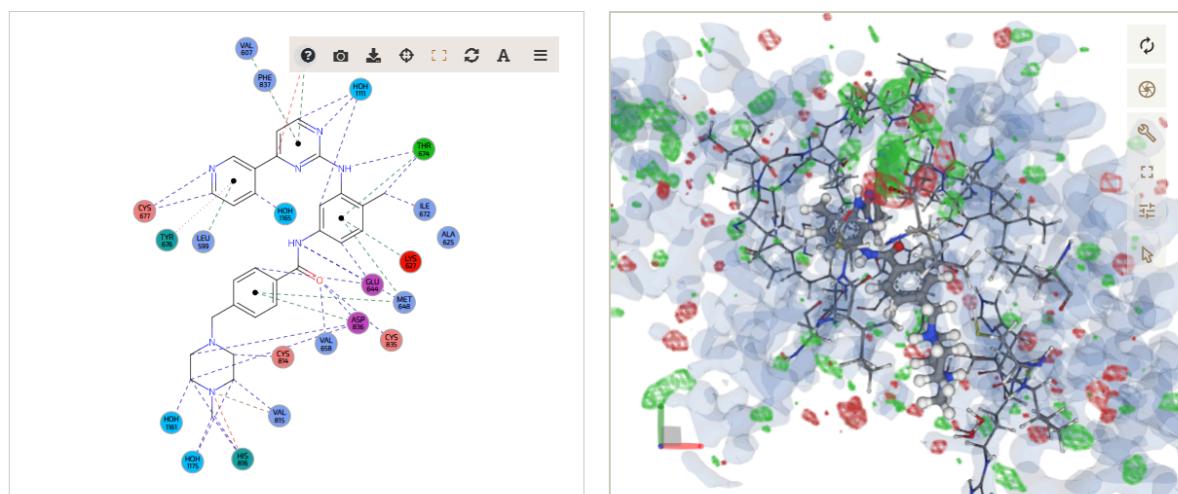
1 bound ligand:
 1 x STI
No modified residues

- This will open the ‘Environment details’ section has two views:

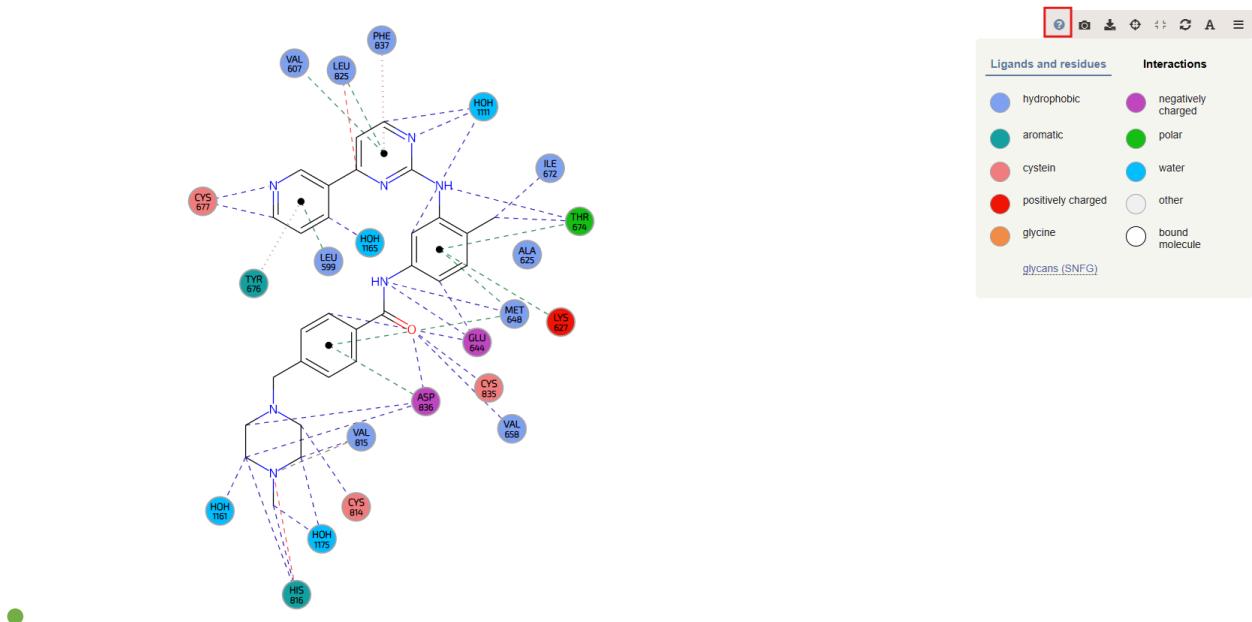
- On the left is an image displaying the small molecule and all of the amino acids that form the binding site for this molecule in a 2D depiction.
- On the right is the Mol* viewer, displaying the same data in 3D. The experimental data (electron density map, since this X-ray crystallography structure) is also shown.
- The image on the left displays the bound small molecule. The amino acids in the binding site are shown in different ways:
 - There is a colour scheme highlights the different amino acids and helps in navigating the type of interactions between the ligand and the protein.
- Maximise the left view (Hint: click on icon which opens the 'Menu' and hit [] button for fullscreen view).

Environment details NEW

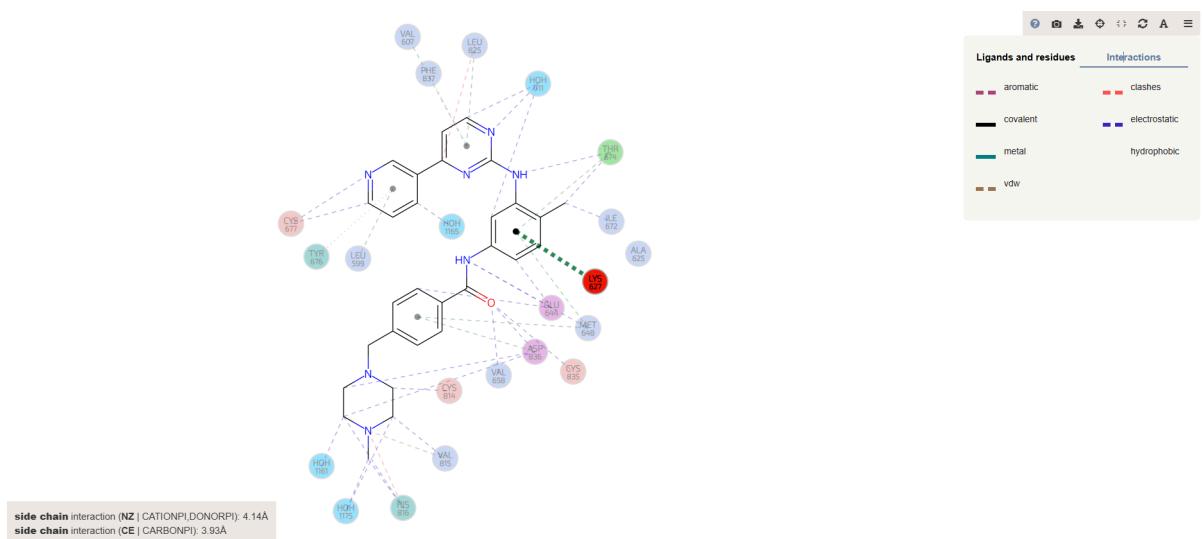
STI 1001 bound to chain A



- Click on the ? button to view the coloring scheme for this view



- List all the of (a) hydrophobic, (b) positively charged, (c) negatively charged, (d) aromatic and (e) polar amino acids that are interacting directly with STI ? (Hint hover over the residue and interaction to see the detailed interaction at the bottom)



- Minimise the screen and go back to the default view with two panels.
- Notice how mousing over amino acids in the left panel results in the amino acid being highlighted in the right panel.

- Try interacting with the Mol* viewer on the right panel.
 - The right panel shows the electron density that the molecule was fitted into.
- Notice how mousing over the amino acid in the Mol* viewer results in the highlighting in the 2D depiction.
- How well do the atoms fit into the electron density maps?

Section 3: Access and evaluate ligand quality using wwPDB validation reports.

From a given PDBe entry page for that structure, the wwPDB validation report can be viewed using the View button on the right side menu.

The screenshot shows the PDBe entry page for structure 6jol. The main content includes:

- PDBe > 6jol**
- X-ray diffraction 1.9 Å resolution**
- Released: 25 Mar 2020**
- DOI: 10.2210/pdb6jol/pdb**
- Model geometry Fit model/data** (with a red bar indicating poor fit)
- Quick links** (including 6jol overview, Citations, Structure analysis, Function and Biology, Ligands and Environments, and Experiments and Validation).
- View** button highlighted in red.
- Function and Biology** section with reaction catalysed: ATP + a [protein]-L-tyrosine = ADP + a [protein]-L-tyrosine phosphate.
- Ligands and Environments** section showing 1 bound ligand (1 x STI) and No modified residues.
- Reaction catalysed:** ATP + a [protein]-L-tyrosine = ADP + a [protein]-L-tyrosine phosphate.
- Biochemical function:** ATP binding.
- Biological process:** cell surface receptor protein tyrosine kinase signaling pathway.
- Cellular component:** not assigned.
- Sequence domains:**

- Click on the ‘View’ button and then click on the Full report (PDF).
 - This will open the wwPDB full validation report in PDF format in your browser
- Click on the icon shown in the red box to expand the document outline

Full wwPDB X-ray Structure Validation Report [\(i\)](#)

Nov 15, 2023 – 04:52 PM JST

PDB ID : 6JOL
 Title : Crystal structure of PDGFRA in complex with imatinib by co-crystallization
 Authors : Liang, L.; Yan, X.E.; Yun, C.H.
 Deposited on : 2019-03-22
 Resolution : 1.90 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
 A user guide is available at <https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
 with specific help available everywhere you see the [\(i\)](#) symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

- Click on the ‘Model quality’ and then ‘ligand geometry’ to view ligand geometric outliers

5.6 Ligand geometry [\(i\)](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	STI	A	1001	-	40,41,41	1.90	6 (15%)	51,56,56	1.81	6 (11%)

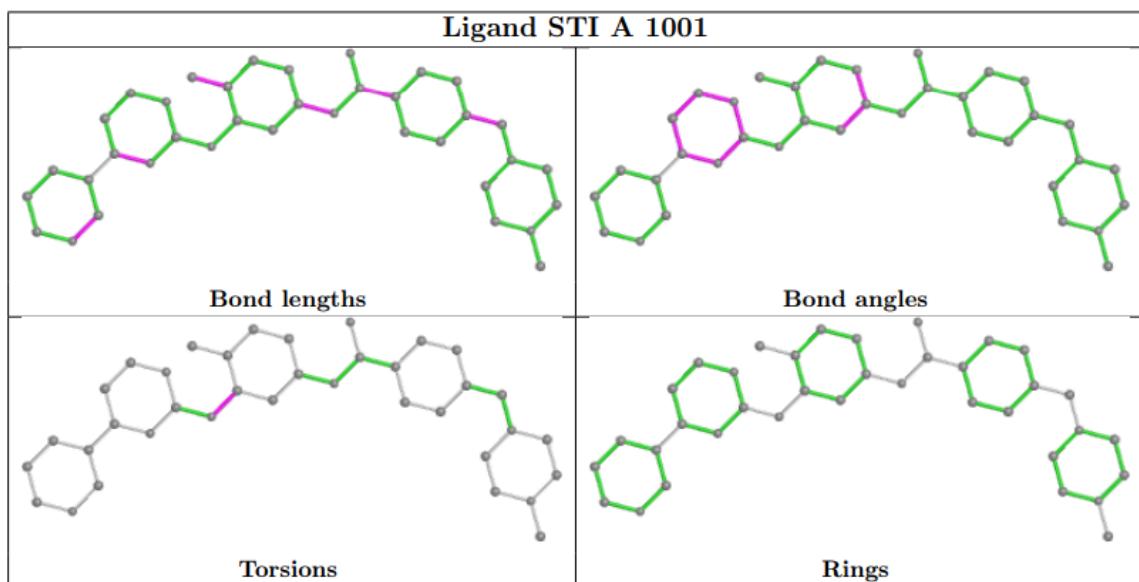
In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STI	A	1001	-	-	2/16/30/30	0/5/5/5

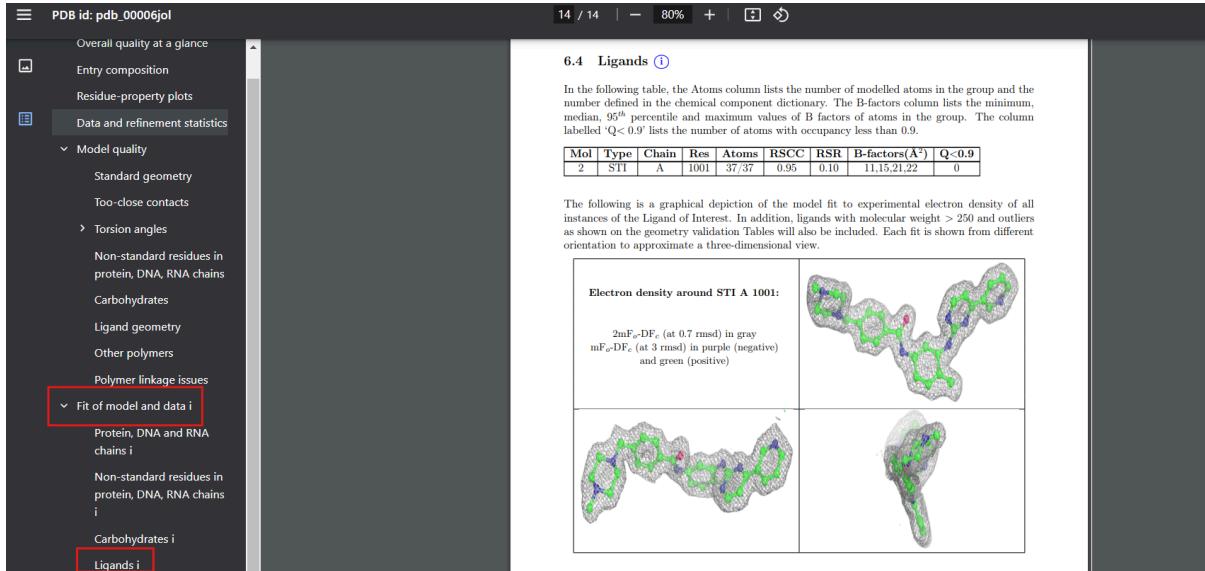
All (6) bond length outliers are listed below:

wwPDB
PROTEIN DATA BANK

- Using the program Mogul, these reports evaluate ligand geometry against the small molecule structures in the Cambridge Structural Database (CSD). The results are shown in tabular format which shows :
 - Z-scores that are calculated to quantify deviations in bond lengths, angles, torsion angles, and ring geometry, with values above 2.0 flagged as outliers and highlighted in yellow.
 - The RMSZ score, which summarises the overall ligand geometry, should ideally range between 0 and 1.
 - For torsion angles, deviations are flagged if their local density measure is below 5%, while rings are flagged if their torsion angle RMSD exceeds 60°.
- Find all the geometry outliers for STI in this structure**
- The two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry is also shown.



- Commonly observed values are shown in green, unusual values in magenta, and features with insufficient data in grey.
- Click on ‘Fit of model and data’ and the ‘Ligands’**



- This will open the section for ligand fit to the electron density is assessed using metrics like the RSR (Real-Space R-value) and RSCC (Real-Space Correlation Coefficient).
- Ligands with RSCC values below 0.8 or RSR values above 0.4 are highlighted as outliers and indicate poor fit quality.
- The 3D view for the ligand atomic model fit the experimental electron density map (shown in grey) with positive and negative difference density maps shown in green and magenta respectively.
- Evaluate the model-fit quality and determine if STI is mapped good fit or a poor fit to electron density data.**

- Find all the other structures of PDGFRA in complex with imatinib
 - Hint: Go to UniProt ID mentioned on the PDBe entry page

 Platelet-derived growth factor receptor alpha

Chain: A  Molecule details >

Length: 356 amino acids

Theoretical weight: 40.59 KDa

Source organism: *Homo sapiens*

Expression system: *Spodoptera frugiperda*

UniProt:

- Canonical:  P16234  (Residues: 550-973; Coverage: 33%)
- Best match:  P16234-3  (Residues: 550-706)

Gene names: PDGFR2, PDGFRA, RHEPDGFRA

Sequence domains: Protein tyrosine and serine/threonine kinase 

- This will take you to PDBe-KB protein page for that protein where you can see all the aggregated data including structures, ligands, other macromolecules, various annotations and similar proteins.
- How many other structure did you find for this protein ?
- How many other ligands does it bind to apart from Imatinib ?

2. PDBe-KB protein pages

Introduction

This tutorial guides accessing ligand-related information on PDBe-KB protein pages. It will show how to identify key binding residues

using PDBe-KB's aggregated protein views and locate important ligand binding sites through a 3D view of superimposed ligands.

Example used: Tyrosine-protein kinase ABL1 from human (UniProt accession: P00519)

In this tutorial, all the tasks are marked in red.

Section 1: Navigating PDBe-KB Protein page

There are three ways you can access the PDBe-KB Protein page for the protein of interest.

1. Using PDBe search - pdbe.org
2. Using PDBe entry Page - pdbe.org/7n9g
3. Using PDBe-KB landing page (pdbekb.org)

For 1, use the search box to search for the protein of interest. Choose the protein of interest from the hits. Click on UniProt accession mentioned in PDBe-KB to open the PDBe-KB protein page for that entry.

□ 7n9g Crystal structure of the Abl 1b Kinase domain in complex with Dasatinib and Imatinib

Miller DJ, Xie T
J Mol Biol (2022) [PMID: 34774565]

Source organism: *Homo sapiens*

Assembly composition: protein only structure

Bound ligands: 1N1 STI STI 1N1 PO4

Assembly name: Tyrosine-protein kinase ABL1 (Preferred) [search this complex](#)

PDBe complex ID: PDB-CPX-132602 (Preferred) [search this ID](#)

PDBe-KB: P00519

[3D Visualisation](#) [Download files](#)

X-ray diffraction
2.2Å resolution
Released: 27 Apr 2022
DOI: 10.2210/pdb7n9g
Model geometry Fit model/data

For 2, so the entry page of the structure of your interest (for e.g pdbe.org/7n9g). In the 'Structure analysis' section, click on UniProt

accession from UniProt field and this will take you to its PDBe-KB protein page.

☰ Tyrosine-protein kinase ABL1

Chains: A, B, C Molecule details >

Length: 271 amino acids

Theoretical weight: 31.49 KDa

Source organism: *Homo sapiens*

Expression system: *Escherichia coli*

UniProt:

- Canonical: P00519 (Residues: 229-499; Coverage: 24%)

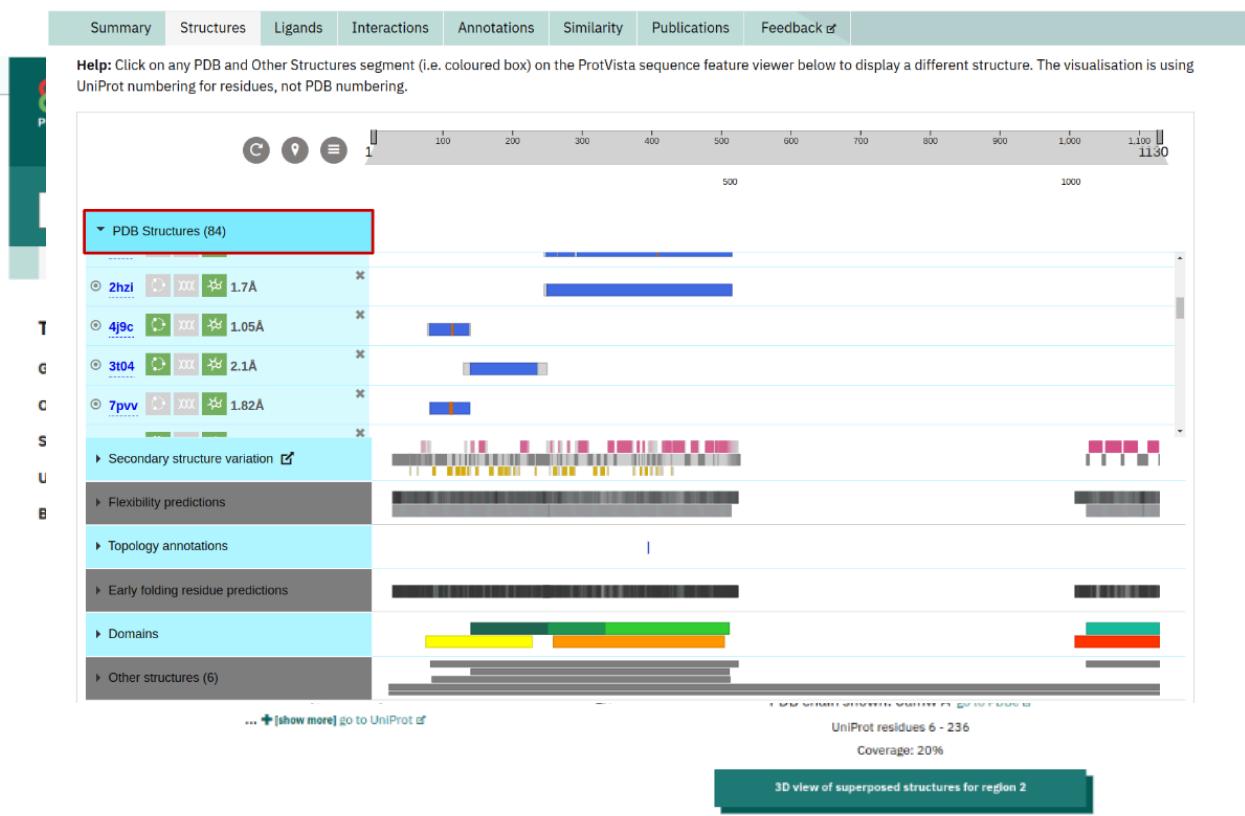
Gene names: *ABL*, *ABL1*, *JTK7*

Sequence domains: Protein tyrosine and serine/threonine kinase

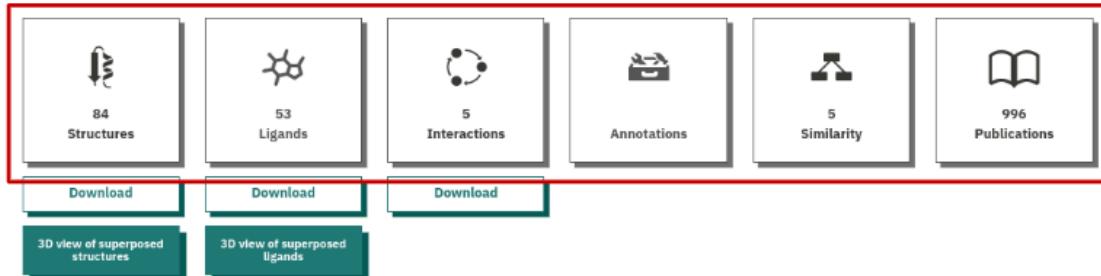
[]

For 3, go to the PDBe-KB landing page (pdbe.org), and search by PDB ID or UniProt accession number. This will take you to that protein's PDBe-KB Protein page available at
<https://www.ebi.ac.uk/pdbe/pdbe-kb/proteins/P00519>

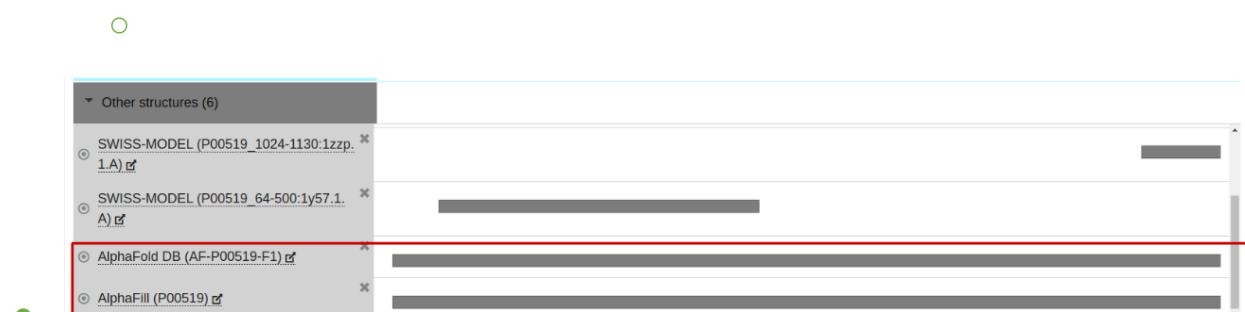
- The icons on the summary page provide a quick overview, showing the total number of structures of that protein in the PDB, the unique ligands bound to it, the unique macromolecules that form complexes with it, similar proteins, and the publications associated with that protein.
- Find the total number of structures present in the PDB.
- Is there an experimental structure solved for the entire protein sequence?
 - All the experimental structures are shown in 'PDB structures' in the ProtVista sequence feature viewer in the 'Structures' tab.



Click on the icons below to view the relevant page:



- Scroll through the structures to see - if you can find the experimental structure solved for the entire protein.
- Find any other structures which are solved for the entire protein sequence. (Hint: 'Other structures' tab)



- In the other structures, you will find all the predicted 3D structures for that protein from various resources like SWISS-MODEL, AlphaFold DB and more.

Section 2- Ligand binding residues

The ligand binding residues are accessible via ‘Ligands’ tab.

‘Ligands and Environments’ section

1. first shows a gallery of ligands which bind to this protein. These images are arranged according to similarity, so the similar-looking molecules are seen together in one frame.
2. Ligand binding residues are shown in the ProtVista viewer.

Use ligand gallery view to answer the following:

- Can you group these ligands based on visual similarity (I.e. they look like similar chemical structures)? Note: this does not have to accurate matching - structures with rings, structures with extended chains etc. is enough.
- Which ligands are most commonly found bound to this structure in PDB entries?
- Were there any ligands that you found difficult to fit into any groups?

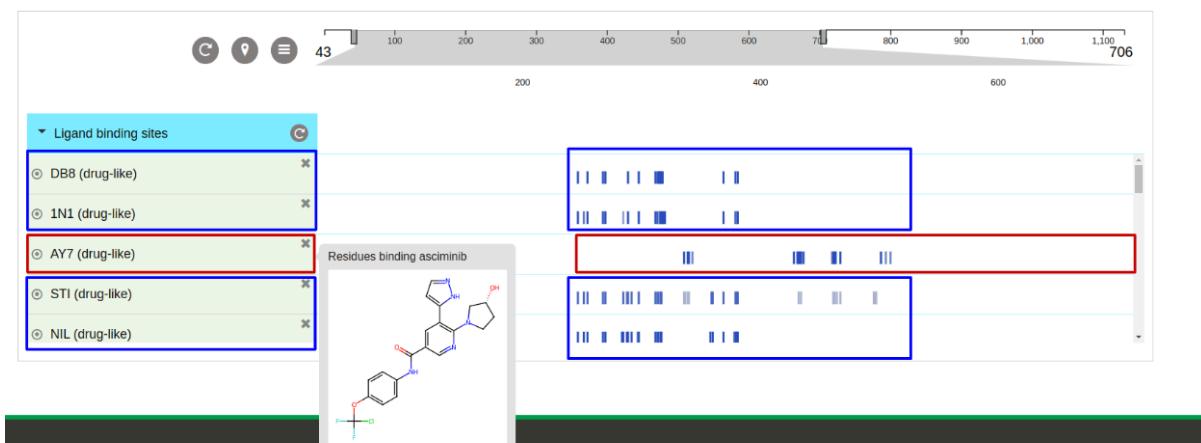
Using ligand binding residues in ProtVista viewer, answer the following:

- Group the ligands into groups according to their binding residues
- Do all the drug-like ligands fall in one group
 - Hint - Look for ligand ID that has ‘drug-like’ annotation

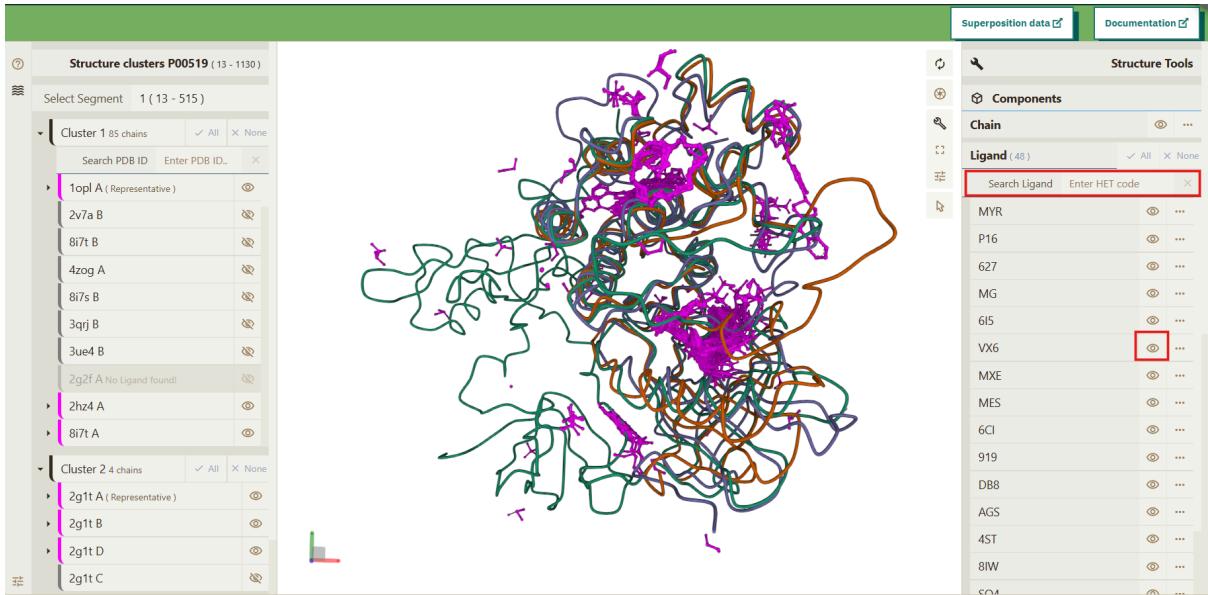
- Hint Asciminib (AY7) seems to bind differently compared to other drug-like molecules like Imatinib (STI), Bosutinib (DB8) and more.

Ligand-binding Residues

The visualisation is using UniProt numbering for residues, not PDB numbering.



- You can also quickly see all the binding site of various ligands on the protein 3D structure using ‘3D view of superposed ligands’ button.
 - This shows all the ligand binding sites this will open a 3D view of all the ligands bound to superposed structures of your query protein in Mol*.
 - Using the controls in the right-hand side of Mol* window, one can hide and unhide the various bound ligands.
- Identify the total number of ligand binding sites from the 3D view of the superposed ligands. Then, check if this aligns with the grouping based on binding residues that you previously created.



- (Hint: Use the search box to locate a ligand of interest and the eye button to hide or unhide it. When you hover over a ligand, its ID and name will display at the bottom of the screen.)
- Navigate the annotation section of this protein page and see if you find any overlap between the observed binding residues and predicted binding residues.
 - (Hint: Compare the binding residues in the blue track labelled “Ligand binding sites” with those in the grey track labelled “Predicted ligand binding sites” to assess consistency between observed and predicted binding locations.)
- Are the common observed and predicted binding residues, conserved?
 - (Hint: Use the ‘Sequence conservation’ track and zoom in to 150 or fewer residues to see the sequence conservation)

3. PDBe-KB ligand pages (Beta version)

Introduction

This is a tutorial for PDBe-KB ligand pages (Beta version). Please note that these pages are not officially released and may contain known or unknown bugs.

To view these pages, identify the PDB ligand identifier for your ligand of interest.

Example used: IMATINIB, which has the PDB ligand identifier: STI.

PDBe-KB ligand page for STI:

<https://wwwdev.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/STI>

In this tutorial, all the tasks are marked in red.

Section 1: Description

- On the top of this page, you will see a description for this ligand with molecular name, synonyms, formula, and essential identifiers of the small-molecule
- On the right side of this section, you will find an image gallery, showing various structural representations of ligand.
- Find the scaffold of this small molecule.

- Find various fragments in this small molecule.

(Hint: Use the arrows next to the ligand 2D image to see various ligand representation)

PDBe-KB Ligands
Protein Data Bank in Europe - Knowledge Base

View PDBe-KB ligand pages by PDB ligand ID (CCD/PRD/CLC) Explore

Examples: STI GLC XRS NAG HEM

This page is currently under active development, and its features and content may change frequently.

Description

STI Drug-like

4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE

View 3D Download as ▾

Description

Synonyms Imatinib, Mitinab, Enliven, Celonib, STI-571, Imatinib, IMATIN...
Show more ▾

Formula C29H31N7O

IUPAC InChI InChI=1S/C29H31N7O/c1-21-5-10-25(18-27(21)34-29-31-13-11-26(33-29)24-4-3-12-30-19-24)32-28(37)23-8-6-22(7-9-23)20-36-16-...
Show more ▾

IUPAC InChIKey KTUFNOKKBMGRW-UHFFFAOYSA-N

SMILES Cc1ccc(cc1Nc2nccc(n2)c3ccnc3)NC(=O)c4ccc(cc4)CN5CCN(CC5)C

Source OpenEye

View Atoms **View Bonds**

Overall view, and highlighted scaffolds and fragments ⓘ

Displayed: 1 / 9
Atom Labelled STI

- Using the button ‘Download as’ you can download the ligand file in various formats.
- Download the ligand in CIF format
- Can this molecule be a drug ?
- Scroll to Physicochemical properties
- How many heavy atoms are present this ligand ?
- How many rings are present in this ligand ?
- How many aromatic rings are present in this ligand ?

Lipinski's 'rule-of-five' is the first qualitative attempt to develop tools to help chemists design orally active compounds, and is now

extensively used in selecting drug molecules for further development.

Lipinski's rule states that, in general, an orally active drug has no more than one violation of the following criteria:

1. No more than 5 hydrogen bond donors (the total number of nitrogen–hydrogen and oxygen–hydrogen bonds)
 2. No more than 10 hydrogen bond acceptors (all nitrogen or oxygen atoms)
 3. A molecular mass less than 500 daltons
 4. A calculated octanol–water partition coefficient (Clog P) that does not exceed 5
- Which Lipinski's 'rule-of-five' does this molecule satisfy?

Section 2: Ligand bound structures

- The 'Bound Structures' section provides an overview of the macromolecules to which a specific ligand binds. The data in this table is organised by 'Proteins' and 'Structures.' The Protein View aggregates all structures associated with the same protein and includes information such as the protein name, EC number, and the functional role of the ligand (indicating whether it acts as a reactant, cofactor, or drug-like molecule). In the Structure View, this table is further expanded to include detailed PDB structure information.

Bound structures

[Download structures \(csv\)](#) [Download coordinates \(mmCIF\)](#)

Protein name	PDBe-KB link	Total structures	Organism	EC number	Ligand function
Tyrosine-protein kinase ABL1	P00520	7	<i>Mus musculus</i> (Mouse)	2.7.10.2	Unannotated
Tyrosine-protein kinase ABL1	P00519	6	<i>Homo sapiens</i> (Human)	2.7.10.2	Drug-like
Proto-oncogene tyrosine-protein kinase Src	P00523	2	<i>Gallus gallus</i> (Chicken)	2.7.10.2	Unannotated
Broad substrate specificity ATP-binding cassette transporter ABCG2	Q9UNQ0	1	<i>Homo sapiens</i> (Human)	7.6.2.2	Unannotated
Deoxycytidine kinase	P27707	1	<i>Homo sapiens</i> (Human)	2.7.1.113, 2.7.1.74, 2.7.1.76	Unannotated
Tyrosine-protein kinase Lck	P06239	1	<i>Homo sapiens</i> (Human)	2.7.10.2	Unannotated

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- How many proteins have this ligand bound to it ?
- How many PDB structures have this ligand bound to it ?

Bound structures

[Download structures \(csv\)](#) [Download coordinates \(mmCIF\)](#)

Protein name	PDBe-KB link	Total structures	Organism	EC number	Ligand function
Tyrosine-protein kinase ABL1	P00520	7	<i>Mus musculus</i> (Mouse)	2.7.10.2	Unannotated
Tyrosine-protein kinase ABL1	P00519	6	<i>Homo sapiens</i> (Human)	2.7.10.2	Drug-like
Proto-oncogene tyrosine-protein kinase Src	P00523	2	<i>Gallus gallus</i> (Chicken)	2.7.10.2	Unannotated
Broad substrate specificity ATP-binding cassette transporter ABCG2	Q9UNQ0	1	<i>Homo sapiens</i> (Human)	7.6.2.2	Unannotated
Deoxycytidine kinase	P27707	1	<i>Homo sapiens</i> (Human)	2.7.1.113, 2.7.1.74, 2.7.1.76	Unannotated
Tyrosine-protein kinase Lck	P06239	1	<i>Homo sapiens</i> (Human)	2.7.10.2	Unannotated

Page Size: 1 to 10 of 16 ⌂ < Page 1 of 2 > ⌂

2.1: Navigating to PDBe entry pages from PDBe-KB ligand pages

- Find the PDB structure for Human Abl kinase domain in complex with imatinib

(Hint: For now, use pdbe.org/search for search but search functionality is coming soon on these web pages)

Entry	Resolution	Release Date	DOI	PDBx-KB ID
7n9g	2.2 Å	27 Apr 2022	10.2210/pdb/7n9g/pdb	P00519
2hyv	2.4 Å	16 Jan 2007	10.2210/pdb/2hyv/pdb	P00519

- Find this ligand's interacting residues for the top hit of task 10.

(Hint: Click on the top hit of task 10. This will take you to the PDBe entry page, now click on the ligand image to view interacting residues)

- Find the water molecule clashing with the ligand in this structure.
 - Can you identify this water molecule in the 3D viewer and measure the distance between the ligand and this water molecule?
- Do any of the ligand binding residues exhibit a poor fit to the electron density(i.e. RSRZ outliers)?

(Hint: Click on the ‘Details’ in the Structure analysis section, scroll down and compare ‘Chains’ and ‘Ligand binding sites’ track in ProtVista viewer)



- The biological assembly (also sometimes referred to as the biological unit) is the macromolecular assembly that has either been shown to be or is believed to be the functional form of the molecule. For example, the functional form of hemoglobin

has four chains.

- What is the biological assembly for the top hit of task 10?
- What is the assembly (complex) name for it?
- Find all the other PDB structures for this assembly (complex) name.

- Filter the above list to include only human PDB structures.

(Hint: Click on the assembly name and then use filter options from the menu on left handside)

- Filter the above list to include PDB structures from the same assembly composition and species as the top hit of task 10.

(Hint: Click on the ‘PDBe Complex ID’)

2.2: Navigating to PDBe-KB Proteins pages from PDBe entry pages

- Let's explore all the other ligands that Human Tyrosine-protein kinase ABL1 binds to. Navigate back to the PDB entry page for the top hit of task 10 and click on the UniProt accession. This will redirect you to the PDBe-KB Protein page for this protein.

Structure analysis Details

Assembly composition: monomeric (preferred)

Assembly name: Tyrosine-protein kinase ABL1 (preferred)

PDBe Complex ID: PDB-CPX-132602 (preferred)

Entry contents: 1 distinct polypeptide molecule

Macromolecule:

Tyrosine-protein kinase ABL1

Chains: A, B, C [Molecule details >](#)

Length: 271 amino acids

Theoretical weight: 31.49 KDa

Source organism: *Homo sapiens*

Expression system: *Escherichia coli*

UniProt:

- Canonical: [P00519](#) (Residues: 229-499; Coverage: 24%)

Gene names: *ABL*, *ABL1*, *JTK7*

Sequence domains: Protein tyrosine and serine/threonine kinase

- On this page, you'll find aggregated PDB data for the specific protein, including information on all the PDB structures, ligands bound to the protein, macromolecule interactions, and related proteins. Additionally, you'll find various structural and functional annotations from PDBe-KB collaborators, providing insights into the biological context of the protein.
- Find all the ligands bound to this protein.

1. 

Ligands [What's new?](#)

Tyrosine-protein kinase ABL1

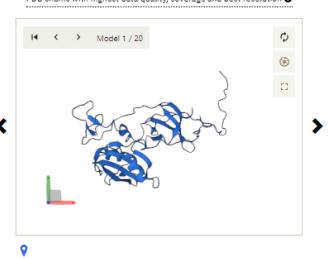
Gene: ABL1 [Enzyme: EC 2.7.10.2](#) [Disease](#)

Organism: *Homo sapiens (Human)*

Synonyms: ABL, JTK7

Uniprot: P00519 [go to UniProt](#)

Biological function: Non-receptor tyrosine-protein kinase that plays a role in many key processes linked to cell growth and survival such as cytoskeleton remodeling in response to extracellular stimuli, cell motility and adhesion, receptor endocytosis, autophagy, DNA damage response and apoptosis. Coordinates actin remodeling through tyrosine phosphorylation of proteins controlling cytoskeleton dynamics like WASF3 (involved in branch formation); ANXA1 (involved in membrane anchoring); ... [\[show more\]](#) [go to UniProt](#)



Representative structures for UniProt P00519
PDB chains with highest data quality, coverage and best resolution [\[more\]](#)

PDB chain shown: 6amv A [go to PDBe](#)
UniProt residues 6 - 236
Coverage: 20%

3D view of superposed structures for region 2

Click on the icons below to view the relevant page:

 81 Structures Download	 50 Ligands Download	 5 Interactions Download	 Annotations	 5 Similarity	 991 Publications
3D view of superposed structures					
3D view of superposed ligands					

- Filter all the ligands which are drugs from this list
- View all the ligands superposed on this protein and investigate if all the drugs found in task 16 a. bind in the same binding site.
- Do all the STI molecules binds to the same binding site?

Section 3: Interaction statistics

- Now let's go back to PDBe-KB ligand pages. After Structures section, you will see is the 'Interaction statistics' section. This sections aggregates the interactions data over all PDB entries in which this ligand is bound. It shows 1) the frequency of interaction between each atom of the small molecule and each amino acid across all the PDB structures to which it is bound 2) It also highlights the interaction frequency on each atom in the ligand's 2D interactive image.



- What kind of amino acids does this ligand generally binds to ?

- Which is the most frequently interacting amino-acid with ligand ?
- Which is the most interacting ligand atom in the heatmap and where it is located in the ligand 2D image.
- Which ligand atoms generally involved in aromatic interactions ?

Section 4: Related ligands

- Next section, you will see is the ‘Related ligands’ section. This section shows all the ligands which are similar to this ligand. In general, this section will show (whenever applicable): 1) Ligands with same scaffold 2) Ligands with 60 % or more similarity 3) Stereoisomers
- Now let’s look at the ligands which are similar to this ligand.
- Which ligand has the same scaffold as STI ?
- Which ligands are 70 % or more similar to STI ?
- Do the similar ligands identified in task 24, interact with similar kind of amino-acids ?