

How to Run 2P2I_{INSPECTOR}

Using a 4 letter PDB code :

The screenshot shows the 2P2IInspector web interface with four numbered steps indicated by arrows:

- Search for a PDB entry :** A text input field contains "1BXL".
- OR**
- Upload your PDB file :** A button labeled "Choisissez un fichier" and the text "Aucun fichier choisi".
- Chain1 :** A dropdown menu with "A" selected. **Chain2 :** A dropdown menu with "B" selected.
- Enter Job Title (optional) :** A text input field containing "1BXL NMR Complex (Chain A and B)". Below it is an example: "Example : 1BXL" with a small square icon.
- Calculate Interface Parameters** button and a **Reset** button.

- 1 Enter a valid PDB code
- 2 Select two Chains in contact
- 3 Enter a Job Title (optional)
- 4 Run 2P2I_{INSPECTOR}

Using a PDB File from a local Directory:

The screenshot shows the web interface for 2P2IInspector. It features a search bar for PDB entries, an 'OR' option, and a file upload section. The upload section includes a file selection button labeled 'Choisissez un fichier' with '1BXL.pdb' as an example. Below this are two dropdown menus for 'Chain1' (set to 'A') and 'Chain2' (set to 'B'). A text input field for 'Enter Job Title (optional)' contains '1BXL uploaded from local directory'. Below the input field is a checkbox labeled 'Example : 1BXL'. At the bottom, there is a large 'Calculate Interface Parameters' button and a smaller 'Reset' button. Four numbered callouts (1-4) point to the file selection button, the chain selection dropdowns, the job title input field, and the 'Calculate Interface Parameters' button, respectively.

- 1 Upload a PDB File
- 2 Select two Chains in contact
- 3 Enter a Job Title (optional)
- 4 Run 2P2I_{INSPECTOR}

(To see an example simply tick the **1BXL example box** and run 2P2I_{INSPECTOR})

2P2I_{INSPECTOR} Results

1 BCL-XL/BAK PEPTIDE COMPLEX

1BXL
2A
3B
4

5 3D View of the Complex

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Download Results

PDB File of the dimer
HTML Files with results for both chains
List of Contacts, H-Bonds, Salt Bridges
List of Parameters and Glossary

Interface Properties for 1BXL Complex

Summary Properties ? 9

Summary Properties		Contacts	
Total Interface Area (Å ²)	1843.7	Atom	Atom Res Res no. name name no. Chain
Gap Volume (Å ³)	2892.37	1.	924 C2 PHE 97 A <-> 2939 CD2 LEU 578 B
% Charged Residues	23.1	2.	924 CE1 PHE 97 A <-> 2939 CD2 LEU 578 B
Total Nb of Segments	5	3.	924 CE1 PHE 97 A <-> 2937 CQ LEU 578 B
Nb of non-bonded contacts List	12	4.	924 CE1 PHE 97 A <-> 2987 CD1 ILE 581 B
Nb of hydrogen bonds List	1	5.	922 CE1 PHE 97 A <-> 2987 CD1 ILE 581 B
Nb of salt bridges List	0	6.	973 O ARG 100 A <-> 2986 CD2 ILE 581 B
Total Nb of Disulfide bonds	0	7.	978 C2 ARG 100 A <-> 3025 CD2 ASP 584 B
Secondary Structure at Interface	Alpha	8.	977 NE ARG 100 A <-> 3025 CD2 ASP 584 B
		9.	977 NE ARG 100 A <-> 3023 CQ ASP 584 B
		10.	977 NE ARG 100 A <-> 3022 CQ ASP 584 B
		11.	1005 OH TYR 101 A <-> 2873 CQ1 VAL 574 B
		12.	1004 C2 TYR 101 A <-> 2873 CQ1 VAL 574 B
		13.	1005 OH TYR 101 A <-> 2869 CQ VAL 574 B
		14.	1005 OH TYR 101 A <-> 2872 CQ VAL 574 B
		15.	1002 CE1 TYR 101 A <-> 2938 CD1 LEU 578 B
		16.	1000 CD1 TYR 101 A <-> 2938 CD1 LEU 578 B
		17.	1002 CE1 TYR 101 A <-> 2937 CQ LEU 578 B
		18.	1002 CE1 TYR 101 A <-> 2932 H LEU 578 B
		19.	1005 OH TYR 101 A <-> 2938 CD1 LEU 578 B
		20.	1004 C2 TYR 101 A <-> 2938 CD1 LEU 578 B
		21.	1000 CD1 TYR 101 A <-> 2987 CD1 ILE 581 B
		22.	1083 C2 PHE 105 A <-> 2920 CQ GLN 577 B
		23.	1082 CE2 PHE 105 A <-> 2920 CQ GLN 577 B
		24.	1082 CE2 PHE 105 A <-> 2919 CQ GLN 577 B
		25.	1080 CD2 PHE 105 A <-> 2919 CQ GLN 577 B
		26.	1080 CD2 PHE 105 A <-> 2920 CQ GLN 577 B
		27.	1078 CQ PHE 105 A <-> 2920 CQ GLN 577 B
		28.	1081 CE1 PHE 105 A <-> 2920 CQ GLN 577 B

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- 1 Job Title
- 2 PDB Code or PDB Filename
- 3 4 Show detailed properties for chain A or B
- 5 Visualize complex using Jmol applet and customized menus
- 6 Download Results (2P2Iinspector-results.tgz)
- 7 Result table for global interface parameters
- 8 Open popup menus with list of contacts, hydrogen bonds or salt bridges
- 9 Open a popup menu with parameter definitions

Detailed Properties (by Chain)

SEGMENTS & BASA

Number of Segments	4
Interface Accessible Surface Area	873.4
% Interface Accessible Surface Area	7.2
% Neutral contribution	45.9
% Polar contribution	56.2
% Non polar contribution	43.8
% Charged contribution	27.3

CONTACTS

Number of Non-Bonded	Residues	Atoms
All	13	34
Neutral	5	18
Polar	6	15
Hydrophobic	7	19
Charged	3	6

Detailed Properties (by Chain)

⊗ GENERAL PROPERTIES

Properties	Residues	Atoms
% Aromatic	21.7	30.7
% Acidic	8.7	5.4
% Basic	17.4	15.1
% Acyclic	78.3	69.3
% Cyclic	21.7	30.7
% Aliphatic	39.1	41.6
% Small	21.7	12.7
% Medium	4.3	7.8
% Large	73.9	79.5
% Alpha character	78.3	79.5
% Beta character	0.0	0.0
% Coil	8.7	7.2

⊗ ATOM PROPERTIES

Atom Types	%
Carbon	34.3
(O)xygen	7.2
(N)itrogen	3.6
(S)ulfur	0.0
Hydrogen	54.8
(P)hosphorus	0.0
Fluor	0.0
N+O+P+S	4.8

List of Parameters and Jmol Help File

List of interface parameters

BASA	All	BASAT	Total Interface Accessible Surface Area
	by Chain	BASA1	Interface Accessible Surface Area for Chain A
		%BASA1	Interface Accessible Surface Area for Chain A (%)
		BASA2	Interface Accessible Surface Area for Chain B
	%	%BASA2	Interface Accessible Surface Area for Chain B (%)
		BASAN	% Neutral contribution
		BASAP	% Polar contribution
BASANP		% Non polar contribution	
BASAC	% Charged contribution		
GAP Volume	All	GAPV	Gap Volume
SEGMENTS	All	SEGT	Nb Segments Total
	by Chain	SEG1	Nb Segments for Chain A
		SEG2	Nb Segments for Chain B
SSBONDS	All	Disulnt	Number of Disulfide bonds
HBONDS		Hb30	Number of hydrogen bonds
SALT BRIDGES		SBAB	Number of Salt Bridges
		CONTACT	All
Atom (by Chain)	ContCh		Number of all non-bonded atoms
	ContN		Number of neutral non-bonded atoms
	ContP		Number of polar non-bonded atoms
	ContHyd		Number of hydrophobic non-bonded atoms
	ContC		Number of charged non-bonded atoms
Resid (by Chain)	ContRes		Number of all non-bonded residues
	ContRN		Number of neutral non-bonded residues
	ContRP		Number of polar non-bonded residues
	ContRHyd		Number of hydrophobic non-bonded residues
	ContRC	Number of charged non-bonded residues	

Page menu

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References

2P2I_{INSPECTOR} : Jmol Help File

Protein-Protein Complexes

Click [3D View of the Complex](#) to open the Jmol viewer. **Ctrl-Click** to open in a new Tab. **Shift-Click** to open in a new window.

The protein-protein complex is shown as a cartoon representation colored by chain. The PDB code is shown in the top left corner of the Jmol window.