Identify the binding site residues in 6CRO using the distance cutoff of 3.5 Å.

Steps:

- 1. Enter the PDB code (case sensitive)
- 2. Check "Identification of binding site" and Click on "Submit". This will open up a new page
- 3. Check Protein-DNA/RNA
- 4. Give the distance (default: 3.5 Å)
- 5. Click on "Submit"

For protein-protein complexes it is necessary to provide the second chain name.



Identification of binding site - Protein-DNA/RNA

PDB ID : 6CRO.pdb

Residue name	Residue number	Atom name	Chain name	Residue name	Residue number	Atom name	Chain name	Distance
PHE	14	0	Α	DT	1	O2	U	3.140
GLN	16	N	Α	DT	3	OP2	R	3.000
GLN	16	N	Α	DT	3	OP2	U	3.000
THR	17	OG1	Α	DT	3	C7	R	3.436
THR	17	OG1	Α	DT	3	C7	U	3.436
VAL	25	CG2	Α	DT	15	OP2	R	2.791
VAL	25	CG2	Α	DT	15	OP2	U	2.792
TYR	26	N	Α	DT	15	OP2	R	2.843
TYR	26	N	Α	DT	15	OP2	U	2.844
TYR	26	CB	Α	DT	15	OP2	R	3.390
TYR	26	CB	Α	DT	15	OP2	U	3.390
TYR	26	CD2	Α	DG	16	C8	R	3.174
TYR	26	CD2	Α	DG	16	C8	U	3.174
TYR	26	CE1	Α	DG	16	OP2	R	3.361
TYR	26	CE1	Α	DG	16	OP2	U	3.362
TYR	26	CE2	Α	DG	16	C5'	R	3.308
TYR	26	CE2	Α	DG	16	C5'	U	3.309
TYR	26	CZ	Α	DG	16	OP2	R	3.083

Calculate the contact order and the number of contacts for all the residues (C-alpha atoms) within 8 Å limit (6CRO).

Steps:

- 1. Enter the PDB code (case sensitive)
- 2. Check "Inter-residue interactions" and Click on "Submit". This will open up a new page
- 3. Check "contact order and number of contacts (8 Å, CA atoms)"
- 4. Click on "Submit"

Please enter the follo	wing						
 Enter a PDB-id 6cro Ex: PDB-id=2TRX, Chain=A Or 	Chain name (optional)						
O Upload a PDB File Browse No file selected. Chain name (optional)							
Select one of the follo	owing						
 Identification of binding site 	•						
 Inter-residue interactions 							
Secondary structure propensities							
 Physicochemical properties 							
Submit Clear							
Inter-residue interac	tions						
Short range interactions Medium range interactions	Long range interactions						
Contact order Contact order LRO	Total contact distance						
✓ No. of Contacts (8A, CA atoms)	No. of Contacts (14A, CA atoms)						
No. of Contacts (8A, CB atoms)	□ No. of Contacts (14A, CB atoms)						
Multiple contact index for 2 state proteins	□ Multiple contact index for 3 state proteins						
	•						
Example Submit Clear Back							

Contact order

PDB ID : 6CRO.pdb

Contact order = 16.901

Number of contacts (Distance less than 8Å CA atoms)

PDB name : 6CRO.pdb

Residue name	Residue number	Chain	No. of contacting residues	Contacting residues
GLU	2	Α	5	GLN3 , ARG4 , THR43 , ILE44 , ASN45
GLN	3	Α	6	GLU2 , ARG4 , ILE5 , THR43 , ILE44 , ASN45
ARG	4	Α	8	GLU2, GLN3, ILE5, THR6, PHE41, LEU42, THR43, ILE44
ILE	5	A	9	GLN3, ARG4, THR6, LEU7, ASP9, TYR10, PHE41, LEU42, THR43
THR	6	Α	9	ARG4, ILE5, LEU7, LYS8, ASP9, TYR10, ILE40, PHE41, LEU42
LEU	7	Α	10	ILE5, THR6, LYS8, ASP9, TYR10, ALA11, ILE34, ILE40, PHE41, LEU42
LYS	8	Α	7	THR6, LEU7, ASP9, TYR10, ALA11, MET12, ILE34
ASP	9	Α	8	ILE5, THR6, LEU7, LYS8, TYR10, ALA11, MET12, ARG13
TYR	10	A	12	ILE5, THR6, LEU7, LYS8, ASP9, ALA11, MET12, ARG13, PHE14, GLY15, THR19, LEU42
ALA	11	A	10	LEU7, LYS8, ASP9, TYR10, MET12, ARG13, PHE14, GLY15, GLN16, THR19
MET	12	Α	8	LYS8, ASP9, TYR10, ALA11, ARG13, PHE14, GLY15, GLN16
ARG	13	Α	6	ASP9, TYR10, ALA11, MET12, PHE14, GLY15
PHE	14	A	9	TYR10, ALA11, MET12, ARG13, GLY15, GLN16, THR17, LYS18, THR19

Calculate the alpha helical tendency of 4MBN

Steps:

- 1. Enter the PDB code (case sensitive)
- 2. Check "Secondary structure propensities" and Click on "Submit". This will open up a new page
- 3. Check "alpha-helical tendency"
- 4. Click on "Submit"

Please enter the following										
 Enter a PDB-id 4mbn Ex: PDB-id Upload a PDB File Browse. 	Chain name (optional) =2TRX, Chain=A Or No file selected. Chain name (optional)									
Se	lect one of the following									
0	Identification of binding site									
0	Inter-residue interactions									
۲	Secondary structure propensities									
0	Physicochemical properties									
	Submit Clear									



Secondary structure propensities										
Amino acid compositions in high B-value regions	Frequency of occurance in beta-bends	Normalised frequency of turn	Normalised frequency of N-Helix	□ Normalised frequency of C-Helix	□ Normalised frequency of middle-Helix					
Propensity to form MCI for 2 state proteins	Propensity to form MCI for 3 state protei	Alpha-helical tendency	Beta-sheet tendency	Coil tendency	□ A11					
	Example Submit Clear Back									

Frequency of occurence of amino acids in alpha helix

PDB ID : 4MBN.pdb

Residue name	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
Residue	17	4	1	7	0	4	14	7	6	8	16	11	2	4	3	4	4	2	2	7
Residue total	17	4	1	7	0	5	14	11	12	9	18	19	2	6	4	6	5	2	3	8
Frequency	1.2	1.2	1.2	1.2	0	1.0	1.2	0.8	0.6	1.1	1.1	0.7	1.2	0.8	0.9	0.8	1.0	1.2	0.8	1.1

Calculate the centre of mass, disulphide bridges, ionic interactions and surrounding hydrophobicity of 5PTI

Steps:

- 1. Enter the PDB code (case sensitive)
- 2. Check "Physicochemical properties" and Click on "Submit". This will open up a new page
- 3. Check "Centre of mass, disulphide interactions, ionic interactions and surrounding hydrophobicity"
- 4. Click on "Submit"

	-
Pleas	e enter the following
 Enter a PDB-id 5pti Ex: PDB-id=27 Upload a PDB File Browse 	Chain name (optional) TRX, Chain=A Or No file selected. Chain name (optional)
Select	t one of the following
○ Id	lentification of binding site
O Ir	iter-residue interactions
O Se	condary structure propensities
De Pl	hysicochemical properties
	Submit Clear

	· · · · · · · · · · · · · · · · · · ·									
	Physicochemical properties									
>	Centre of mass	Rog Radius of gyration	Disulphide interactions	✓ Ionic Interactions	Hydrophobic interactions	Aromatic-Aromatic interactions				
1	Aromatic-sulphur interactions	Cation- pi interactions	Accessible surface area for the native protein	Surrounding hydrophobicity	Surface hydrophobicity	ASA of Hydrophobic residues				
	Hydrophobic free energy	Free energy due to Disulphide interactions	Main chain Ma chain Hydrogen bond interactions	Main chain side chain hydrogen bond interactions	Side chain side chain Hydrogen bond interactions	Average gain in surrounding hydrophobicity or hydrophobic enrichment				
	Average gain ratio in surrounding hydrophobicity	Br Buriedness	Ra Solvent accessible reduction ratio or Mean fractional area loss	Mean area buried on transfer	Ns Average number of surrounding residues	 Normalized flexibility parameters (B-values), average 				
	Normalized flexibility surrounded by none rigid	y parameters (B-values) fe 1 neighbours	or each residue	Normalized flexibility surrounded by one rigid	v parameters (B-values) f neighbours	or each residue				
	Normalized flexibility parameters (B-values) for each residue surrounded by two rigid neighbours									
				All						
			Example Submi	t Clear Back						

Center of Mass

PDB ID : 5PTI.pdb

Molecular weight =7.689 kilodaltons Center of mass: x = 27.885 y = 9.524 z = 0.247

Disulphide bridge

PDB ID : 5PTI.pdb

Residue name	Residue number	Chain name	Residue name	Residue number	Chain name	Distance
5	CYS	A	55	CYS	A	2.043
14	CYS	A	38	CYS	A	2.030
30	CYS	A	51	CYS	A	2.022

Ionic interactions

PDB ID : 5PTI.pdb

Residue name	Residue number	Atom name	Chain name	Residue name	Residue number	Atom name	Chain name	Distance
GLU	7	OE1	A	LYS	41	NZ	A	5.915
GLU	7	OE1	A	ARG	42	NH2	A	4.573
GLU	7	OE2	A	ARG	42	NH2	A	5.751
ASP	50	OD1	A	ARG	53	NH2	A	4.026
ASP	50	OD2	A	ARG	53	NH2	A	5.678

Surrounding hydrophobicity

PDB ID : 5PTI.pdb

Residue name	Residue number	Chain	Surrounding hydrophobicity
ARG	1	A	7.49
PRO	2	A	12.43
ASP	3	A	11.51
PHE	4	A	11.6
CYS	5	A	17.6
LEU	6	A	17.06
GLU	7	A	13.52
PRO	8	A	11.23