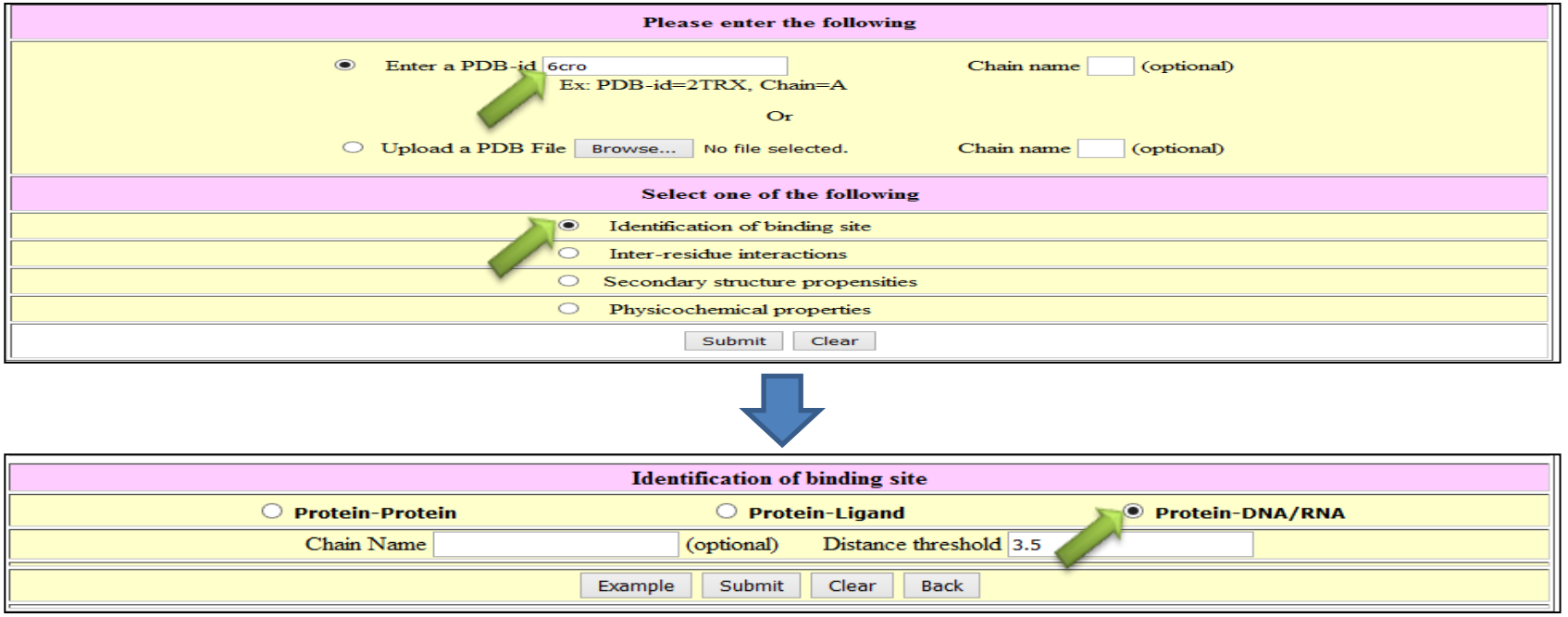
Tutorial 1

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.



Sample output

Identification of binding site - Protein-DNA/RNA

PDB ID : 6CRO.pdb

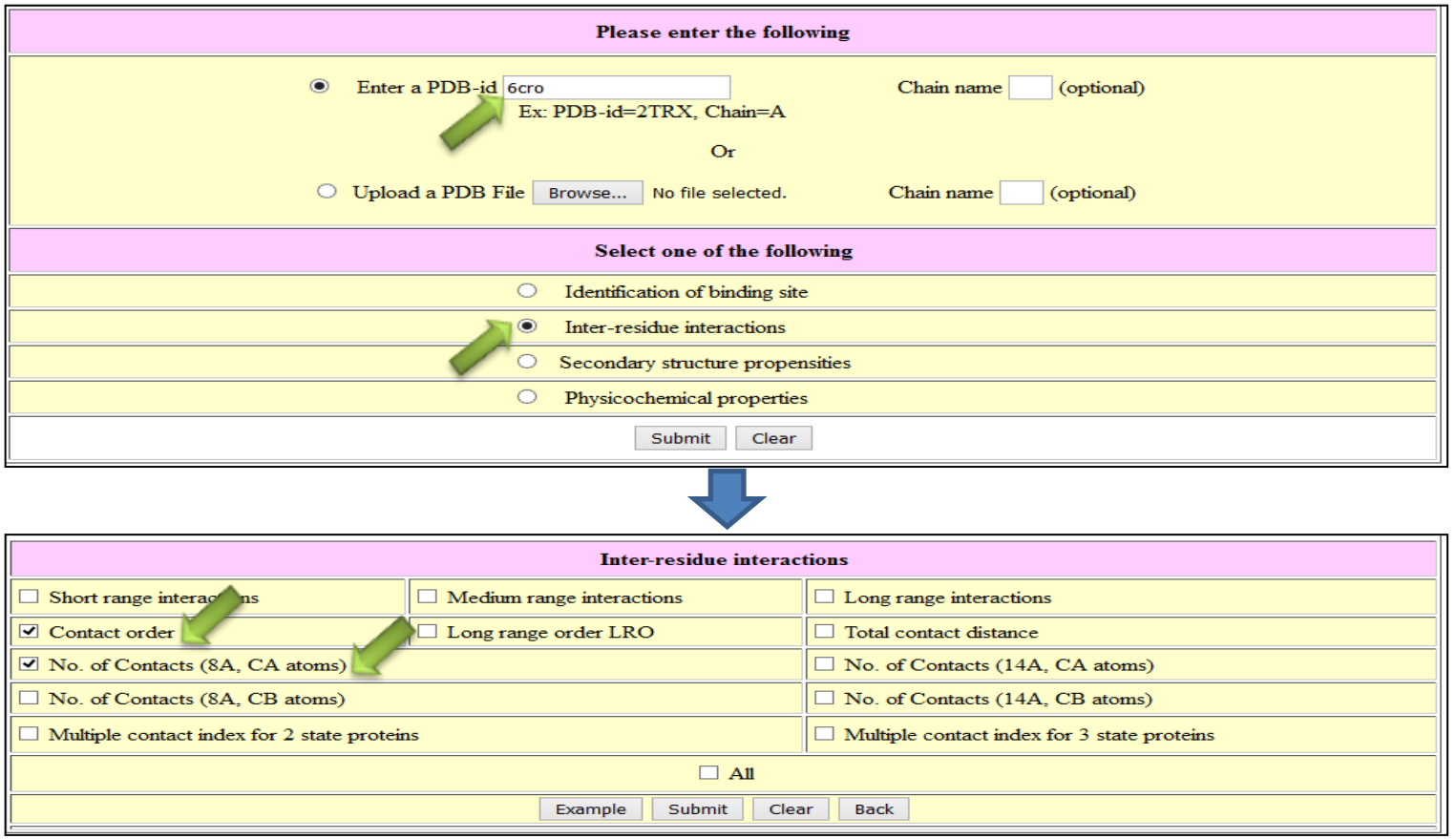
Residue name	Residue number	Atom name	Chain name	Residue name	Residue number	Atom name	Chain name	Distance
PHE	14	O	A	DT	1	O2	U	3.140
GLN	16	N	A	DT	3	OP2	R	3.000
GLN	16	N	A	DT	3	OP2	U	3.000
THR	17	OG1	A	DT	3	C7	R	3.436
THR	17	OG1	A	DT	3	C7	U	3.436
VAL	25	CG2	A	DT	15	OP2	R	2.791
VAL	25	CG2	A	DT	15	OP2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

Tutorial 2

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"



Sample output

Contact order

PDB ID : 6CRO.pdb

Contact order = 16.901

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

PDB name : 6CRO.pdb

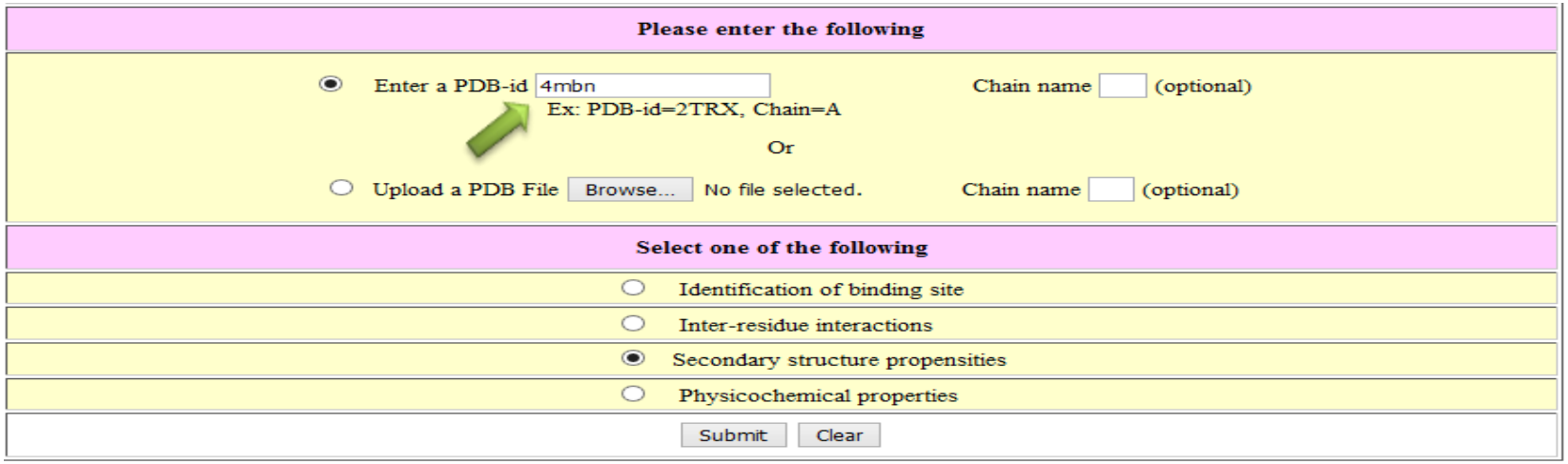
Residue name	Residue number	Chain	No. of contacting residues	Contacting residues
GLU	2	A	5	GLN3 , ARG4 , THR43 , ILE44 , ASN45
GLN	3	A	6	GLU2 , ARG4 , ILE5 , THR43 , ILE44 , ASN45
ARG	4	A	8	GLU2 , GLN3 , ILE5 , THR6 , PHE41 , LEU42 , THR43 , ILE44
ILE	5	A	9	GLN3 , ARG4 , THR6 , LEU7 , ASP9 , TYR10 ,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

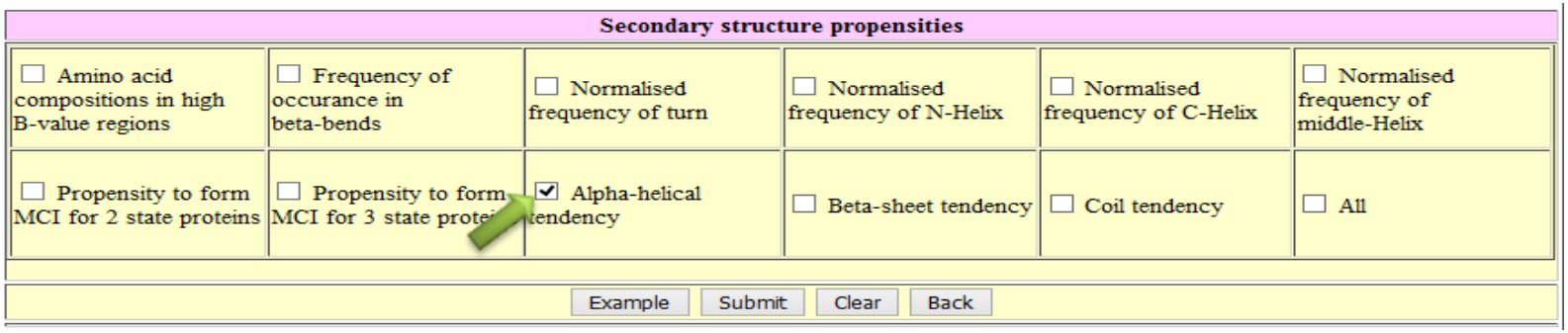
Tutorial 3

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”





Sample output

Frequency of occurence of amino acids in alpha helix

PDB ID : 4MBN.pdb

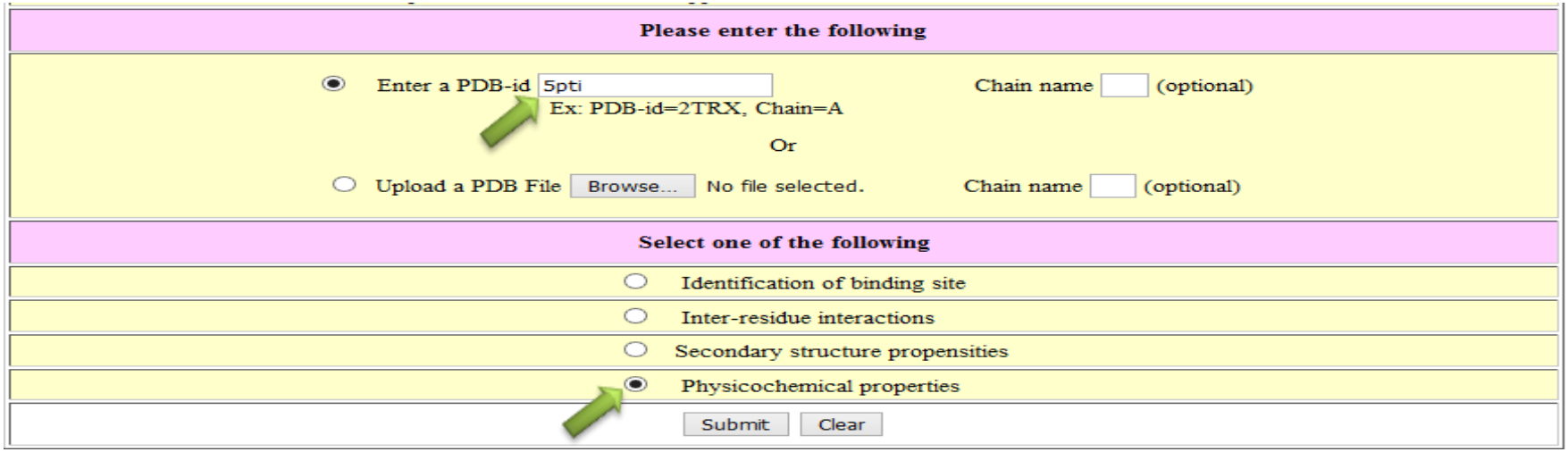
Residue name	ALA	ARG	ASN	ASP	CYS	GLN	GLU	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO	SER	THR	TRP	TYR	VAL
Residue	17	4	1	7	0	4	14	7	6	8	16	11	2	4	3	4	4	2	2	7
Residue total	17	4	1	7	0	5	14	11	12	9	18	19	2	6	4	6	5	2	3	8
Frequency	1.2	1.2	1.2	1.2	0	1.0	1.2	0.8	0.6	1.1	1.1	0.7	1.2	0.8	0.9	0.8	1.0	1.2	0.8	1.1

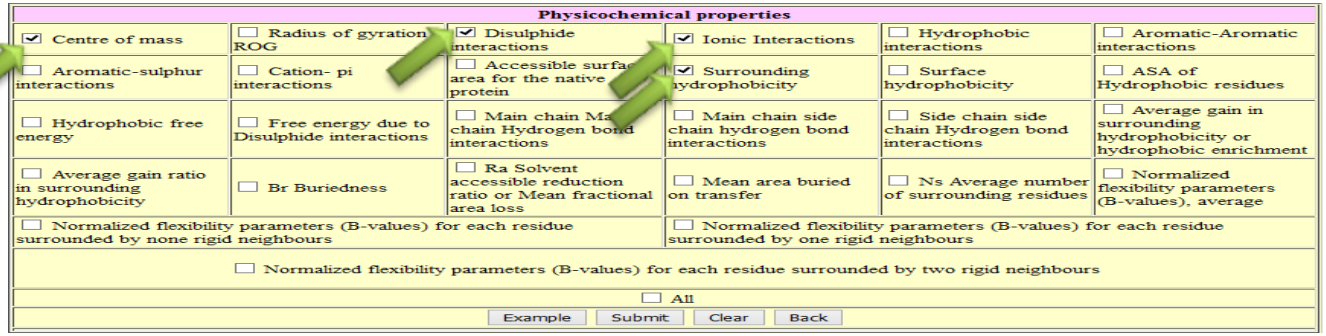
Tutorial 4

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”





Sample output

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