SeamDock

Simple and accessible docking web server
Interactive and Collaborative on-line docking

General information

Please Bookmark the page: https://seamless.rpbs.univ-paris-diderot.fr/cloudless/instance/7264387/ctx/index.html Copy page location

If you'd like that other viewers of the web page to follow the page visualisation state, tick the following checkbox:

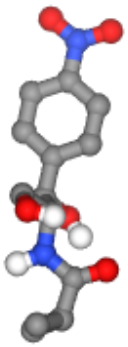
☐ Master receptor view

Ligand preparation

Ligand (`.pdb` , `.mol2` , `.sdf`):

Choose File lig1.pdb

SMILES:



ligand.pdbqt

Receptor preparation

Receptor (`.pdb`):

Choose File No file chosen

PDB Id:

to select a chain add `".Chain(s)"` , *eg.* `"3EAM.AE"`

4dx5.ABC

Box Coordinates

Center:

x : 0 Å

y : -10 Å

z : 5 Å

Size:

x : 50 Å

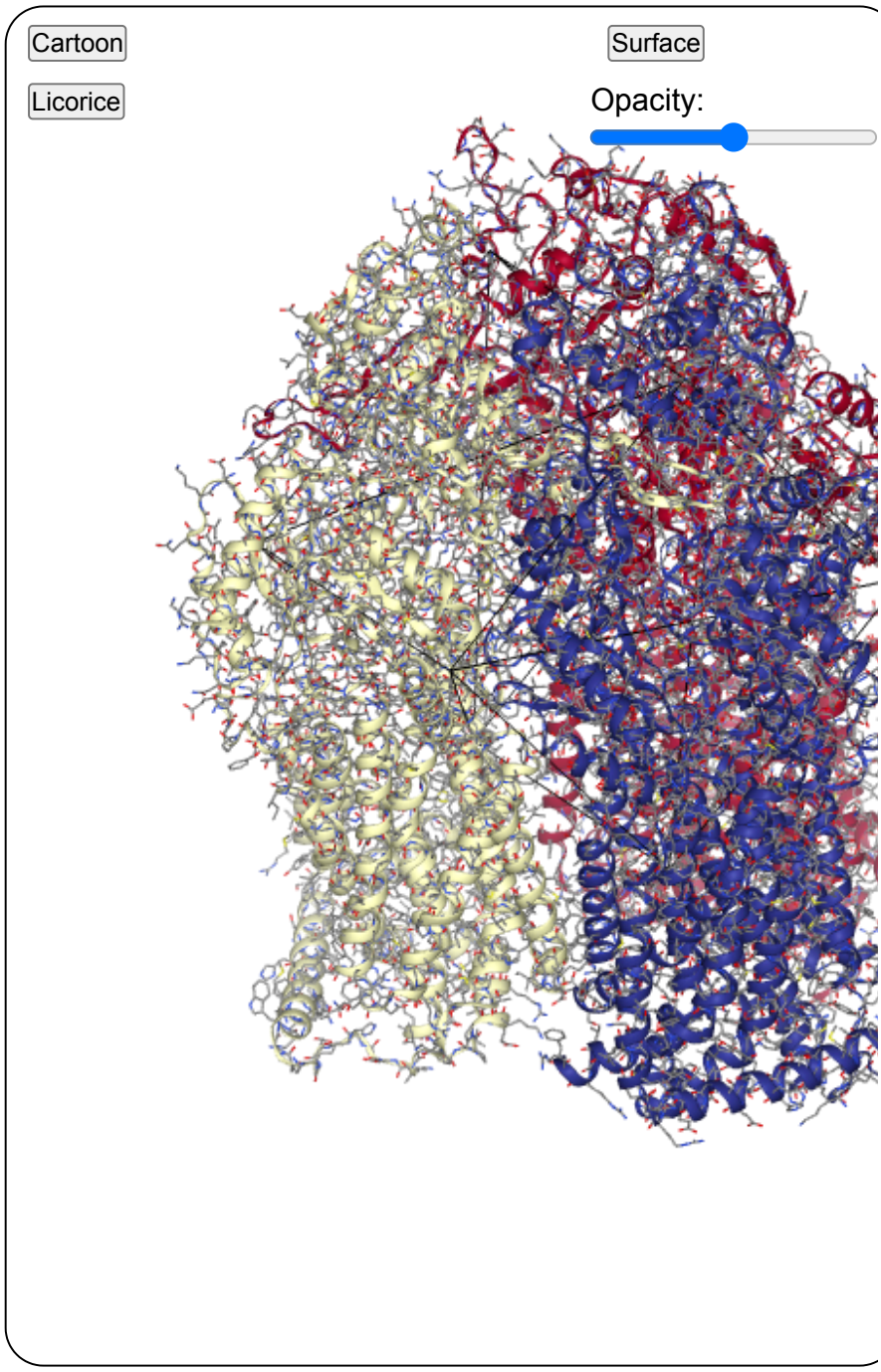
y : 50 Å

z : 50 Å

Box Appearance

Opacity:

Color: Wireframe :



receptor.pdbqt

Reset Ligand/Receptor Inputs

Docking parameters

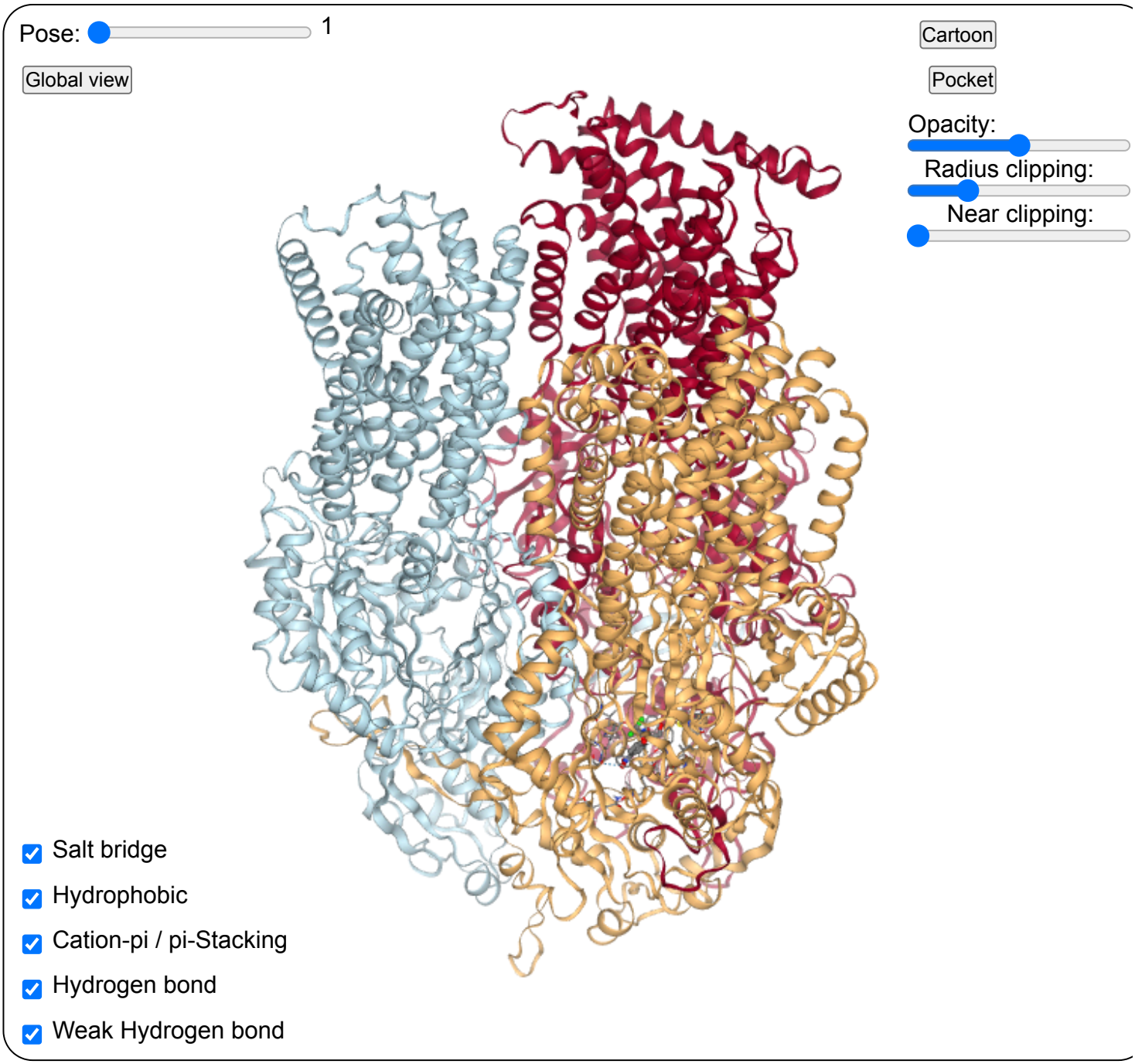
Software Vina

Spacing 1 Mode number 5

Energy Range 5 Exhaustiveness 8

Docking Results

#	affinity (kcal/mol)
1	**-7.5**
2	-7.3
3	-7.2
4	-7.2
5	-7.1



hydrophobic contact

Ligand atom	Receptor
8	F178(B) CG
10	I277(B) CG2
11	V612(B) CG1
7	V612(B) CG2
11	F615(B) CD1

hydrogen bond

Ligand atom	Receptor
5	F178(B) O

dock_log
dock.pdb