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/2866270/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:

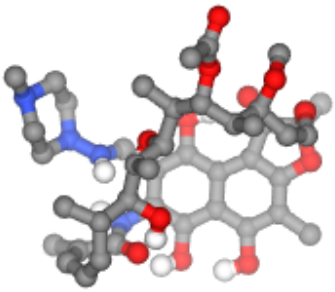
☐ Master receptor view

Ligand preparation

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

Choose File lig2.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

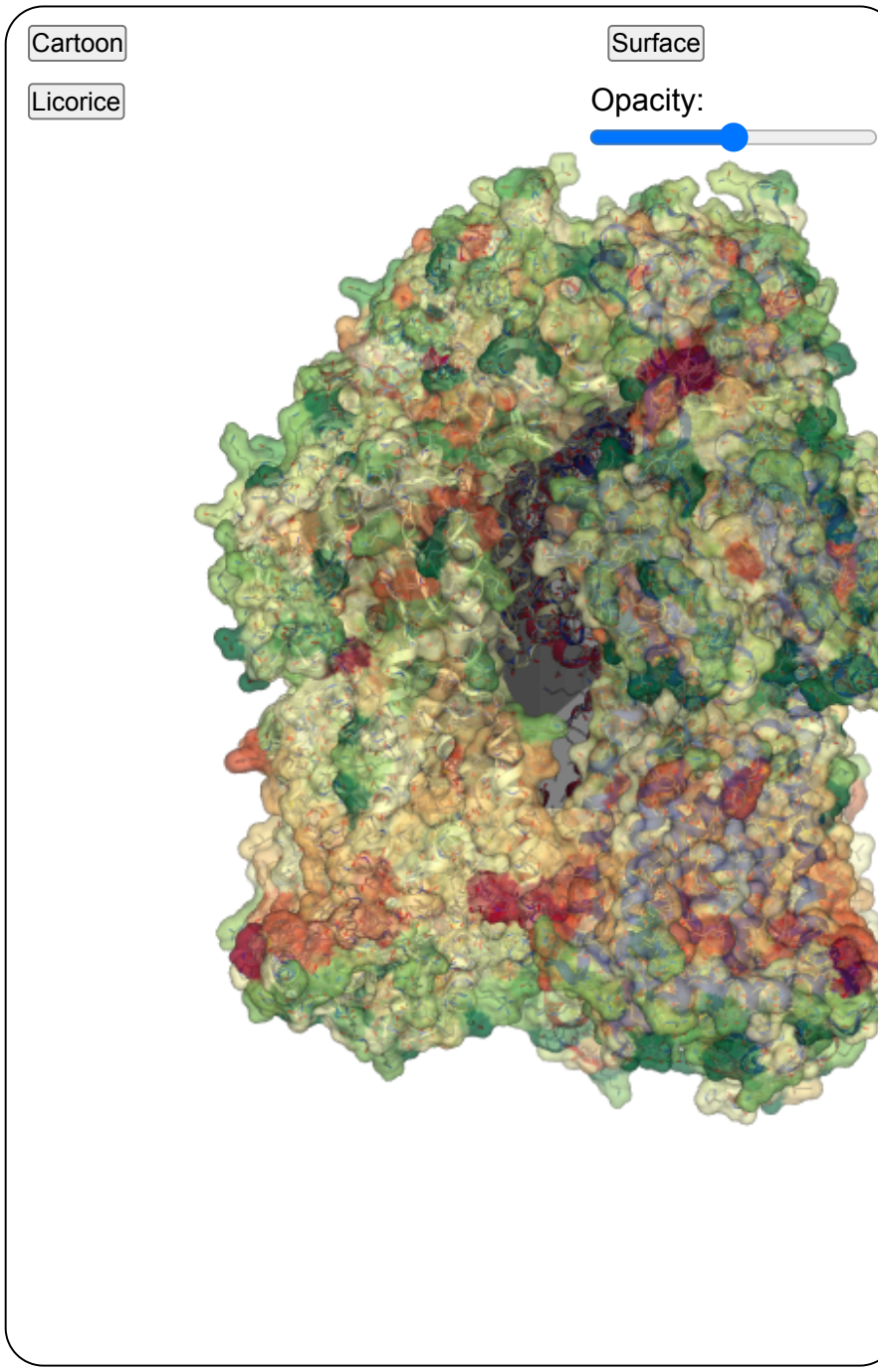
y : 50 Å

z : 50 Å

Box Appearance

Opacity:

Color: Wireframe :



receptor.pdbqt

Reset Ligand/Receptor Inputs

Docking parameters

Software Vina

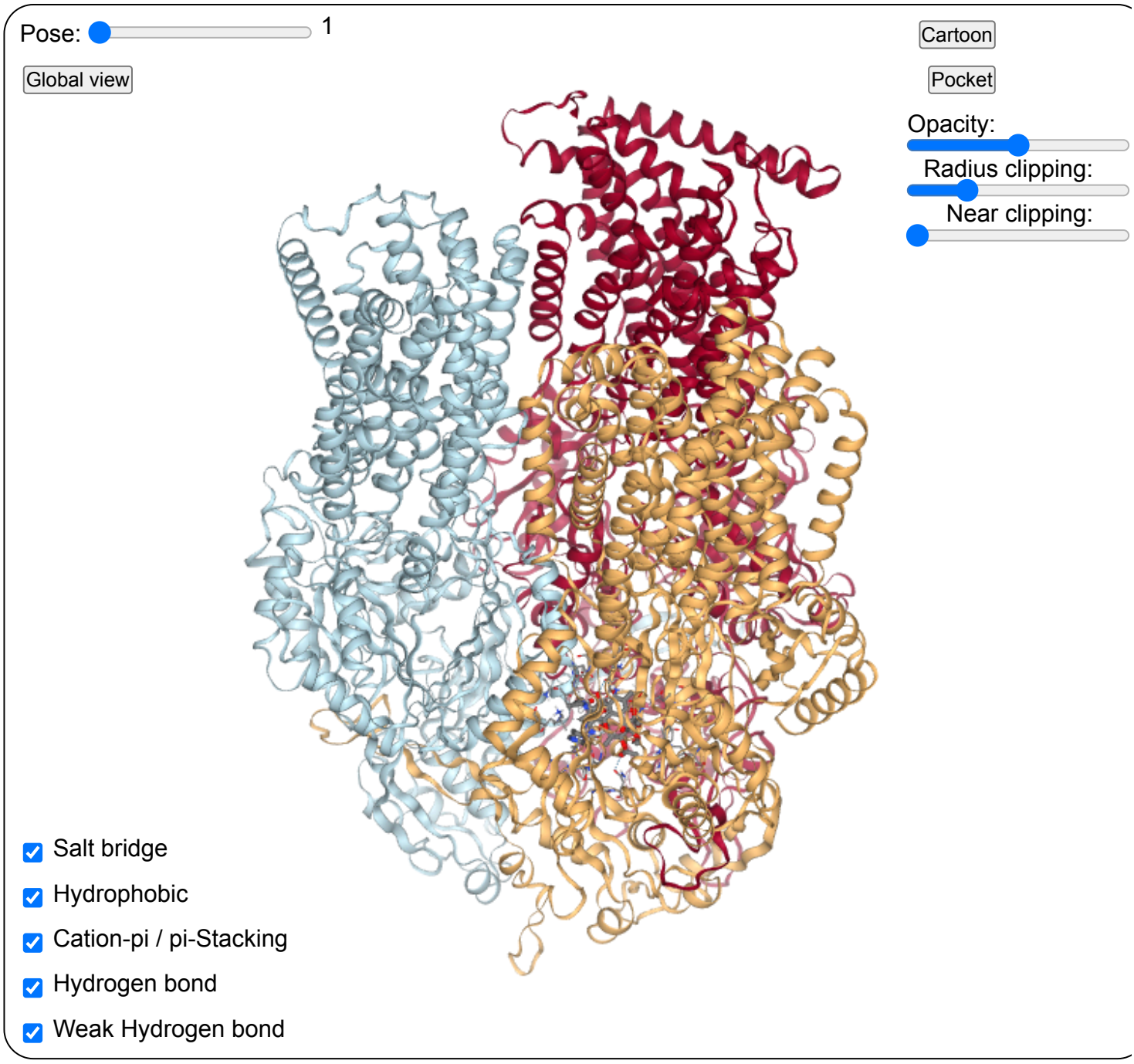
Spacing 1.0 Mode number 5

Energy Range 5 Exhaustiveness 8

Launch Docking

Docking Results

#	affinity (kcal/mol)
1	**-9.8**
2	-9.5
3	-9.4
4	-9.1
5	-9



ionic interaction

Ligand atom	Receptor
OE1	NaN() N3

hydrophobic contact

Ligand atom	Receptor
10	Q176(B) CB
40	Q176(B) CG
24	L113(C) CB
27	L117(C) CD1

hydrogen bond

Ligand atom	Receptor
7	S128(B) OG
12	E130(B) OE1
12	E130(B) OE2
11	E130(B) OE2
5	L177(B) O
2	G179(B) O

10	N274(B) OD1
OG	NaN() O7

dock_log
dock.pdb