

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](#)

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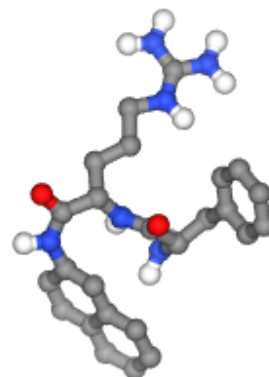
☐ Master receptor view

Ligand preparation

Ligand ([.pdb](#) , [.mol2](#) , [.sdf](#)):

lig3.pdb

SMILES:



[ligand.pdbqt](#)

Receptor preparation

Receptor (.pdb):

No file chosen

PDB Id:

to select a chain add " .Chain(s) ", eg.

"3EAM.AE"

Box Coordinates

Center:

x : 0 Å

y : -10 Å

z : 5 Å

Size:

x : 50 Å

y : 50 Å

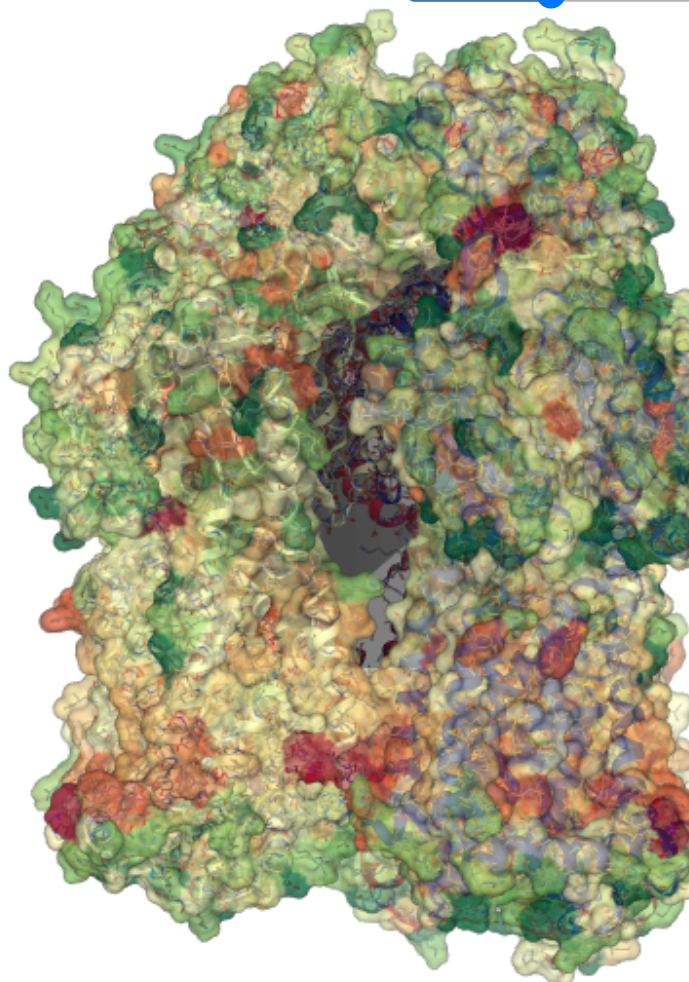
z : 50 Å

Box Appearance

Opacity:

Color: Wireframe : ☐

Opacity:



receptor.pdbqt

Docking parameters

Software

Spacing Mode number

Energy Range Exhaustiveness

Docking Results

#	affinity (kcal/mol)
1	-10.2
2	-10.2
3	-10
4	-9.8
5	-9.8

Pose: 

Global view

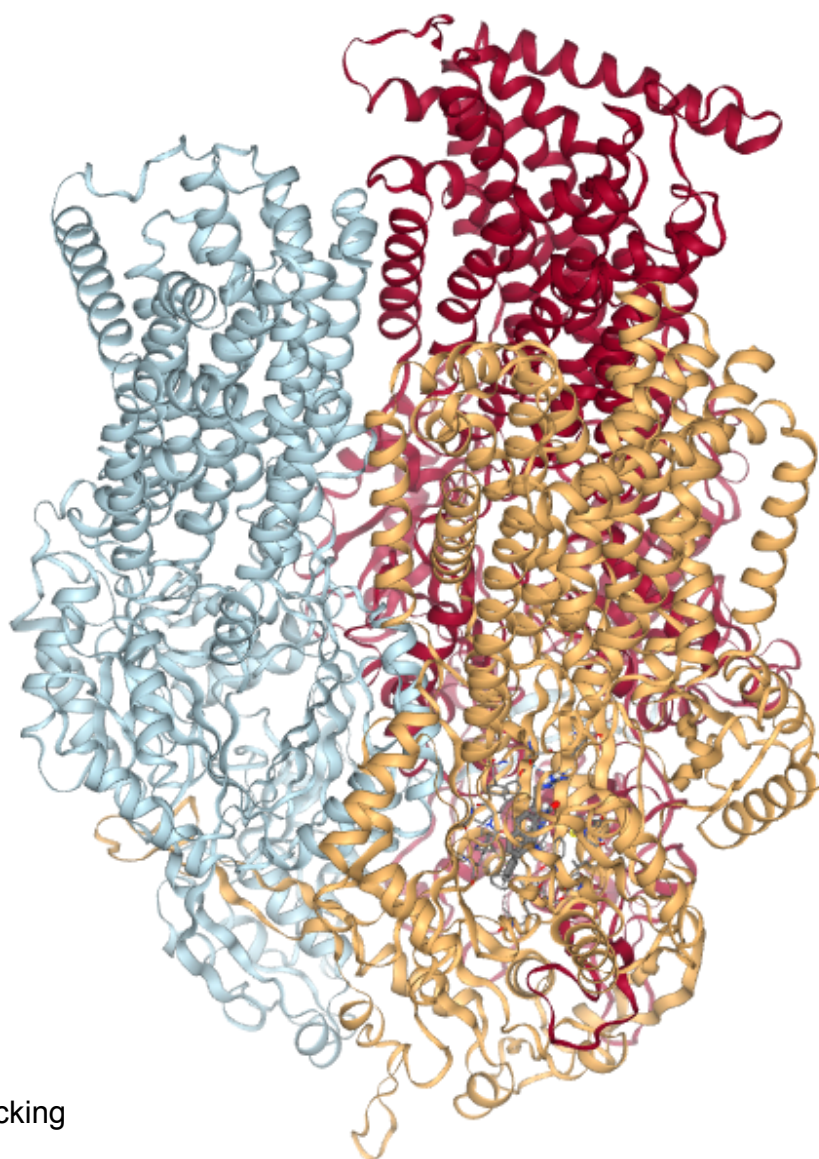
Cartoon

Pocket

Opacity: 

Radius clipping: 

Near clipping: 



- ☒ Salt bridge
- ☒ Hydrophobic
- ☒ Cation-pi / pi-Stacking
- ☒ Hydrogen bond
- ☒ Weak Hydrogen bond

hydrophobic contact

Ligand atom	Receptor
11	F136(B) CE2
22	V139(B) CG1
24	V139(B) CG2
6	F178(B) CB

pi-pi stacking

Ligand atom	Receptor
6	F178(B) CE2
23	F628(B) CE2

hydrogen bond

Ligand atom	Receptor
5	S134(B) O

weak hydrogen bond

Ligand atom	Receptor
14	S134(B) O

2	F178(B) CZ
6	A279(B) CB
24	Y327(B) CB
20	F610(B) CG
21	F610(B) CD2
7	F610(B) CE1
5	V612(B) CG1
7	V612(B) CG2
19	F628(B) CB
22	F628(B) CD2

[dock_log](#)
[dock.pdb](#)