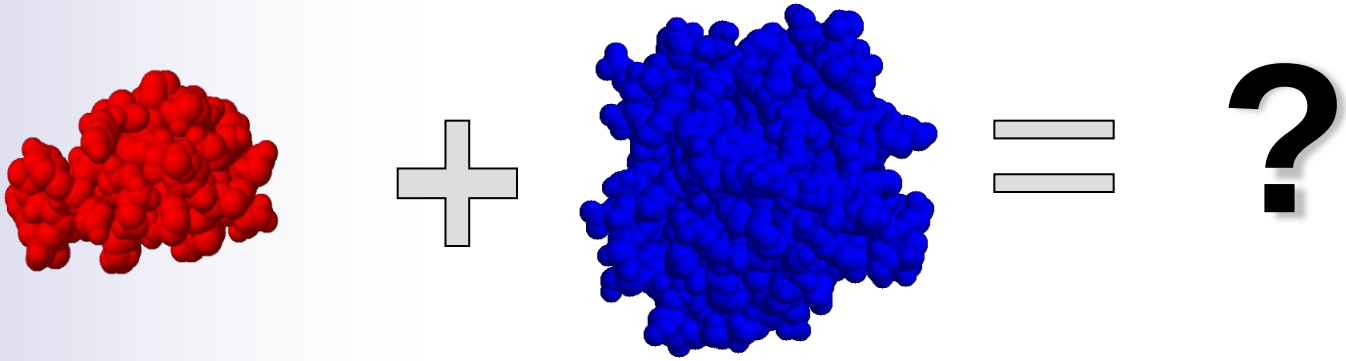
אוניברסיטת תל-אביב

http://bioinfo3d.cs.tau.ac.il/

protein-protein docking



BioInfo3D group page

http://bioinfo3d.cs.tau.ac.il

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- Datasets
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Main Page

Welcome to the BioInfo3D group page!

Latest Updates

24.10.11: New web server: PepCrawler - refinement and binding-affinity estimation of peptide inhibitors.

07.07.11: New web server: ParaDock - rigid protein, flexible DNA Docking.

25.06.11: The new group website is up and running.

BioInfo3D group page

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Servers & Software

Contents [hide]

Protein Structural Alignment (pairwise, multiple, flexible)

GOSSIP - Global Structural Superposition of Proteins

TriangleMatch - Pairwise Protein Structure Alignment based on Ca atoms. With P-value.

FlexProt - Pairwise Alignment of Flexible Protein Structures

MultiProt - Multiple Protein Structure Alignment

MASS - Multiple Protein Structure Alignment by Secondary Structures

STACCATO - Structure Based Multiple Sequence Alignment

Docking (rigid, symmetric, protein-protein, protein-drug, protein-DNA, protein-peptide)

PatchDock - Rigid Unbound Docking of Molecules

SymmDock - Prediction of Complexes with C_n Symmetry

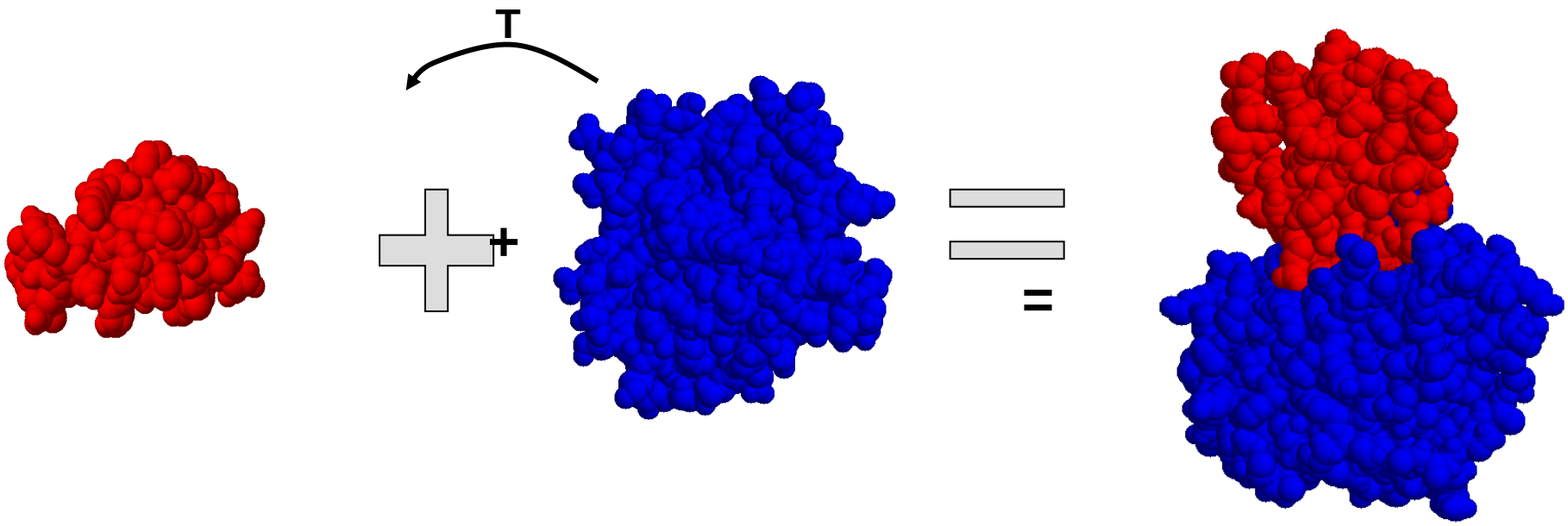
CombDock - COMBinatorial ssembly by mutiple DOCKing

FireDock - Refinement and re-scoring of rigid-body protein-protein docking solutions

FiberDock - Flexible backbone and side-chain refinement and re-scoring of rigid-body protein-protein docking solutions

PatchDock – Rigid Geometric Docking

Given 2 input molecules in their native conformation, the goal is to find their correct association as it appears in nature.



Schneidman-Duhovny et al. Proteins 2003
Duhovny (Schneidman), D., Nussinov, R. Wolfson,HJ. WABI 2002

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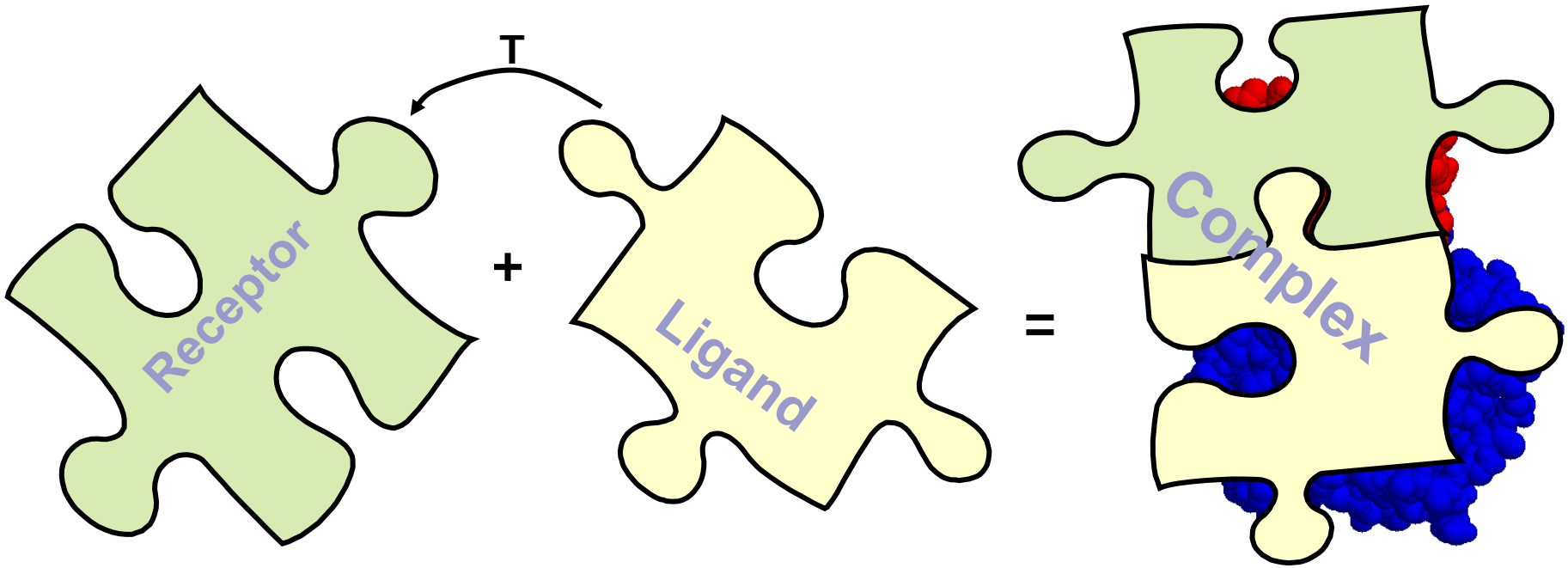

Schneidman-Duhovny et al. Proteins 2003
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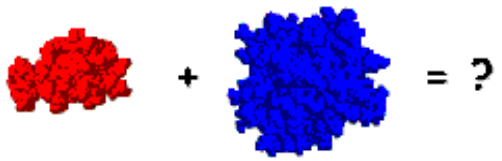
WWW server: http://bioinfo3d.cs.tau.ac.il/PatchDock



Molecular Docking Algorithm Based on Shape Complementarity Principles

[About PatchDock] [Web Server] [Download] [Help] [FAQ] [References]

Type PDB codes of receptor and ligand molecules or upload files in PDB format

Receptor Molecule: (PDB:chainId e.g. 2kai:AB) **or** upload file: Browse...

Ligand Molecule: (PDB:chainId e.g. 2kai:l) **or** upload file: Browse...

e-mail address: (the results are sent to this address)

Clustering RMSD: 4.0

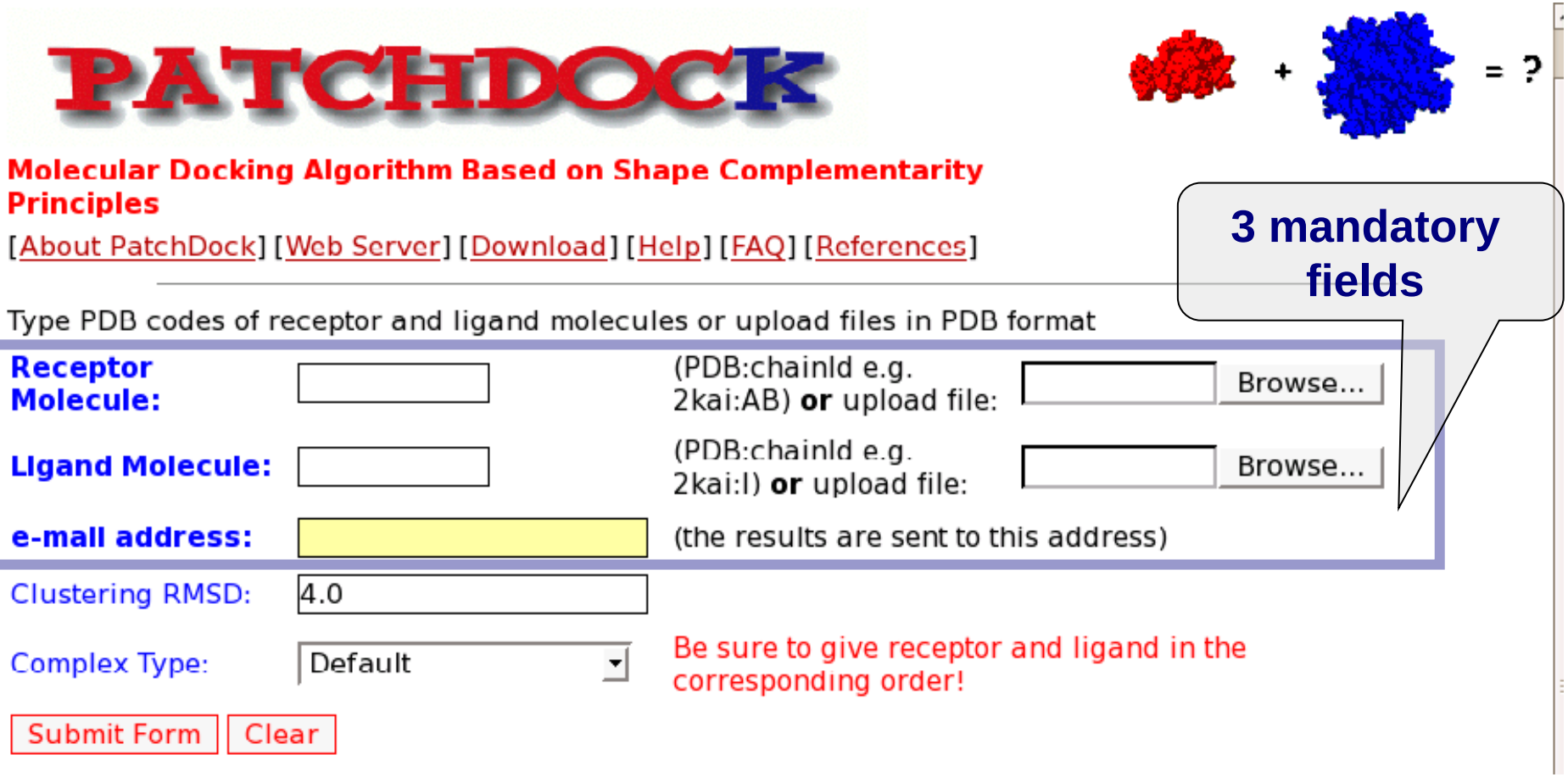
Complex Type: Default

Be sure to give receptor and ligand in the corresponding order!

Submit Form Clear

Schneidman-Duhovny D, Inbar Y, Nussinov R, Wolfson HJ. NAR 2005

WWW server: http://bioinfo3d.cs.tau.ac.il/PatchDock

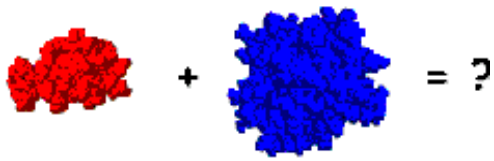


If you are not sure, use the bigger molecule as the receptor.

Schneidman-Duhovny D, Inbar Y, Nussinov R, Wolfson HJ. NAR 2005

WWW server: http://bioinfo3d.cs.tau.ac.il/PatchDock

PATCHDOCK



Molecular Docking Algorithm Based on Shape Complementarity Principles

[About PatchDock] [Web Server] [Download] [Help] [FAQ] [References]

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Receptor Molecule: (PDB:chainId e.g. 2kai:AB) **or** upload file: Browse...

Ligand Molecule: (PDB:chainId e.g. 2kai:l) **or** upload file: Browse...

e-mail address: (the results are sent to this address)

Clustering RMSD: 4.0

Complex Type: Default

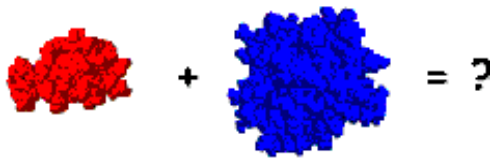
Be sure to give receptor and ligand in the corresponding order!

Submit Form Clear

Clustering RMSD:
Used for defining distance between similar results which should be clustered together.
The higher the RMSD - the less results you get.
For protein-protein docking use 4A.
For protein-small molecule 1.5A.

WWW server: http://bioinfo3d.cs.tau.ac.il/PatchDock

PATCHDOCK



Molecular Docking Algorithm Based on Shape Complementarity Principles

[About PatchDock] [Web Server] [Download] [Help] [FAQ] [References]

Type PDB codes of receptor and ligand molecules

Receptor Molecule:

Ligand Molecule:

e-mail address:

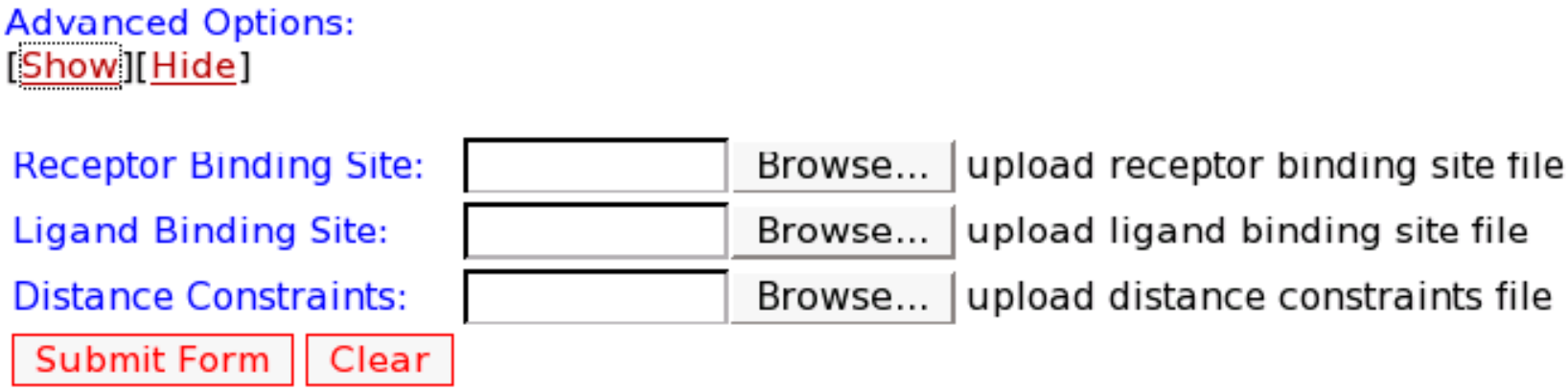
Clustering RMSD: 4.0

Complex Type: Default

Submit Form Clear

Complex Type:
Enzyme-Inhibitor - limits search space to cavities of the enzyme. (The enzyme should be denoted as the receptor.)
Antibody-Antigen - Automatically detects CDRs and limits search space to those regions. (The antibody should be denoted as receptor.)
Protein-Ligand - Use parameters optimized for small sized molecule docked into protein. (The small sized molecule should be denoted as the ligand.)
Default- For other cases.

Optional parameters



Binding Site – list the residues of the receptor potential binding site. Only patches that include these residues will be used for matching.

Format: ***[residue index] [chain ID]***

Example:

88 L
89 L
90 L
91 L
92 L
96 H
101 H
102 H

Optional parameters

Advanced Options:
[Show][Hide]

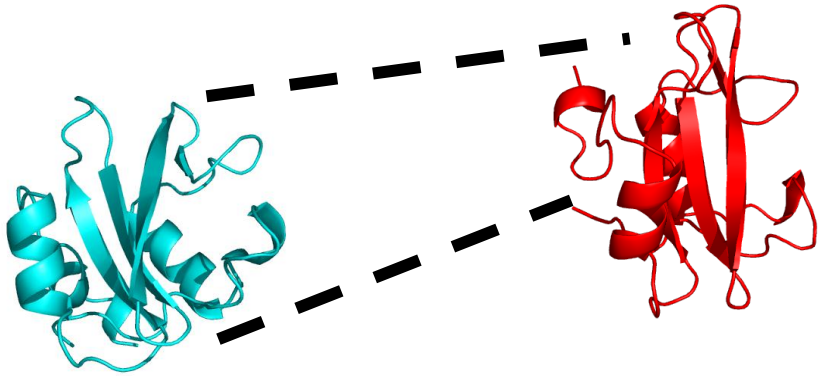
Receptor Binding Site: Browse... upload receptor binding site file
Ligand Binding Site: Browse... upload ligand binding site file
Distance Constraints: Browse... upload distance constraints file
Submit Form Clear

Distance Constraints –between pairs of atoms from the receptor and the ligand.

Format: ***[receptor_atom_index] [ligand_atom_index] [min_dist] [max_dist]***

For example:

25 377 0.0 5.0
340 5603 5.0 10.0



Output:

Receptor	Ligand	Complex Type	Clustering RMSD	User e-mail	Receptor Site	Ligand Site
A.pdb.tr	B.pdb.tr	Default	4.0	duhovka@tau.ac.il	-	-

Solution No	Score	Area	ACE	Transformation	PDB file of the complex
1	10166	1528.90	-12.07	-1.15 -0.37 -0.32 -11.03 -15.21 22.35	result.1.pdb
2	9740	1285.70	129.52	-2.07 -0.40 -1.44 -3.43 9.43 18.35	result.2.pdb
3	9380	1284.70	-8.60	0.77 0.16 -0.54 -1.20 8.06 -10.85	result.3.pdb
4	9122	1298.80	203.84	2.45 -0.57 -1.59 13.45 2.35 14.25	result.4.pdb
5	9048	1185.20	-243.82	3.11 0.11 1.04 -16.19 -29.02 2.25	result.5.pdb
6	9034	1094.70	301.73	2.09 -0.49 -1.37 6.24 3.03 10.96	result.6.pdb
7	8972	1182.40	-39.65	-2.07 -1.05 -2.85 6.41 -17.96 28.59	result.7.pdb
8	8890	1163.80	-165.52	0.59 0.92 2.17 12.62 -23.69 -10.70	result.8.pdb
9	8886	1195.40	-31.63	0.92 0.49 3.07 18.21 -10.46 -11.65	result.9.pdb
10	8850	1240.20	-149.90	-1.43 0.72 0.57 -14.80 -28.15 -1.02	result.10.pdb
11	8768	962.70	19.42	-1.12 -0.24 -0.71 -13.34 -9.72 21.55	result.11.pdb
12	8740	1110.70	2.06	0.34 0.78 2.56 2.98 3.29 -6.48	result.12.pdb
13	8700	973.80	-79.03	-1.32 -0.69 -0.86 -7.61 -8.97 26.23	result.13.pdb
14	8696	1012.60	-161.10	0.23 0.68 2.24 14.51 -28.88 -3.17	result.14.pdb
15	8644	1206.50	-46.74	-1.89 -0.36 1.91 5.66 -34.25 17.10	result.15.pdb
16	8628	1192.00	330.84	-0.75 0.74 0.78 -0.58 0.95 23.63	result.16.pdb
17	8602	1285.20	17.88	-2.71 0.40 -1.13 0.42 4.95 -2.29	result.17.pdb
18	8574	1342.30	118.56	2.27 -0.07 0.36 -10.58 13.53 29.87	result.18.pdb
19	8526	1039.50	-111.44	-0.65 0.10 -1.60 -11.41 7.24 13.05	result.19.pdb
20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

NEW: Jmol view

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DOWNLOAD best solutions as a ZIP file: 10 (solutions number, from 2 to 100) GO (this takes few seconds, please wait patiently)

DOWNLOAD solutions table transformations file

REFINE best solutions with FireDock: 1000 (solutions number, from 1 to 1000) GO

Output:

Input data

Receptor	Ligand	Complex Type	Clustering RMSD	User e-mail	Receptor Site	Ligand Site
A.pdb.tr	B.pdb.tr	Default	4.0	duhovka@tau.ac.il	-	-

Solution No	Score	Area	ACE	Transformation	PDB file of the complex
1	10166	1528.90	-12.07	-1.15 -0.37 -0.32 -11.03 -15.21 22.35	result.1.pdb
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4	9122	1298.80	203.84	2.45 -0.57 -1.59 13.45 2.35 14.25	result.4.pdb
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6	9034	1094.70	301.73	2.09 -0.49 -1.37 6.24 3.03 10.96	result.6.pdb
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12	8740	1110.70	2.06	0.34 0.78 2.56 2.98 3.29 -6.48	result.12.pdb
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20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

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7	8972	1182.40	-39.65	-2.07 -1.05 -2.85 6.41 -17.96 28.59	result.7.pdb
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13	8700	973.80	-79.03	-1.32 -0.69 -0.86 -7.61 -8.97 26.23	result.13.pdb
14	8696	1012.60	-161.10	0.23 0.68 2.24 14.51 -28.88 -3.17	result.14.pdb
15	8644	1206.50	-46.74	-1.89 -0.36 1.91 5.66 -34.25 17.10	result.15.pdb
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18	8574	1342.30	118.56	2.27 -0.07 0.36 -10.58 13.53 29.87	result.18.pdb
19	8526	1039.50	-111.44	-0.65 0.10 -1.60 -11.41 7.24 13.05	result.19.pdb
20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

NEW: Jmol view

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Output:

shape complementarity score

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A.pdb.tr	B.pdb.tr	Defaul	duhovka@tau.ac.il	-	-

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8	8890	1163.80	-165.52	0.59 0.92 2.17 12.62 -23.69 -10.70	result.8.pdb
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12	8740	1110.70	2.06	0.34 0.78 2.56 2.98 3.29 -6.48	result.12.pdb
13	8700	973.80	-79.03	-1.32 -0.69 -0.86 -7.61 -8.97 26.23	result.13.pdb
14	8696	1012.60	-161.10	0.23 0.68 2.24 14.51 -28.88 -3.17	result.14.pdb
15	8644	1206.50	-46.74	-1.89 -0.36 1.91 5.66 -34.25 17.10	result.15.pdb
16	8628	1192.00	330.84	-0.75 0.74 0.78 -0.58 0.95 23.63	result.16.pdb
17	8602	1285.20	17.88	-2.71 0.40 -1.13 0.42 4.95 -2.29	result.17.pdb
18	8574	1342.30	118.56	2.27 -0.07 0.36 -10.58 13.53 29.87	result.18.pdb
19	8526	1039.50	-111.44	-0.65 0.10 -1.60 -11.41 7.24 13.05	result.19.pdb
20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

NEW: Jmol view

show next 20 »»

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DOWNLOAD solutions table transformations file

REFINE best solutions with FireDock: 1000 (solutions number, from 1 to 1000) GO

Output:

The estimated interface area

Receptor	Ligand	Complex Ty	il	Receptor Site	Ligand Site
A.pdb.tr	B.pdb.tr	Default	dunovka@tau.ac.il	-	-

Solution No	Score	Area	ACE	Transformation	PDB file of the complex
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4	9122	1298.80	203.84	2.45 -0.57 -1.59 13.45 2.35 14.25	result.4.pdb
5	9048	1185.20	-243.82	3.11 0.11 1.04 -16.19 -29.02 2.25	result.5.pdb
6	9034	1094.70	301.73	2.09 -0.49 -1.37 6.24 3.03 10.96	result.6.pdb
7	8972	1182.40	-39.65	-2.07 -1.05 -2.85 6.41 -17.96 28.59	result.7.pdb
8	8890	1163.80	-165.52	0.59 0.92 2.17 12.62 -23.69 -10.70	result.8.pdb
9	8886	1195.40	-31.63	0.92 0.49 3.07 18.21 -10.46 -11.65	result.9.pdb
10	8850	1240.20	-149.90	-1.43 0.72 0.57 -14.80 -28.15 -1.02	result.10.pdb
11	8768	962.70	19.42	-1.12 -0.24 -0.71 -13.34 -9.72 21.55	result.11.pdb
12	8740	1110.70	2.06	0.34 0.78 2.56 2.98 3.29 -6.48	result.12.pdb
13	8700	973.80	-79.03	-1.32 -0.69 -0.86 -7.61 -8.97 26.23	result.13.pdb
14	8696	1012.60	-161.10	0.23 0.68 2.24 14.51 -28.88 -3.17	result.14.pdb
15	8644	1206.50	-46.74	-1.89 -0.36 1.91 5.66 -34.25 17.10	result.15.pdb
16	8628	1192.00	330.84	-0.75 0.74 0.78 -0.58 0.95 23.63	result.16.pdb
17	8602	1285.20	17.88	-2.71 0.40 -1.13 0.42 4.95 -2.29	result.17.pdb
18	8574	1342.30	118.56	2.27 -0.07 0.36 -10.58 13.53 29.87	result.18.pdb
19	8526	1039.50	-111.44	-0.65 0.10 -1.60 -11.41 7.24 13.05	result.19.pdb
20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

NEW: Jmol view

show next 20 »»

DOWNLOAD best solutions as a ZIP file: 10 (solutions number, from 2 to 100) GO (this takes few seconds, please wait patiently)

DOWNLOAD solutions table transformations file

REFINE best solutions with FireDock: 1000 (solutions number, from 1 to 1000) GO

Output:

Atomic Contact Energy

Receptor	Ligand	Complex Type	Clus		Receptor Site	Ligand Site	
A.pdb.tr	B.pdb.tr	Default	4.0	dunovka@tau.ac.il	-	-	-

Solution No	Score	Area	ACE	Transformation	PDB file of the complex
1	10166	1528.90	-12.07	-1.15 -0.37 -0.32 -11.03 -15.21 22.35	result.1.pdb
2	9740	1285.70	129.52	-2.07 -0.40 -1.44 -3.43 9.43 18.35	result.2.pdb
3	9380	1284.70	-8.60	0.77 0.16 -0.54 -1.20 8.06 -10.85	result.3.pdb
4	9122	1298.80	203.84	2.45 -0.57 -1.59 13.45 2.35 14.25	result.4.pdb
5	9048	1185.20	-243.82	3.11 0.11 1.04 -16.19 -29.02 2.25	result.5.pdb
6	9034	1094.70	301.73	2.09 -0.49 -1.37 6.24 3.03 10.96	result.6.pdb
7	8972	1182.40	-39.65	-2.07 -1.05 -2.85 6.41 -17.96 28.59	result.7.pdb
8	8890	1163.80	-165.52	0.59 0.92 2.17 12.62 -23.69 -10.70	result.8.pdb
9	8886	1195.40	-31.63	0.92 0.49 3.07 18.21 -10.46 -11.65	result.9.pdb
10	8850	1240.20	-149.90	-1.43 0.72 0.57 -14.80 -28.15 -1.02	result.10.pdb
11	8768	962.70	19.42	-1.12 -0.24 -0.71 -13.34 -9.72 21.55	result.11.pdb
12	8740	1110.70	2.06	0.34 0.78 2.56 2.98 3.29 -6.48	result.12.pdb
13	8700	973.80	-79.03	-1.32 -0.69 -0.86 -7.61 -8.97 26.23	result.13.pdb
14	8696	1012.60	-161.10	0.23 0.68 2.24 14.51 -28.88 -3.17	result.14.pdb
15	8644	1206.50	-46.74	-1.89 -0.36 1.91 5.66 -34.25 17.10	result.15.pdb
16	8628	1192.00	330.84	-0.75 0.74 0.78 -0.58 0.95 23.63	result.16.pdb
17	8602	1285.20	17.88	-2.71 0.40 -1.13 0.42 4.95 -2.29	result.17.pdb
18	8574	1342.30	118.56	2.27 -0.07 0.36 -10.58 13.53 29.87	result.18.pdb
19	8526	1039.50	-111.44	-0.65 0.10 -1.60 -11.41 7.24 13.05	result.19.pdb
20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

NEW: Jmol view

show next 20 »»

DOWNLOAD best solutions as a ZIP file: 10 (solutions number, from 2 to 100) GO (this takes few seconds, please wait patiently)

DOWNLOAD solutions table transformations file

REFINE best solutions with FireDock: 1000 (solutions number, from 1 to 1000) GO

Output:

3D transformation

Receptor	Ligand	Complex Type	Clustering RMSD		Ligand Site	
A.pdb.tr	B.pdb.tr	Default	4.0		-	-

Solution No	Score	Area	ACE	Transformation	PDB file of the complex
1	10166	1528.90	-12.07	-1.15 -0.37 -0.32 -11.03 -15.21 22.35	result.1.pdb
2	9740	1285.70	129.52	-2.07 -0.40 -1.44 -3.43 9.43 18.35	result.2.pdb
3	9380	1284.70	-8.60	0.77 0.16 -0.54 -1.20 8.06 -10.85	result.3.pdb
4	9122	1298.80	203.84	2.45 -0.57 -1.59 13.45 2.35 14.25	result.4.pdb
5	9048	1185.20	-243.82	3.11 0.11 1.04 -16.19 -29.02 2.25	result.5.pdb
6	9034	1094.70	301.73	2.09 -0.49 -1.37 6.24 3.03 10.96	result.6.pdb
7	8972	1182.40	-39.65	-2.07 -1.05 -2.85 6.41 -17.96 28.59	result.7.pdb
8	8890	1163.80	-165.52	0.59 0.92 2.17 12.62 -23.69 -10.70	result.8.pdb
9	8886	1195.40	-31.63	0.92 0.49 3.07 18.21 -10.46 -11.65	result.9.pdb
10	8850	1240.20	-149.90	-1.43 0.72 0.57 -14.80 -28.15 -1.02	result.10.pdb
11	8768	962.70	19.42	-1.12 -0.24 -0.71 -13.34 -9.72 21.55	result.11.pdb
12	8740	1110.70	2.06	0.34 0.78 2.56 2.98 3.29 -6.48	result.12.pdb
13	8700	973.80	-79.03	-1.32 -0.69 -0.86 -7.61 -8.97 26.23	result.13.pdb
14	8696	1012.60	-161.10	0.23 0.68 2.24 14.51 -28.88 -3.17	result.14.pdb
15	8644	1206.50	-46.74	-1.89 -0.36 1.91 5.66 -34.25 17.10	result.15.pdb
16	8628	1192.00	330.84	-0.75 0.74 0.78 -0.58 0.95 23.63	result.16.pdb
17	8602	1285.20	17.88	-2.71 0.40 -1.13 0.42 4.95 -2.29	result.17.pdb
18	8574	1342.30	118.56	2.27 -0.07 0.36 -10.58 13.53 29.87	result.18.pdb
19	8526	1039.50	-111.44	-0.65 0.10 -1.60 -11.41 7.24 13.05	result.19.pdb
20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

NEW: Jmol view

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DOWNLOAD solutions table transformations file

REFINE best solutions with FireDock: 1000 (solutions number, from 1 to 1000) GO

Output:

Receptor	Ligand	Complex Type	Clustering RMSD	User e-mail	Receptor
A.pdb.tr	B.pdb.tr	Default	4.0	duhovka@tau.ac.il	-

The resulted pdb

Solution No	Score	Area	ACE	Transformation	PDB file of the complex
1	10166	1528.90	-12.07	-1.15 -0.37 -0.32 -11.03 -15.21 22.35	result.1.pdb
2	9740	1285.70	129.52	-2.07 -0.40 -1.44 -3.43 9.43 18.35	result.2.pdb
3	9380	1284.70	-8.60	0.77 0.16 -0.54 -1.20 8.06 -10.85	result.3.pdb
4	9122	1298.80	203.84	2.45 -0.57 -1.59 13.45 2.35 14.25	result.4.pdb
5	9048	1185.20	-243.82	3.11 0.11 1.04 -16.19 -29.02 2.25	result.5.pdb
6	9034	1094.70	301.73	2.09 -0.49 -1.37 6.24 3.03 10.96	result.6.pdb
7	8972	1182.40	-39.65	-2.07 -1.05 -2.85 6.41 -17.96 28.59	result.7.pdb
8	8890	1163.80	-165.52	0.59 0.92 2.17 12.62 -23.69 -10.70	result.8.pdb
9	8886	1195.40	-31.63	0.92 0.49 3.07 18.21 -10.46 -11.65	result.9.pdb
10	8850	1240.20	-149.90	-1.43 0.72 0.57 -14.80 -28.15 -1.02	result.10.pdb
11	8768	962.70	19.42	-1.12 -0.24 -0.71 -13.34 -9.72 21.55	result.11.pdb
12	8740	1110.70	2.06	0.34 0.78 2.56 2.98 3.29 -6.48	result.12.pdb
13	8700	973.80	-79.03	-1.32 -0.69 -0.86 -7.61 -8.97 26.23	result.13.pdb
14	8696	1012.60	-161.10	0.23 0.68 2.24 14.51 -28.88 -3.17	result.14.pdb
15	8644	1206.50	-46.74	-1.89 -0.36 1.91 5.66 -34.25 17.10	result.15.pdb
16	8628	1192.00	330.84	-0.75 0.74 0.78 -0.58 0.95 23.63	result.16.pdb
17	8602	1285.20	17.88	-2.71 0.40 -1.13 0.42 4.95 -2.29	result.17.pdb
18	8574	1342.30	118.56	2.27 -0.07 0.36 -10.58 13.53 29.87	result.18.pdb
19	8526	1039.50	-111.44	-0.65 0.10 -1.60 -11.41 7.24 13.05	result.19.pdb
20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

NEW: Jmol view

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DOWNLOAD best solutions as a ZIP file: 10 (solutions number, from 2 to 100) GO (this takes few seconds, please wait patiently)

DOWNLOAD solutions table transformations file

REFINE best solutions with FireDock: 1000 (solutions number, from 1 to 1000) GO

Output:

Receptor	Ligand	Complex Type	Clustering RMSD	User e-mail	Receptor Site	Ligand Site
A.pdb.tr	B.pdb.tr	Default	4.0	duhovka@tau.ac.il	-	-

Solution No	Score	Area	ACE	Transformation	PDB file of the complex
1	10166	1528.90	-12.07	-1.15 -0.37 -0.32 -11.03 -15.21 22.35	result.1.pdb
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3	9380	1284.70	-8.60	0.77 0.16 -0.54 -1.20 8.06 -10.85	result.3.pdb
4	9122	1298.80	203.84	2.45 -0.57 -1.59 13.45 2.35 14.25	result.4.pdb
5	9048	1185.20	-243.82	3.11 0.11 1.04 -16.19 -29.02 2.25	result.5.pdb
6	9034	1094.70	301.73	2.09 -0.49 -1.37 6.24 3.03 10.96	result.6.pdb
7	8972	1182.40	-39.65	-2.07 -1.05 -2.85 6.41 -17.96 28.59	result.7.pdb
8	8890	1163.80	-165.52	0.59 0.92 2.17 12.62 -23.69 -10.70	result.8.pdb
9	8886	1195.40	-31.63	0.92 0.49 3.07 18.21 -10.46 -11.65	result.9.pdb
10	8850	1240.20	-149.90	-1.43 0.72 0.57 -14.80 -28.15 -1.02	result.10.pdb
11	8768	962.70	19.42	-1.12 -0.24 -0.71 -13.34 -9.72 21.55	result.11.pdb
12	8740	1110.70	2.06	0.34 0.78 2.56 2.98 3.29 -6.48	result.12.pdb
13	8700	973.80	-79.03	-1.32 -0.69 -0.86 -7.61 -8.97 26.23	result.13.pdb
14	8696	1012.60	-161.10	0.23 0.68 2.24 14.51 -28.88 -3.17	result.14.pdb
15	8644	1206.50	-46.74	-1.89 -0.36 1.91 5.66 -34.25 17.10	result.15.pdb
16	8628	1192.00	330.84	-0.75 0.74 0.78 -0.58 0.95 23.63	result.16.pdb
17	8602	1285.20	17.88	-2.71 0.40 -1.13 0.42 4.95 -2.29	result.17.pdb
18	8574	1342.30	118.56	2.27 -0.07 0.36 -10.58 13.53 29.87	result.18.pdb
19	8526	1039.50	-111.44	-0.65 0.10 -1.60 -11.41 7.24 13.05	result.19.pdb
20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

NEW: Jmol view

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DOWNLOAD best solutions as a ZIP file: 10 (solutions number, from 2 to 100) GO (this takes few seconds, please wait patiently)

DOWNLOAD solutions table transformations file

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Output:

Receptor	Ligand	Complex Type	Clustering RMSD	User e-mail	Receptor Site	Ligand Site
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Solution No	Score	Area	ACE	Transformation	PDB file of the complex
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3	9380	1284.70	-8.60	0.77 0.16 -0.54 -1.20 8.06 -10.85	result.3.pdb
4	9122	1298.80	203.84	2.45 -0.57 -1.59 13.45 2.35 14.25	result.4.pdb
5	9048	1185.20	-243.82	3.11 0.11 1.04 -16.19 -29.02 2.25	result.5.pdb
6	9034	1094.70	301.73	2.09 -0.49 -1.37 6.24 3.03 10.96	result.6.pdb
7	8972	1182.40	-39.65	-2.07 -1.05 -2.85 6.41 -17.96 28.59	result.7.pdb
8	8890	1163.80	-165.52	0.59 0.92 2.17 12.62 -23.69 -10.70	result.8.pdb
9	8886	1195.40	-31.63	0.92 0.49 3.07 18.21 -10.46 -11.65	result.9.pdb
10	8850	1240.20	-149.90	-1.43 0.72 0.57 -14.80 -28.15 -1.02	result.10.pdb
11	8768	962.70	19.42	-1.12 -0.24 -0.71 -13.34 -9.72 21.55	result.11.pdb
12	8740	1110.70	2.06	0.34 0.78 2.56 2.98 3.29 -6.48	result.12.pdb
13	8700	973.80	-79.03	-1.32 -0.69 -0.86 -7.61 -8.97 26.23	result.13.pdb
14	8696	1012.60	-161.10	0.23 0.68 2.24 14.51 -28.88 -3.17	result.14.pdb
15	8644	1206.50	-46.74	-1.89 -0.36 1.91 5.66 -34.25 17.10	result.15.pdb
16	8628	1192.00	330.84	-0.75 0.74 0.78 -0.58 0.95 23.63	result.16.pdb
17	8602	1285.20	17.88	-2.71 0.40 -1.13 0.42 4.95 -2.29	result.17.pdb
18	8574	1342.30	118.56	2.27 -0.07 0.36 -10.58 13.53 29.87	result.18.pdb
19	8526	1039.50	-111.44	-0.65 0.10 -1.60 -11.41 7.24 13.05	result.19.pdb
20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

NEW: Jmol view

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DOWNLOAD best solutions as a ZIP file: 10 (solutions number, from 2 to 100) GO (this takes few seconds, please wait patiently)

DOWNLOAD solutions table transformations file

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Output:

Receptor	Ligand	Complex Type	Clustering RMSD	User e-mail	Receptor Site	Ligand Site
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Solution No	Score	Area	ACE	Transformation	PDB file of the complex
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3	9380	1284.70	-8.60	0.77 0.16 -0.54 -1.20 8.06 -10.85	result.3.pdb
4	9122	1298.80	203.84	2.45 -0.57 -1.59 13.45 2.35 14.25	result.4.pdb
5	9048	1185.20	-243.82	3.11 0.11 1.04 -16.19 -29.02 2.25	result.5.pdb
6	9034	1094.70	301.73	2.09 -0.49 -1.37 6.24 3.03 10.96	result.6.pdb
7	8972	1182.40	-39.65	-2.07 -1.05 -2.85 6.41 -17.96 28.59	result.7.pdb
8	8890	1163.80	-165.52	0.59 0.92 2.17 12.62 -23.69 -10.70	result.8.pdb
9	8886	1195.40	-31.63	0.92 0.49 3.07 18.21 -10.46 -11.65	result.9.pdb
10	8850	1240.20	-149.90	-1.43 0.72 0.57 -14.80 -28.15 -1.02	result.10.pdb
11	8768	962.70	19.42	-1.12 -0.24 -0.71 -13.34 -9.72 21.55	result.11.pdb
12	8740	1110.70	2.06	0.34 0.78 2.56 2.98 3.29 -6.48	result.12.pdb
13	8700	973.80	-79.03	-1.32 -0.69 -0.86 -7.61 -8.97 26.23	result.13.pdb
14	8696	1012.60	-161.10	0.23 0.68 2.24 14.51 -28.88 -3.17	result.14.pdb
15	8644	1206.50	-46.74	-1.89 -0.36 1.91 5.66 -34.25 17.10	result.15.pdb
16	8628	1192.00	330.84	-0.75 0.74 0.78 -0.58 0.95 23.63	result.16
17	8602	1285.20	17.88	-2.71 0.40 -1.13 0.42 4.95 -2.29	result.17
18	8574	1342.30	118.56	2.27 -0.07 0.36 -10.58 13.53 29.87	result.18
19	8526	1039.50	-111.44	-0.65 0.10 -1.60 -11.41 7.24 13.05	result.19
20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

NEW: Jmol view

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Download output

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DOWNLOAD solutions table transformations file

REFINE best solutions with FireDock: 1000 (solutions number, from 1 to 1000) GO

Output:

Receptor	Ligand	Complex Type	Clustering RMSD	User e-mail	Receptor Site	Ligand Site
A.pdb.tr	B.pdb.tr	Default	4.0	duhovka@tau.ac.il	-	- -

Solution No	Score	Area	ACE	Transformation	PDB file of the complex
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4	9122	1298.80	203.84	2.45 -0.57 -1.59 13.45 2.35 14.25	result.4.pdb
5	9048	1185.20	-243.82	3.11 0.11 1.04 -16.19 -29.02 2.25	result.5.pdb
6	9034	1094.70	301.73	2.09 -0.49 -1.37 6.24 3.03 10.96	result.6.pdb
7	8972	1182.40	-39.65	-2.07 -1.05 -2.85 6.41 -17.96 28.59	result.7.pdb
8	8890	1163.80	-165.52	0.59 0.92 2.17 12.62 -23.69 -10.70	result.8.pdb
9	8886	1195.40	-31.63	0.92 0.49 3.07 18.21 -10.46 -11.65	result.9.pdb
10	8850	1240.20	-149.90	-1.43 0.72 0.57 -14.80 -28.15 -1.02	result.10.pdb
11	8768	962.70	19.42	-1.12 -0.24 -0.71 -13.34 -9.72 21.55	result.11.pdb
12	8740	1110.70	2.06	0.34 0.78 2.56 2.98 3.29 -6.48	result.12.pdb
13	8700	973.80	-79.03	-1.32 -0.69 -0.86 -7.61 -8.97 26.23	result.13.pdb
14	8696	1012.60	-161.10	0.23 0.68 2.24 14.51 -28.88 -3.17	result.14.pdb
15	8644	1206.50	-46.74	-1.89 -0.36 1.91 5.66 -34.25 17.10	result.15.pdb
16	8628	1192.00	330.84	-0.75 0.74 0.78 -0.58 0.95 23.63	result.16.pdb
17	8602	1285.20	17.88	-2.71 0.40 -1.13 0.42 4.95 -2.29	result.17.pdb
18	8574	1342.30	118.56	2.27 -0.07 0.36 -10.58 13.53 29.87	result.18.pdb
19	8526	1039.50	-111.44	-0.65 0.10 -1.60 -11.41 7.24 13.05	result.19.pdb
20	8524	1098.60	-27.75	0.71 -0.70 2.28 24.54 7.03 47.47	result.20.pdb

NEW: Jmol view

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DOWNLOAD solutions table transformations file

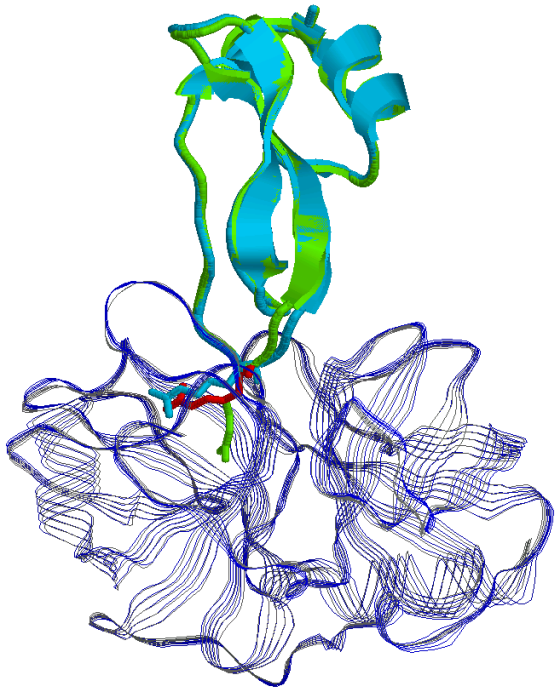
REFINE best solutions with FireDock: 1000 (solutions number, from 1 to 1000) GO

Send for refinement

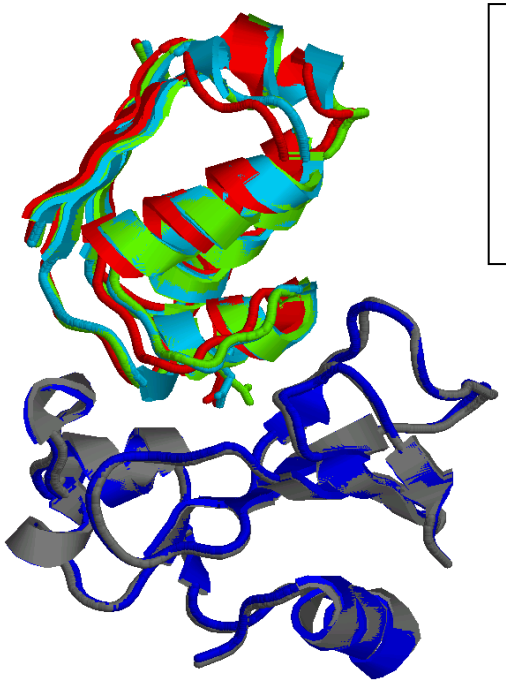
FireDock

Fast Interaction Refinement in Molecular Docking

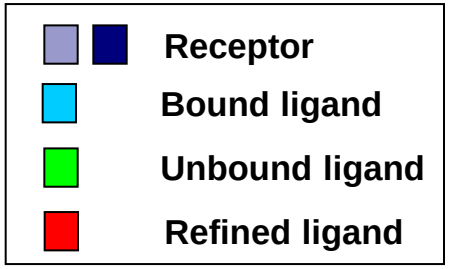
- Allows residue flexibility.
- Refinement and re-scoring of docking solutions



1BRS
BARNASE-BARSTAR
Arg15



1BRC
TRYPSIN-APPI
Asp39



Andrusier N, Nussinov R, Wolfson HJ Proteins 07

FireDock

Fast Interaction REfinement in molecular DOCKing

[Web Server] [About] [Download] [FAQ] [Help] [References] Contact: ppdock@tau.ac.il

FireDock is an efficient method for refinement and re-scoring of rigid-body protein-protein docking solutions.

Please choose one of the options below

Option 1 (use transformation file, a faster option)

Receptor Molecule: (PDB:chainId e.g. 2kai:AB) **or** upload file: Browse...

Ligand Molecule: (PDB:chainId e.g. 2kai:I) **or** upload file: Browse...

Transformations File: Browse... (up to 1000 transformations)

(Example: Receptor Molecule: *2kai:AB*, Ligand Molecule: *2kai:I*, Transformations File: 2kai_trans.txt)

Option 2 (use models file, a much slower option)

Models File: Browse... (up to 100) Receptor chains: Ligand chains:

(Example: Models File: models_example.ent, Receptor chain: *E*, Ligand chain: *I*)

Number of output structures: 10 (up to 100)

Your e-mail address:

Submit Query Clear

Advanced Options: (optional)
[show][hide]

E. Mashiach, D. Schneidman-Duhovny, N. Andrusier, R. Nussinov, H. J. Wolfson. NAR 08

FireDock

Fast Interaction REfinement in molecular DOCKing

[Web Server] [About] [Download] [FAQ] [Help] [References] Contact: ppdock@tau.ac.il

FireDock is an efficient method for refinement and re-scoring of rigid-body protein-protein docking solutions.

Please choose one of the options below

Option 1 (use transformation file, a faster option)

Receptor Molecule: (PDB:chainId e.g. 2kai:AB) **or** upload file: Browse...

Ligand Molecule: (PDB:chainId e.g.

Transformations File: Browse... (up t

(Example: Receptor Molecule: *2kai:AB*, Ligand Molecule: *2kai:I*, Transfo

Option 2 (use models file, a much slower option)

Models File: Browse... (up t

(Example: Models File:models_example.ent, Receptor chain: *E*, Ligand

Number of output structures: 10 (up to 100)

Your e-mail address:

Submit Query Clear

Advanced Options: (optional)
[show][hide]

Transformations File:
A file containing the ligand's transformations in the following format:
index X-rotation Y-rotation Z-rotation
X-translation Y-translation Z-translation

For example:
1 2.11363 0.153389 2.82412 10.8802 -4.53751 -7.76723
2 1.3353 -0.0999924 -2.60445 44.0002 4.52072 8.73591
3 1.99255 0.159889 2.81949 12.0745 -2.47299 -9.35544
4 1.3353 -0.0999924 -2.49973 43.5566 7.54644 8.73591
5 1.32362 0.0314778 -2.64412 42.0512 3.61016 5.47968

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Please choose one of the options below

Option 1 (use transformation file, a faster option)

Receptor Molecule: (PDB:chainId e.g. 2kai:AB) **or** upload file: Browse...

Ligand Molecule: (PDB:chainId e.g. 2kai:I) **or** upload file: Browse...

Transformations File: Browse... (up to 1000 transformations)

(Example: Receptor Molecule: *2kai:AB*, Ligand Molecule: *2kai:I*, Transformations File: 2kai_trans.txt)

Option 2 (use models file, a much slower option)

Models File: Browse... (up to 100) Receptor chains: Ligand chains:

(Example: Models File: models_example.ent, Receptor chain: *E*, Ligand chain: *I*)

Number of output structures: 10 (up to 100)

Your e-mail address:

Submit Query Clear

Advanced Options: (optional)
[show][hide]

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FireDock

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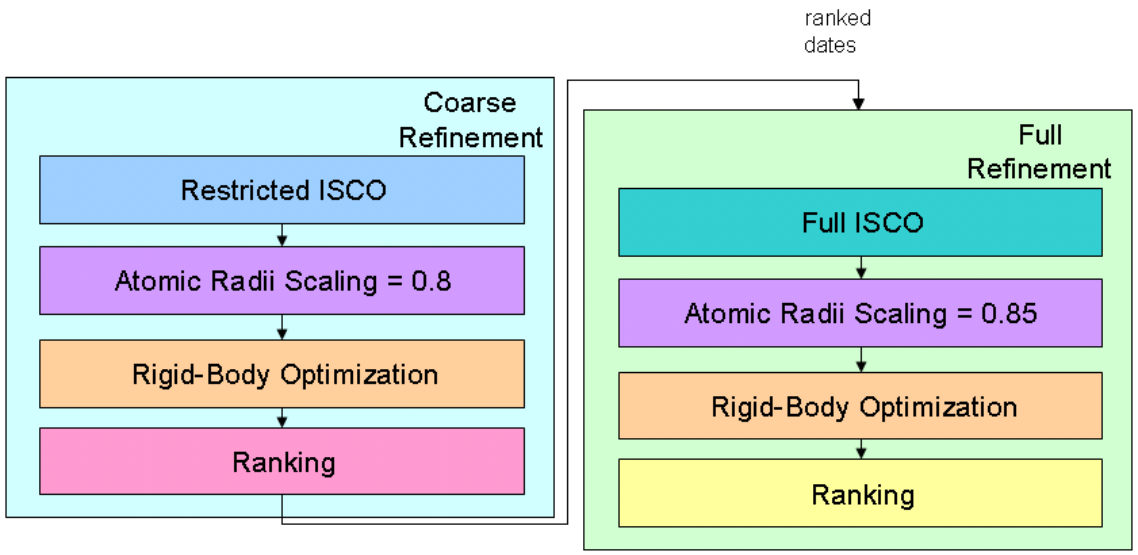
Advanced Options: (optional)
[show][hide]

Complex Type:	Default	
Refinement Level:	Restricted	
Number of RBO Cycles:	50	
Atomic Radius Scale:	0.8	
Bound/Unbound:	Receptor: Unbound	Ligand: Unbound
Fixed Residues Files:	Receptor: Browse...	Ligand: Browse...
Flexible Residues Files:	Receptor: Browse...	Ligand: Browse...

Submit Query Clear



FireDock

Fast Interaction REfinement in molecular DOCKing

[Web Server] [About] [Download] [FAQ] [Help] [References] Contact: ppdock@tau.ac.il

Advanced Options: (optional)
[show][hide]

Complex Type:	Default			
Refinement Level:	Restricted			
Number of RBO Cycles:	50			
Atomic Radius Scale:	0.8			
Bound/Unbound:	Receptor: Unbound		Ligand: Unbound	
Fixed Residues Files:	Receptor:	Browse...	Ligand:	Browse...
Flexible Residues Files:	Receptor:	Browse...	Ligand:	Browse...

Submit Query Clear

Fixed/Flexible Residues Files:
Files that specify fixed/flexible residues of the receptor and the ligand, in the following format:

<residue-index> <chain>

For example:
88 A
89 A
90 A
91 A

FireDock

Receptor	Ligand	TransFile	User e-mail
A.pdb	C.pdb	trans.txt	efratmas@gmail.com

Rank	Solution Number	Global Energy ↓	Attractive VdW	Repulsive VdW	ACE	HB	Structure show/hide
1	4	-22.88	-27.16	16.96	-11.83	-4.93	☑
2	64	-21.95	-21.95	7.16	-11.61	-3.60	☐
3	26	-21.50	-22.47	6.91	-11.01	-2.63	☐
4	112	-21.40	-25.74	16.40	-11.18	-3.96	☐
5	27	-20.67	-18.88	6.81	-9.82	-2.82	☐
6	158	-20.00	-26.22	9.17	-10.38	-2.59	☐
7	117	-19.27	-27.51	12.51	-11.22	-2.54	☐
8	131	-17.37	-21.60	8.38	-13.76	-1.44	☐
9	128	-17.01	-25.25	14.27	-9.50	-3.64	☐
10	97	-16.46	-17.62	5.80	-10.33	-4.85	☐
11	118	-16.40	-24.34	15.17	-9.13	-3.45	☐
12	154	-15.38	-23.17	16.41	-12.05	-3.80	☐
13	46	-15.22	-28.68	15.75	-10.95	-3.17	☐
14	36	-15.21	-19.25	8.58	-8.62	-4.05	☐
15	38	-14.84	-17.85	2.36	-8.15	-5.32	☐
16	156	-13.58	-22.35	15.07	-9.46	-3.92	☐
17	139	-12.25	-17.74	7.82	-11.66	-2.97	☐
18	120	-10.88	-25.93	20.57	-13.12	-1.73	☐
19	52	-9.29	-19.63	6.51	-8.62	-3.60	☐
20	111	-9.15	-21.51	10.50	-7.28	-2.76	☐

show next 20 »»

☐ show all/hide all

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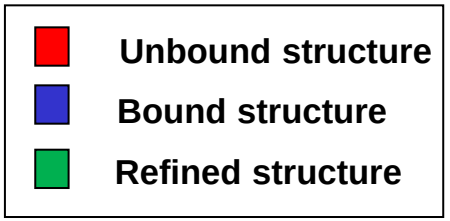
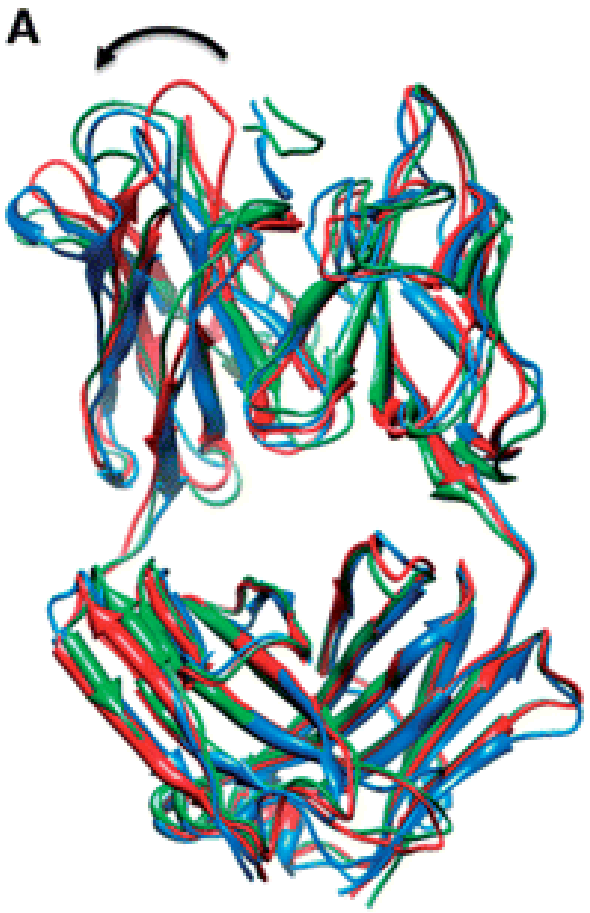
FiberDock

Flexible Induced-fit Backbone Refinement in Molecular Docking

- Refinement and re-scoring of docking solutions
- Allows residues and backbone flexibility.

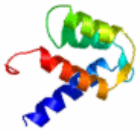


1GGI
HIV-1 NEUTRALIZING
ANTIBODY - V3 LOOP
PEPTIDE ANTIGEN



FiberDock

Flexible Induced-fit Backbone Refinement in Molecular Docking



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FiberDock is an efficient method for flexible refinement and re-scoring of rigid-body protein-protein docking solutions.

Option 1 (use transformation file)

(Example: Receptor Molecule: *1ukr:A*, Ligand Molecule: *1t6g:B*, Transformations File:1t6g_trans.txt)

Receptor Molecule: (PDB:chainId e.g. 1ukr:A) **or** upload file: בחר קובץ לא נבחר קובץ

Refine receptor's backbone conformation? Yes No

Ligand Molecule: (PDB:chainId e.g. 1t6g:B) **or** upload file: בחר קובץ לא נבחר קובץ

Refine ligand's backbone conformation? Yes No

Rigid Docking Solutions: File format: PatchDock transformations file / ZDOCK output file — upload file: בחר קובץ לא נבחר קובץ (up to 100 solutions)

* If no file is uploaded a zero-transformation will be used.

Option 2 (use models file)

(Example: Models File:models_example.ent, Receptor chain: *E*, Ligand chain: *I*)

Models file: בחר קובץ לא נבחר קובץ Receptor chain: Ligand chain: (up to 100 models)

the backbone conformation of the proteins must be **the same** in all the models!

Refine receptor's backbone conformation? Yes No

Refine ligand's backbone conformation? Yes No

Your e-mail address: (optional)

A link to the results page will be sent to this address when FiberDock will finish running.

If you use this program, please cite:

1. E. Mashiach, R. Nussinov and H. J. Wolfson. FiberDock: Flexible induced-fit backbone refinement in molecular docking. *Proteins* 2009 Dec 9;78(6):1503-1519.
2. E. Mashiach, R. Nussinov and H. J. Wolfson. FiberDock: a web server for flexible induced-fit backbone refinement in molecular docking. *Nucleic Acids Res.* 2010 Jul 1;38

שלח Clear

FiberDock

Advanced Options: (optional)
[show][hide]

Side-Chain Optimization (SCO)	**Perform SCO for:**	☑ Receptor	☑ Ligand
	SCO Level:	Restricted	
Backbone Refinement	**Number of normal modes:**	50	
	Backbone flexibility level:	0.95	(range: 0-1)
Rigid-Body Optimization	**Number of MC Cycles:**	50	
Scoring	**Complex Type:**	Default	
	Atomic radius scale:	0.8	

שלח Clear

FiberDock

Advanced Options: (optional)
[show][hide]

Side-Chain Optimization (SCO)	**Perform SCO for:**	☑ Receptor ☑ Ligand
	SCO Level:	Restricted
Backbone Refinement	**Number of normal modes:**	50
	Backbone flexibility level:	0.95 (range: 0-1)
Rigid-Body Optimization	**Number of MC Cycles:**	50
Scoring	**Complex Type:**	Default
	Atomic radius scale:	0.8

שלח Clear

Same as FireDock

FiberDock

Advanced Options: (optional)
[show][hide]

Side-Chain Optimization (SCO)	**Perform SCO for:**	☑ Receptor ☑ Ligand
	SCO Level:	Restricted
Backbone Refinement	**Number of normal modes:**	50
	Backbone flexibility level:	0.95 (range: 0-1)
Rigid-Body Optimization	**Number of MC Cycles:**	50
Scoring	**Complex Type:**	Default
	Atomic radius scale:	0.8

שלח Clear

Number of normal modes:

- Small number restricts to relatively global movements
- High number allows also local movements.

FiberDock

Advanced Options: (optional)
[show][hide]

Side-Chain Optimization (SCO)	**Perform SCO for:**	☑ Receptor ☑ Ligand
	SCO Level:	Restricted
Backbone Refinement	**Number of normal modes:**	50
	Backbone flexibility level:	0.95 (range: 0-1)
Rigid-Body Optimization	**Number of MC Cycles:**	50
Scoring	**Complex Type:**	Default
	Atomic radius scale:	0.8

שלח Clear

Backbone felxibility level:

- To prevent the backbone from over distorting, a penalty term is introduced into the backbone minimization step.
- The higher the level, the lower the weight of this penalty term.

FiberDock

Advanced Options: (optional)
[show][hide]

Side-Chain Optimization (SCO)	Perform SCO for:	☑ Receptor ☑ Ligand
	SCO Level:	Restricted
Backbone Refinement	Number of normal modes:	50
	Backbone flexibility level:	0.95 (range: 0-1)
Rigid-Body Optimization	Number of MC Cycles:	50
Scoring	Complex Type:	Default
	Atomic radius scale:	0.8

שלח Clear

Same as FireDock

FiberDock

Flexible Induced-fit Backbone Refinement in Molecular Docking

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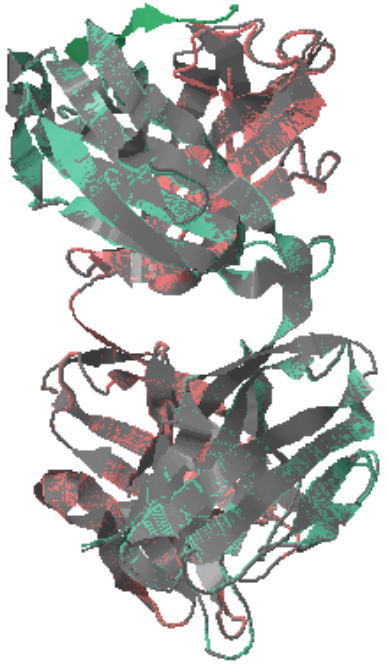
Receptor	Ligand	TransFile
1ggc.pdb	1GGI_ligand.pdb	trans_1ggi.txt

☐ show all/hide all ☑ show original receptor

Rank	Solution Number	Global Energy ↓	Attractive VdW	Repulsive VdW	ACE	HB	Structure show/hide
1	2	-49.10	-24.48	10.81	-12.03	-1.43	☐
2	4	-47.49	-22.19	17.11	-16.06	-0.34	☐
3	5	-30.64	-20.05	7.30	-7.30	0.00	☐
4	3	-17.68	-13.62	5.31	0.01	0.00	☐
5	1	-9.81	-29.05	57.75	-10.43	-0.90	☐
6	6	0.02	-18.67	10.87	-5.23	-0.24	☑



Jmol

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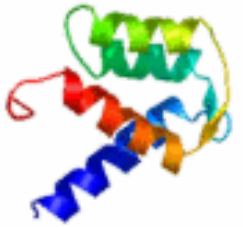
Good Luck

Enjoy the docking!



Good Luck

Enjoy the docking!

FiberDock

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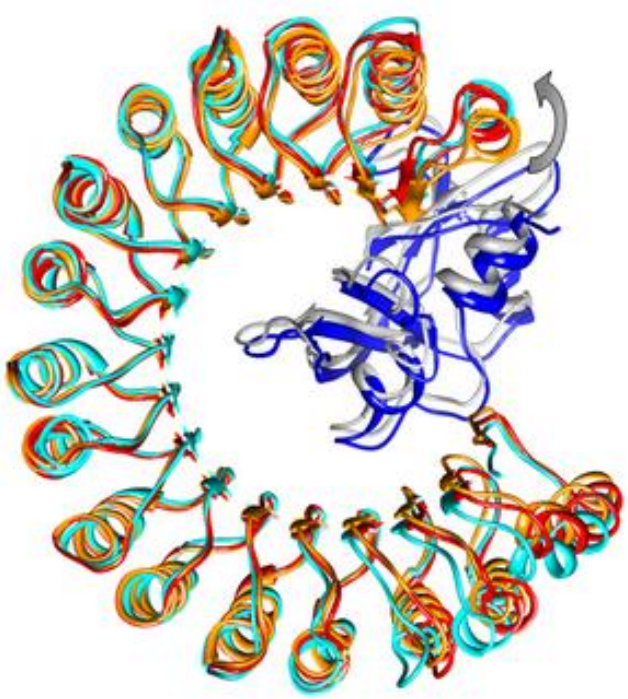

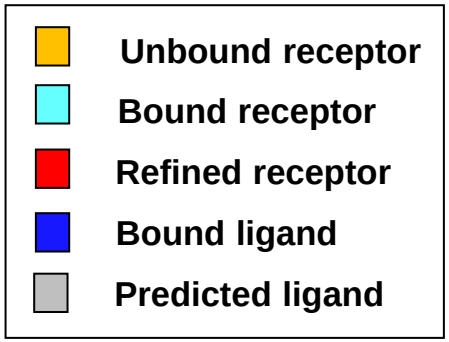

1IBR
Ran-Importin beta