Online Services

- I-TASSER
- I-TASSER-MTD
- C-I-TASSER
- CR-I-TASSER
- QUARK
- C-QUARK
- LOMETS
- MUSTER
- CEthreader
- SEGMER
- DeepFold
- DeepFoldRNA
- FoldDesign
- COFACTOR
- COACH
- MetaGO
- TripletGO
- IonCom
- FG-MD
- ModRefiner
- REMO
- DEMO
- DEMO-EM
- SPRING
- COTH
- Threpp
- PEPPI
- BSpred
- ANGLOR
- EDock
- BSP-SLIM
- SAXSTER
- FUpred
- ThreaDom
- ThreaDomEx
- EvoDesign
- BindProf
- BindProfX
- SSIPe
- GPCR-I-TASSER
- MAGELLAN
- ResQ
- STRUM
- DAMpred
- TM-score
- TM-align

[Server] [Queue] [Forum] [Download] [Example] [Search] [Registration] [Statistics] [Remove] [Potential] [Decoys] [News] [About] [Annotation]

Annotation on the I-TASSER Results

The outputs of the I-TASSER modeling results are generally summarized in a webpage, the link of which is sent to the users after the modeling is completed (see an example of I-TASSER output). This page includes a detailed explanation on the data listed on the I-TASSER output page.

Download the complete set of I-TASSER results

Figure 1. *The tarball of I-TASSER modeling results.*

Predicted Secondary Structure

Figure 2. *The sequence-based prediction of secondary structure by PSSpred.*

Predicted normalized B-factor
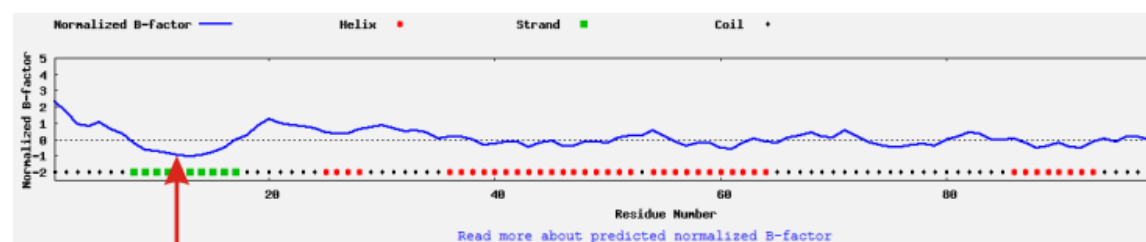
Figure 3. *The predicted normalized B-factor by ResQ.*

Top 10 templates used by I-TASSER

Figure 4. *The top 10 template-query alignments generated by LOMETS.*

Top 5 Models predicted by I-TASSER
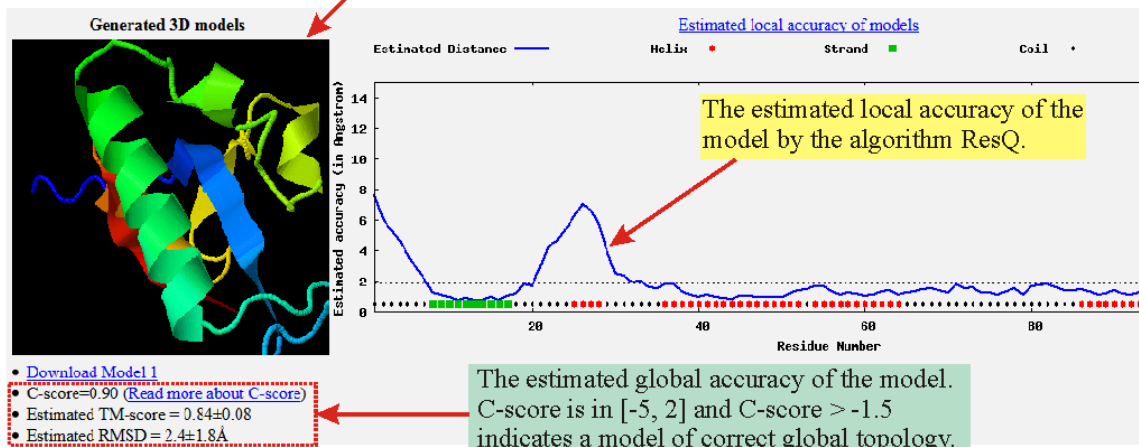
Figure 5. *The predicted 3D model and the estimated global and local accuracy.*

Proteins structurally close to the target in the PDB

Figure 6. *The structure alignment between the first I-TASSER model and the top 10 most similar structure templates in PDB.*

Predicted ligand binding sites

Ligand Binding Sites

Select a radio button to visualize different ligand binding sites.
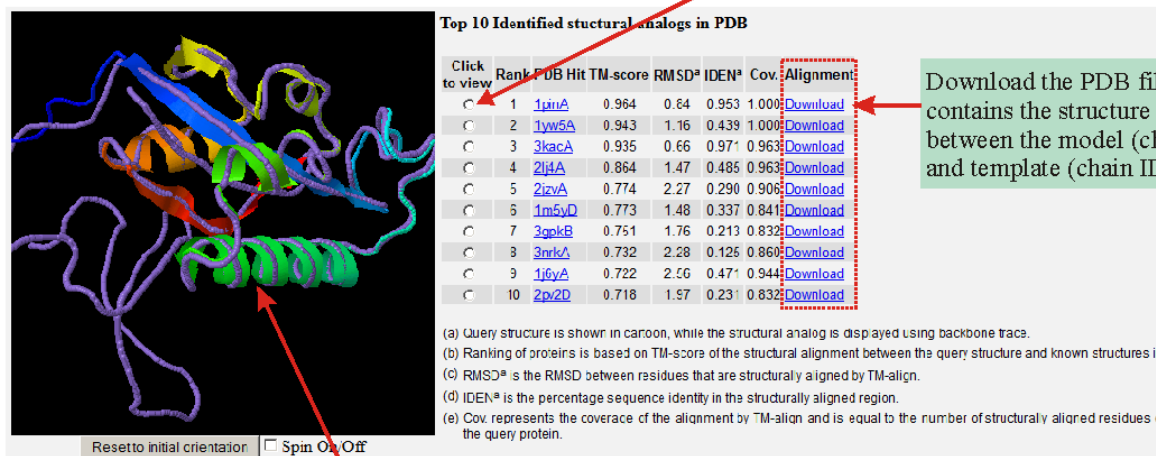
The complex with one binding ligand.

The complex with multiple binding ligands.

Click to view	Rank	C-score	Cluster size	PDB Hit	Lig Name	Download Complex	Ligand Binding Site Residues
◉	1	0.98	94	3kaiA	4FI	Rep, Mult	13,15,17,23,67,68,69,75,76,84,85,88
○	2	0.41	24	2pv1A	PEPTIDE	Rep, Mult	9,11,13,67,69,75,76,77,78,79,80,84,85,88,106,
○	3	0.24	11	3tc5A	3T5	Rep, Mult	17,22,23,76,79,83,84,85,88
○	4	0.09	8	3kceA	12P	Rep, Mult	47,51,100,101,102
○	5	0.08	4	3i6cA	GIA	Rep, Mult	28,29,34,42,64

Download the residue-specific ligand binding probability, which is estimated by SVM.
Download the all possible binding ligands and detailed prediction summary.
Download the templates clustering results.

(a) **C-score** is the confidence score of the prediction. C-score ranges [0-1], where a higher score indicates a more
(b) **Cluster size** is the total number of templates in a cluster.
(c) **Lig Name** is name of possible binding ligand. Click the name to view its information in the BioLiP database.
(d) **Rep** is a single complex structure with the most representative ligand in the cluster, i.e., the one listed in the Lig
     Mult is the complex structures with all potential binding ligands in the cluster.

Predicted binding ligand is shown in greenyellow sphere.

Reset to initial orientation   ☐ Spin On/Off

Binding residues are shown in blue ball & stick.

Figure 7. *The predicted ligand-binding sites.*

Predicted enzyme commission numbers and active sites

Enzyme Commission (EC) numbers and active sites

Select a radio button to visualize dufferent active sites.

Predicted EC numbers of protein.

Click to view	Rank	Cscore^EC	PDB Hit	TM-score	RMSD^a	IDEN^a	Cov.	EC Number	Active Site Residues
○	1	0.677	1nmwA	0.891	1.22	0.981	0.972	5.2.1.8	76,85,87,91,95,100,102,104,106
○	2	0.495	2jzvA	0.774	2.27	0.290	0.906	5.2.1.8	13,15,67,91,95,101
○	3	0.431	2kgjA	0.607	2.22	0.259	0.738	5.2.1.8	10,56,67,75,77,91,98,102
○	4	0.430	1vw5A	0.943	1.16	0.439	1.000	5.2.1.8	NA
○	5	0.428	2pv1A	0.690	2.20	0.231	0.832	5.2.1.8	13,15,60,70,91,103

Click on the radio buttons to visualize predicted active site residues.

(a) Cscore^EC is the confidence score for the EC number prediction.
    where a higher score indicates a more reliable EC number pred
(b) TM-score is a measure of global structural similarity between qu
(c) RMSD^a is the RMSD between residues that are structurally aligned by TM-align.
(d) IDEN^a is the percentage sequence identity in the structurally aligned region.
(e) Cov. represents the coverage of global structural alignment and is equal to the number of structurally aligned resid
    by length of the query protein.

Predicted catalytic site resi of the query protein.

Predicted active site residues are shown in colored ball&stick.

Reset to initial orientation   ☐ Spin On/Off

Figure 8. *The predicted enzyme commission numbers and active sites.*

Predicted gene ontology terms

C-score^GO measures the similarity between the query and template. The range is [0, 1]and the higher the better.

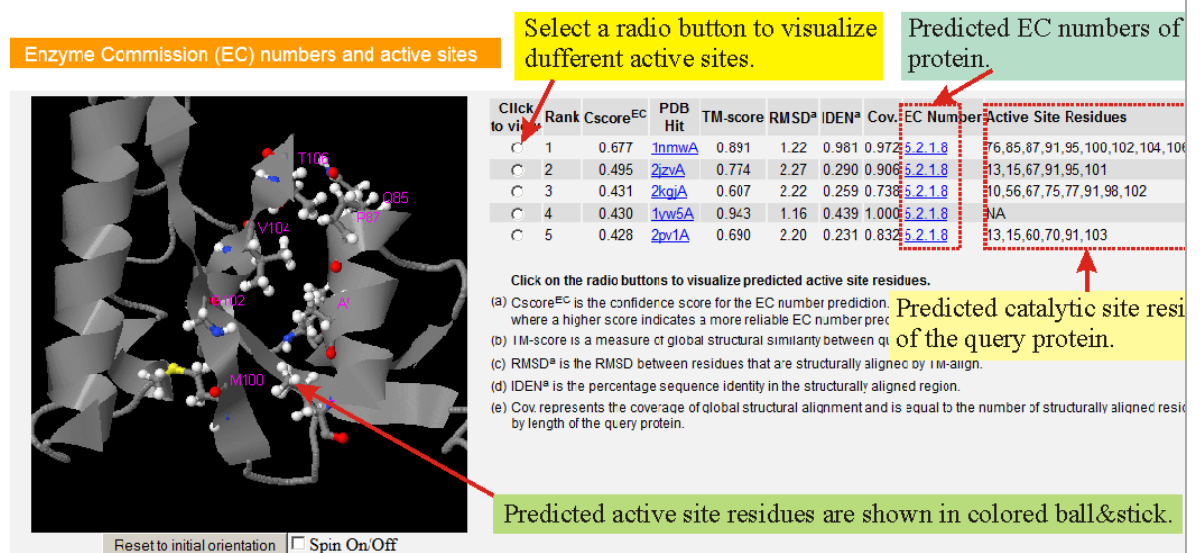**The experimental gene on terms of the templates.**

Gene Ontology (GO) terms

Top 10 homologous GO templates in PDB

Rank	Cscore^GO	TM-score	RMSD^a	IDEN^a	Cov	PDB Hit	Associated GO Terms
1	0.67	0.9135	1.34	0.95	1.00	1nmvA	GO:0007088 GO:0051443 GO:0050816 GO:0005654 GO:0030512 GO:0050815 GO:0007049 GO:0032480 GO:0070373 GO:00037 GO:0032794 GO:0000413 GO:2000146 GO:0005634 GO:0060393 GO:0031434 GO:0006457 GO:0005515 GO:0032321
2	0.65	0.8911	1.22	0.98	0.97	1nmwA	GO:0006457 GO:0031434 GO:0051443 GO:0007088 GO:0032321 GO:0050816 GO:0005654 GO:0030512 GO:0050815 GO:00070 GO:0070373 GO:0003755 GO:0016853 GO:0032794 GO:0000413 GO:2000146 GO:0005634 GO:0060393 GO:0005515
3	0.56	0.9426	1.16	0.44	1.00	1yw5A	GO:0003755 GO:0030448 GO:0006457 GO:0000413 GO:0005515 GO:0016853 GO:0009405
4	0.54	0.6483	1.65	0.43	0.75	2rqsA	GO:0003755 GO:0000413 GO:0016853
5	0.53	0.7217	2.56	0.47	0.94	1j6yA	GO:0006457 GO:0005515 GO:0051726 GO:0000413 GO:0003755 GO:0016853 GO:0005829 GO:0005886
6	0.50	0.7743	2.27	0.29	0.91	2jzvA	GO:0016853
7	0.49	0.6793	1.19	0.44	0.74	1zk6A	GO:0016853
8	0.48	0.6945	1.78	0.38	0.76	3rfwA	GO:0005515 GO:0000413 GO:0016853 GO:0003755 GO:0006457 GO:0015031
9	0.47	0.7051	2.47	0.21	0.87	2pv3A	GO:0051085 GO:0016853 GO:0030288 GO:0050821 GO:0003755 GO:0000413 GO:0043165 GO:0042597 GO:0060274 GO:00422 GO:0006457 GO:0015031
10	0.46	0.7449	1.48	0.22	0.81	3gpkA	GO:0016853

Consensus prediction of GO terms

Molecular Function	GO:0003755	GO:0031434	GO:0050815	GO:0050816	GO:0032794				
GO-Score	0.99	0.89	0.89	0.89	0.89				
Biological Process	GO:0000413	GO:0006457	GO:0051443	GO:0007088	GO:2000146	GO:0070373	GO:0060393	GO:0032321	GO:0030512	GO:0032480
GO-Score	0.99	0.98	0.89	0.89	0.89	0.89	0.89	0.89	0.89	0.89
Cellular Component	GO:0005654	GO:0005886	GO:0005829							
GO-Score	0.89	0.53	0.53							

Consensus prediction derived based on the occurrence of the GO terms among selected templates. The predictions are made for all the three GO categories: (1) Molecular Function, (2) Biological Process, and (3) Cellular Component.

Figure 9. *The top 10 GO templates in PDB and consensus prediction of GO terms in the three function categories of GO.*

Need more help?

If you have more questions about the I-TASSER modeling results, please post them at the I-TASSER Message Board, whereby some members will study and answer the questions asap.