

### I-TASSER results for job id S808440

Submitted Sequence in FASTA format

### Predicted Secondary Structure

### Predicted Solvent Accessibility

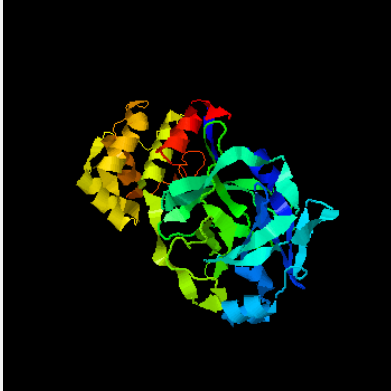
Predicted normalized B-factor

Rank	PDB Hit	Iden1	Iden2	Cov	Norm. Z-score	Download Align.
1	<a href="#">3vb3A</a>	0.96	0.94	0.98	3.91	<a href="#">Download</a>
2	<a href="#">7wo1A</a>	1.00	1.00	1.00	1.99	<a href="#">Download</a>
3	<a href="#">2yy4</a>	0.96	0.96	1.00	2.48	<a href="#">Download</a>
4	<a href="#">2yy4</a>	0.96	0.96	1.00	1.81	<a href="#">Download</a>
5	<a href="#">6xr3A</a>	1.00	1.00	1.00	4.78	<a href="#">Download</a>
6	<a href="#">2yy4</a>	0.96	0.96	1.00	2.73	<a href="#">Download</a>
7	<a href="#">5c5oA</a>	0.96	0.94	0.98	8.66	<a href="#">Download</a>
8	<a href="#">7s3kA</a>	1.00	1.00	1.00	4.26	<a href="#">Download</a>
9	<a href="#">3f9eA</a>	0.96	0.93	0.97	7.69	<a href="#">Download</a>
10	<a href="#">1c3a9A</a>	0.96	0.94	0.98	6.61	<a href="#">Download</a>

- ### Top 5 final models predicted by I-TASSER

- [More about C-score](#)
- Local structure accuracy profile of the top five models

(By right-click on the images, you can export image file or change the configurations, e.g. modifying the background color or stopping the spin of your models)

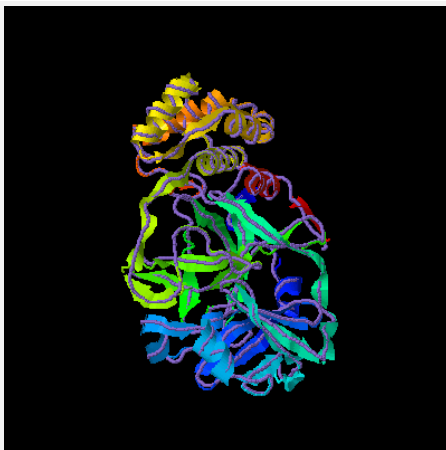


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- [Download Model 1](#)
- C-score=1.41 ([Read more about C-score](#))
- Estimated TM-score = 0.91±0.06
- Estimated RMSD = 3.4±2.4Å

### Proteins structurally close to the target in the PDB (as identified by [TM-align](#))

(After the structure assembly simulation, I-TASSER uses the TM-align structural alignment program to match the first I-TASSER model to all structures in the PDB library. This section reports the top 10 proteins from the PDB that have the closest structural similarity, i.e. the highest [TM-score](#), to the predicted I-TASSER model. Due to the structural similarity, these proteins often have similar function to the target. However, users are encouraged to use the data in the next section 'Predicted function using COACH' to infer the function of the target protein, since COACH has been extensively trained to derive biological functions from multi-source of sequence and structure features which has on average a higher accuracy than the function annotations derived only from the global structure comparison.)



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### Top 10 Identified structural analogs in PDB

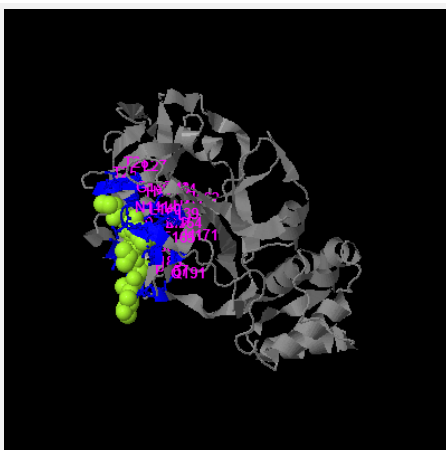
Click to view	Rank	PDB Hit	TM-score	RMSD <sup>a</sup>	IDEN <sup>b</sup>	Cov	Alignment
<input type="radio"/>	1	<a href="#">7wo1A</a>	0.991	0.62	0.997	1.000	<a href="#">Download</a>
<input type="radio"/>	2	<a href="#">4xfqA</a>	0.946	1.15	0.444	0.974	<a href="#">Download</a>
<input type="radio"/>	3	<a href="#">2zu2B</a>	0.946	1.49	0.407	0.984	<a href="#">Download</a>
<input type="radio"/>	4	<a href="#">5gwyB</a>	0.938	1.60	0.440	0.984	<a href="#">Download</a>
<input type="radio"/>	5	<a href="#">3d23D</a>	0.937	1.41	0.483	0.977	<a href="#">Download</a>
<input type="radio"/>	6	<a href="#">2ynaA</a>	0.930	1.57	0.490	0.977	<a href="#">Download</a>
<input type="radio"/>	7	<a href="#">6ijjB</a>	0.929	1.45	0.497	0.971	<a href="#">Download</a>
<input type="radio"/>	8	<a href="#">8cztA</a>	0.926	1.75	0.503	0.984	<a href="#">Download</a>
<input type="radio"/>	9	<a href="#">2ampB</a>	0.925	1.64	0.450	0.977	<a href="#">Download</a>
<input type="radio"/>	10	<a href="#">2q6dB</a>	0.904	1.90	0.409	0.967	<a href="#">Download</a>

- (a) Query structure is shown in cartoon, while the structural analog is displayed using backbone trace.  
(b) Ranking of proteins is based on TM-score of the structural alignment between the query structure and known structures in the PDB library.  
(c) RMSD<sup>a</sup> is the RMSD between residues that are structurally aligned by TM-align.  
(d) IDEN<sup>b</sup> is the percentage sequence identity in the structurally aligned region.  
(e) Cov represents the coverage of the alignment by TM-align and is equal to the number of structurally aligned residues divided by length of the query protein.

### Predicted function using [COFACTOR](#) and [COACH](#)

(This section reports biological annotations of the target protein by COFACTOR and COACH based on the I-TASSER structure prediction. While COFACTOR deduces protein functions (ligand-binding sites, EC and GO) using structure comparison and protein-protein networks, COACH is a meta-server approach that combines multiple function annotation results (on ligand-binding sites) from the COFACTOR, TM-SITE and S-SITE programs.)

### Ligand binding sites

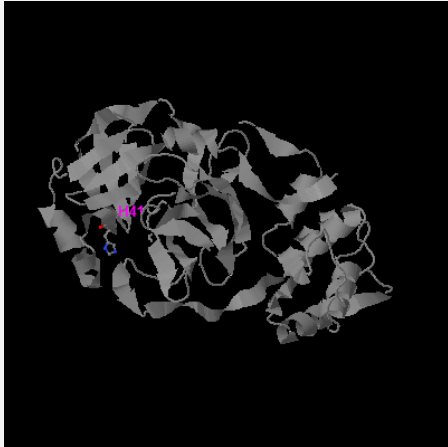


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Click to view	Rank	C-score	Cluster size	PDB Hit	Lig Name	Download Complex	Ligand Binding Site Residues
<input checked="" type="radio"/>	1	0.87	66	<a href="#">2q6gB</a>	<a href="#">PEPTIDE</a>	<a href="#">Rep</a> , <a href="#">Mult</a>	25,26,27,41,49,139,140,141,142,143,144,162,163,164,165,167,171,186,188,189,
<input type="radio"/>	2	0.12	6	<a href="#">3sndB</a>	<a href="#">PEPTIDE</a>	<a href="#">Rep</a> , <a href="#">Mult</a>	139,140,141,142,143,144,162,163,164,165,186
<input type="radio"/>	3	0.06	3	<a href="#">1q2w0</a>	<a href="#">PEPTIDE</a>	<a href="#">Rep</a> , <a href="#">Mult</a>	4,6,7,9,10,11,14,122,123,124,125,126,127,128,137,138,140,289,297,298
<input type="radio"/>	4	0.01	1	N/A	N/A	N/A	6,127,291,294
<input type="radio"/>	5	0.01	1	<a href="#">2bvsH</a>	<a href="#">PEPTIDE</a>	<a href="#">Rep</a> , <a href="#">Mult</a>	22,67

- [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 reliable prediction.  
(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 Name** column.  
**Mult** is the complex structures with all potential binding ligands in the cluster.

## Enzyme Commission (EC) numbers and active sites

 ☐ Spin On/Off

Click to view	Rank	Cscore <sup>EC</sup>	PDB Hit	TM-score	RMSD <sup>a</sup>	IDEN <sup>a</sup>	Cov	EC Number	Active Site Residues
<input type="radio"/>	1	0.728	<a href="#">2yy4A</a>	0.968	1.04	0.941	0.987	<a href="#">3.4.22.69</a>	41
<input type="radio"/>	2	0.525	<a href="#">2zu2B</a>	0.946	1.49	0.407	0.984	<a href="#">3.1.2.15</a>	NA
<input type="radio"/>	3	0.513	<a href="#">1lvoD</a>	0.910	1.91	0.447	0.980	<a href="#">3.4.22.-</a>	NA
<input type="radio"/>	4	0.473	<a href="#">2q6dB</a>	0.904	1.90	0.409	0.967	<a href="#">3.4.22.-</a>	NA
<input type="radio"/>	5	0.454	<a href="#">3d23B</a>	0.927	1.65	0.485	0.980	<a href="#">3.4.22.-</a>	NA

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

- (a) Cscore<sup>EC</sup> is the confidence score for the EC number prediction. Cscore<sup>EC</sup> values range in between [0-1]; where a higher score indicates a more reliable EC number prediction.
- (b) TM-score is a measure of global structural similarity between query and template protein.
- (c) RMSD<sup>a</sup> is the RMSD between residues that are structurally aligned by TM-align.
- (d) IDEN<sup>a</sup> 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 residues divided by length of the query protein.

## Gene Ontology (GO) terms

## Top 10 homologous GO templates in PDB

Rank	Cscore <sup>GO</sup>	TM-score	RMSD <sup>a</sup>	IDEN <sup>a</sup>	Cov	PDB Hit	Associated GO Terms
1	0.82	0.9678	1.04	0.94	0.99	<a href="#">2yy4A</a>	<a href="#">GO:0003824</a> <a href="#">GO:0019082</a>
2	0.52	0.9456	1.49	0.41	0.98	<a href="#">2zu2B</a>	<a href="#">GO:0003824</a> <a href="#">GO:0019082</a>
3	0.51	0.9097	1.91	0.45	0.98	<a href="#">1lvoD</a>	<a href="#">GO:0003824</a> <a href="#">GO:0019082</a>
4	0.47	0.9043	1.90	0.41	0.97	<a href="#">2q6dB</a>	<a href="#">GO:0003824</a> <a href="#">GO:0019082</a>
5	0.45	0.9270	1.65	0.48	0.98	<a href="#">3d23B</a>	<a href="#">GO:0003824</a> <a href="#">GO:0019082</a>
6	0.25	0.4621	3.52	0.09	0.55	<a href="#">3mmeA</a>	<a href="#">GO:0003824</a> <a href="#">GO:0006508</a> <a href="#">GO:0008234</a>
7	0.25	0.4693	3.32	0.12	0.56	<a href="#">1mbmA</a>	<a href="#">GO:0003824</a> <a href="#">GO:0004252</a> <a href="#">GO:0016032</a> <a href="#">GO:0019082</a>
8	0.25	0.4608	3.42	0.09	0.55	<a href="#">3govB</a>	<a href="#">GO:0003824</a> <a href="#">GO:0004252</a> <a href="#">GO:0006508</a>
9	0.24	0.4639	3.68	0.14	0.56	<a href="#">1lvnA</a>	<a href="#">GO:0003824</a> <a href="#">GO:0006508</a> <a href="#">GO:0008234</a>
10	0.24	0.4477	3.33	0.08	0.53	<a href="#">2puxB</a>	<a href="#">GO:0003824</a> <a href="#">GO:0004252</a> <a href="#">GO:0005509</a> <a href="#">GO:0006508</a> <a href="#">GO:0007596</a>

## Consensus prediction of GO terms

Molecular Function	<a href="#">GO:0003824</a>
GO-Score	0.99
Biological Process	<a href="#">GO:0019082</a>
GO-Score	0.99
Cellular Component	None was predicted

- (a) Cscore<sup>GO</sup> is a combined measure for evaluating global and local similarity between query and template protein. It's range is [0-1] and higher values indicate more confident predictions.
- (b) TM-score is a measure of global structural similarity between query and template protein.
- (c) RMSD<sup>a</sup> is the RMSD between residues that are structurally aligned by TM-align.
- (d) IDEN<sup>a</sup> 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 residues divided by length of the query protein.
- (f) The second table shows a consensus GO terms amongst the top scoring templates. The GO-Score associated with each prediction is defined as the average weight of the GO term, where the weights are assigned based on Cscore<sup>GO</sup> of the template.

[Click on [S808440\\_results.tar.bz2](#) to download the tarball file including all modeling results listed on this page]

Please cite the following articles when you use the I-TASSER server:

- Wei Zheng, Chengxin Zhang, Yang Li, Robin Pearce, Eric W. Bell, Yang Zhang. Folding non-homology proteins by coupling deep-learning contact maps with I-TASSER assembly simulations. Cell Reports Methods, 1: 100014 (2021).
- Chengxin Zhang, Peter L. Freddolino, and Yang Zhang. COFACTOR: improved protein function prediction by combining structure, sequence and protein-protein interaction information. Nucleic Acids Research, 45: W291-299 (2017).
- Jianyi Yang, Yang Zhang. I-TASSER server: new development for protein structure and function predictions, Nucleic Acids Research, 43: W174-W181, 2015.