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I-TASSER results for job id S808440

(Click on [S808440 results.tar.bz2](#) to download the tarball file including all modeling results listed on this page. Click on [Annotation of I-TASSER Output](#) to read the instructions for how to interpret the results on this page. Model results are kept on the server for 60 days, there is no way to retrieve the modeling data older than 2 months)

Submitted Sequence in FASTA format

>protein
SFRGFKMAFPGSKVVEGCMVQTCGTTLNLWLDVVYCPRHVICTSEDMLNPNYEDLLIR
KSINHFLVQAGNVQLRVIHGSMONCVLKLVDTANPKTPKYKFVRIQPGQTFSVALCYNG
SPSGVYQCAMPRNFTIKSLNGSCSGVGFNIDYDCVSFCYMHMELPTGVHAGTDLEGNF
YGPFDVROTAQAAGDTITTVNVLAWLYAAVINGDRWFNLRFTTTLNDFLNVAKYNEYEP
LTQDHDVILGLSAQTGIAVLDMCASLKEELQNGMGRTILGSALLEDEEFTFPDVVRQCS
GVTQF

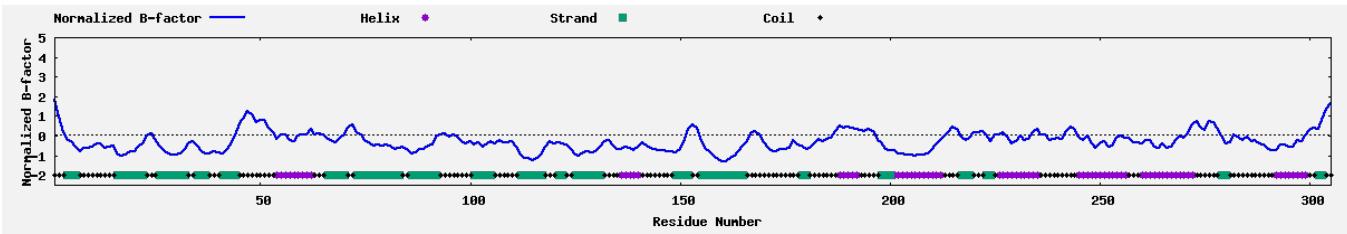
Predicted Secondary Structure

Predicted Solvent Accessibility

Sequence logo showing the distribution of amino acids at each position from 20 to 140. The x-axis is labeled with positions 20, 40, 60, 80, 100, 120, and 140. The y-axis shows amino acid probabilities from 0 to 9. The sequence logo is composed of vertical bars of varying heights representing the probability of each amino acid at each position. A legend at the bottom indicates that values range from 0 (buried residue) to 9 (highly exposed residue).

Predicted normalized B-factor

(B-factor) is a value to indicate the extent of the inherent thermal mobility of residues/atoms in proteins. In I-TASSER, this value is deduced from threading template proteins from the PDB in combination with the sequence profiles derived from sequence databases. The reported B-factor profile in the figure below corresponds to the normalized B-factor of the target protein, defined by $B = (B' - u)/s$, where B' is the raw B-factor value, u and s are respectively the mean and standard deviation of the raw B-factors along the sequence. [Click here to read more about predicted normalized B-factor](#)



Top 10 threading templates used by I-TASSER

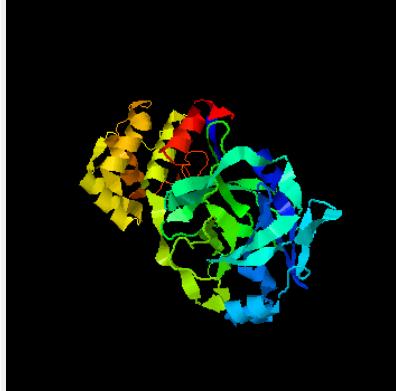
I-TASSER modeling starts from the structure templates identified by LOMETS from the PDB library. LOMETS is a meta-server threading approach containing multiple threading programs, where each threading program can generate tens of thousands of template alignments. I-TASSER only uses the templates of the highest significance in the threading alignments, the significance of which are measured by the Z-score, i.e. the difference between the raw and average scores in the unit of standard deviation. The templates in this section are the 10 best templates selected from the LOMETS threading programs. Usually, one template of the highest Z-score is selected from each threading program, whereas the threading programs are sorted by the average performance in the large-scale benchmark test experiments.)

Top 5 final models predicted by I-TASSER

(For each target, I-TASSER simulations generate a large ensemble of structural conformations, called decoys. To select the final models, I-TASSER uses the SPICKER program to cluster all the decoys based on the pair-wise structure similarity, and reports up to five models which corresponds to the five largest structure clusters. The confidence of each model is quantitatively measured by C-score that is calculated based on the significance of threading template alignments and the convergence parameters of the structure assembly simulations. C-score is typically in the range of [-5, 2], where a C-score of a higher value signifies a model with a higher confidence and vice-versa. TM-score and RMSD are estimated based on C-score and protein length following the correlation observed between these qualities. Since the top 5 models are ranked by the cluster size, it is possible that the lower-rank models have a higher C-score in rare cases. Although the first model has a better quality in most cases, it is also possible that the lower-rank models have a better quality than the higher-rank models as seen in our benchmark tests. If the I-TASSER simulations converge, it is possible to have less than 5 clusters generated; this is usually an indication that the models have a good quality because of the converged simulations.)

- More about C-score
 - Local structure accuracy profile of the top five models

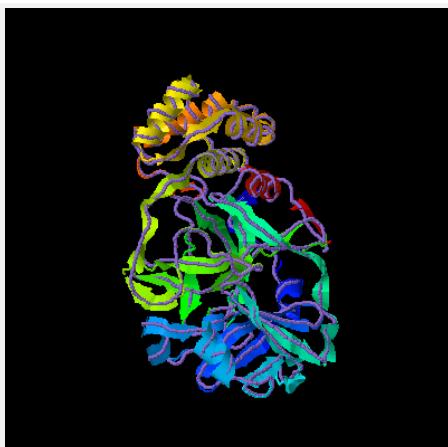
(By right-click on the images, you can export image file or change the configurations, e.g. modifying the background color or stopping the spin of your models)

 Reset to initial orientation Spin On/Off

- [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 COFACTOR' to infer the function of the target protein, since COFACTOR 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.)



Top 10 Identified structural analogs in PDB

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

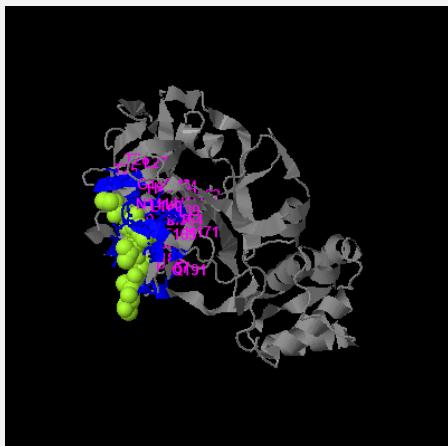
- (a) Query structure is shown in cartoon, while the structural analog is displayed using backbone trace.
 (b) Ranking of proteins is based on TM-score of the structural alignment between the query structure and known structures in the PDB library.
 (c) RMSD^a is the RMSD between residues that are structurally aligned by TM-align.
 (d) IDEN^b 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.

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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



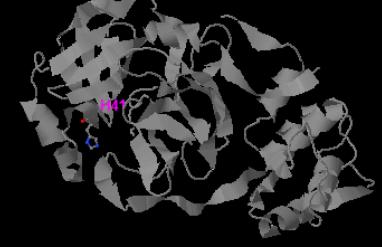
Click to view	Rank	C-score	Cluster size	PDB Hit	Lig Name	Download Complex	Ligand Binding Site Residues
<input checked="" type="radio"/>	1	0.87	66	2q6gB	PEPTIDE	Rep. Mult	25,26,27,41,49,139,140,141,142,143,144,162,163,164,165,167,171,186,188,189,
<input type="radio"/>	2	0.12	6	3sndB	PEPTIDE	Rep. Mult	139,140,141,142,143,144,162,163,164,165,186
<input type="radio"/>	3	0.06	3	1q2w0	PEPTIDE	Rep. Mult	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	2bvsH	PEPTIDE	Rep. Mult	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 BiLoP 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.

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Enzyme Commission (EC) numbers and active sites



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

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

(a) Cscore^{EC} is the confidence score for the EC number prediction. Cscore^{EC} 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^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 residues divided by length of the query protein.

Spin On/Off

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	0.82	0.9678	1.04	0.94	0.99	2yy4A	GO:0003824 GO:0019082
2	0.52	0.9456	1.49	0.41	0.98	2zu2B	GO:0003824 GO:0019082
3	0.51	0.9097	1.91	0.45	0.98	1lvoD	GO:0003824 GO:0019082
4	0.47	0.9043	1.90	0.41	0.97	2q6dB	GO:0003824 GO:0019082
5	0.45	0.9270	1.65	0.48	0.98	3d23B	GO:0003824 GO:0019082
6	0.25	0.4621	3.52	0.09	0.55	3mimgA	GO:0003824 GO:0006508 GO:0008234
7	0.25	0.4693	3.32	0.12	0.56	1mbmA	GO:0003824 GO:0004252 GO:0016032 GO:0019082
8	0.25	0.4608	3.42	0.09	0.55	3govB	GO:0003824 GO:0004252 GO:0006508
9	0.24	0.4639	3.68	0.14	0.56	1lvmA	GO:0003824 GO:0006508 GO:0008234
10	0.24	0.4477	3.33	0.08	0.53	2pxub	GO:0003824 GO:0004252 GO:0005509 GO:0006508 GO:0007596

Consensus prediction of GO terms

Molecular Function	GO:0003824
GO-Score	0.99
Biological Process	GO:0019082
GO-Score	0.99
Cellular Component	None was predicted

(a) Cscore^{GO} is a combined measure for evaluating global and local similarity between query and template protein. Its 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^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 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^{GO} 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.