

- Here are the Top 10 threading templates. Based on the sequence identity, coverage, and Normalized Z-score, is thymidylate synthase from W.g.b. an easy or hard target?
- The sequence identity is not very high but in a reasonable range for homology modeling. The coverage is very high and Normalized Z-score is also high, so this not a hard target for I-TASSER.

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 detecting 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 results, the significance of which are assessed by the Z-score, i.e. the difference between the score and coverage 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, where the ranking programs are sorted by the average performance in the large-scale benchmark test experiments.)

Rank	PDB Hit	Iden1	Iden2	Cov	Norm. Z-score	Download Align.
1	3qj7A	0.56	0.58	0.98	4.34	Download
2	1jcn2	0.62	0.62	1.00	5.42	Download
3	3qj7A	0.56	0.58	0.98	5.67	Download
4	1jcn2	0.51	0.52	1.00	2.98	Download
5	1jcn2	0.51	0.52	1.00	1.67	Download
6	3qj7A	0.56	0.58	0.98	0.57	Download
7	1jcn2	0.51	0.52	1.00	2.51	Download
8	6y38A	0.44	0.45	1.00	6.47	Download
9	3qj7A	0.56	0.58	0.98	0.54	Download
10	1jcn2	0.43	0.46	1.00	12.11	Download

(a) All the residues are colored in black; however, those residues in template which are identical to the residue in the query sequence are highlighted in color. Coloring scheme is based on the property of amino acids, where polar are brightly colored while non polar or residues are colored in dark shade. ([more about the colors used](#))

(b) Rank of template represents the top 10 best threading templates used by I-TASSER.

(c) iden1 is the percentage sequence identity of the templates in the threading aligned region with the query sequence.

(d) iden2 is the percentage sequence identity of the whole template chains with the query sequence.

(e) Cov represents the coverage of the threading alignment and is equal to the number of aligned residues divided by the length of query protein.

(f) Norm. Z-score is the normalized Z-score of the threading alignments. Alignment with a Normalized Z-score >1 means a good alignment and vice versa.

(g) Download Align. provides the 3D structure of the aligned regions of the threading templates.

(h) The top 10 alignments reported above (in order of their ranking) are from the following threading programs:

1: MUSTER 2: PFAS-SC 3: SPARKS-X 4: HHSEARCH2 5: HHSEARCH1 6: NCIPFAS 7: HHSEARCH 8: pGenTHREADER 9: PROSPECT2 10: PRO

Top 10 threading templates used by I-TASSER

(1-TASSER modeling starts from the structure templates identified by LOMETS from the PDB library. LOMETS is a meta-server threading approach containing multiple 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 sorted by the average performance in the large-scale benchmark test experiments.)

Rank	PDB Hit	Ident1	Ident2	Cov	Norm. Z-score	Download Align.
						<div style="text-align: center;"> </div>
						Sec.Str Seq
1	3qj7A	0.56	0.55	0.98	4.34	Download
2	1an5A	0.62	0.62	1.00	5.42	Download
3	3qj7A	0.56	0.55	0.98	5.67	Download
4	1vza	0.51	0.52	1.00	2.28	Download
5	1vza	0.51	0.52	1.00	1.67	Download
6	3qj7A	0.56	0.55	0.98	5.07	Download
7	1vza	0.51	0.52	1.00	2.51	Download
8	6pf8A	0.44	0.45	1.00	6.47	Download
9	3qj7A	0.56	0.55	0.98	5.04	Download
10	1qzfA	0.43	0.45	1.00	12.11	Download

(a) All the residues are colored in black; however, those residues in template which are identical to the residue in the query sequence are highlighted in color. Coloring scheme is based on the property of amino acids, where polar are brightly coloured while non-polar residues are colored in dark shade. ([more about the colors used](#))

(b) Rank of templates represents the top ten threading templates used by I-TASSER.

(c) Ident1 is the percentage sequence identity of the templates in the threading aligned region with the query sequence.

(d) Ident2 is the percentage sequence identity of the whole template chains with query sequence.

(e) Cov represents the coverage of the threading alignment and is equal to the number of aligned residues divided by the length of query protein.

(f) Norm. Z-score is the normalized Z-score of the threading alignments. Alignment with a Normalized Z-score >1 mean a good alignment and vice versa.

(g) Download Align. provides the 3D structure of the aligned regions of the threading templates.

(h) The top 10 alignments reported above (in order of their ranking) are from the following threading programs:

1: MUSTER 2: FFAS-3D 3: SPARKS-X 4: HHSEARCH2 5: HHSEARCH I 6: Neff-PPAS 7: HHSEARCH 8: pGenTHREADER 9: PROSPECT2 10: PRC

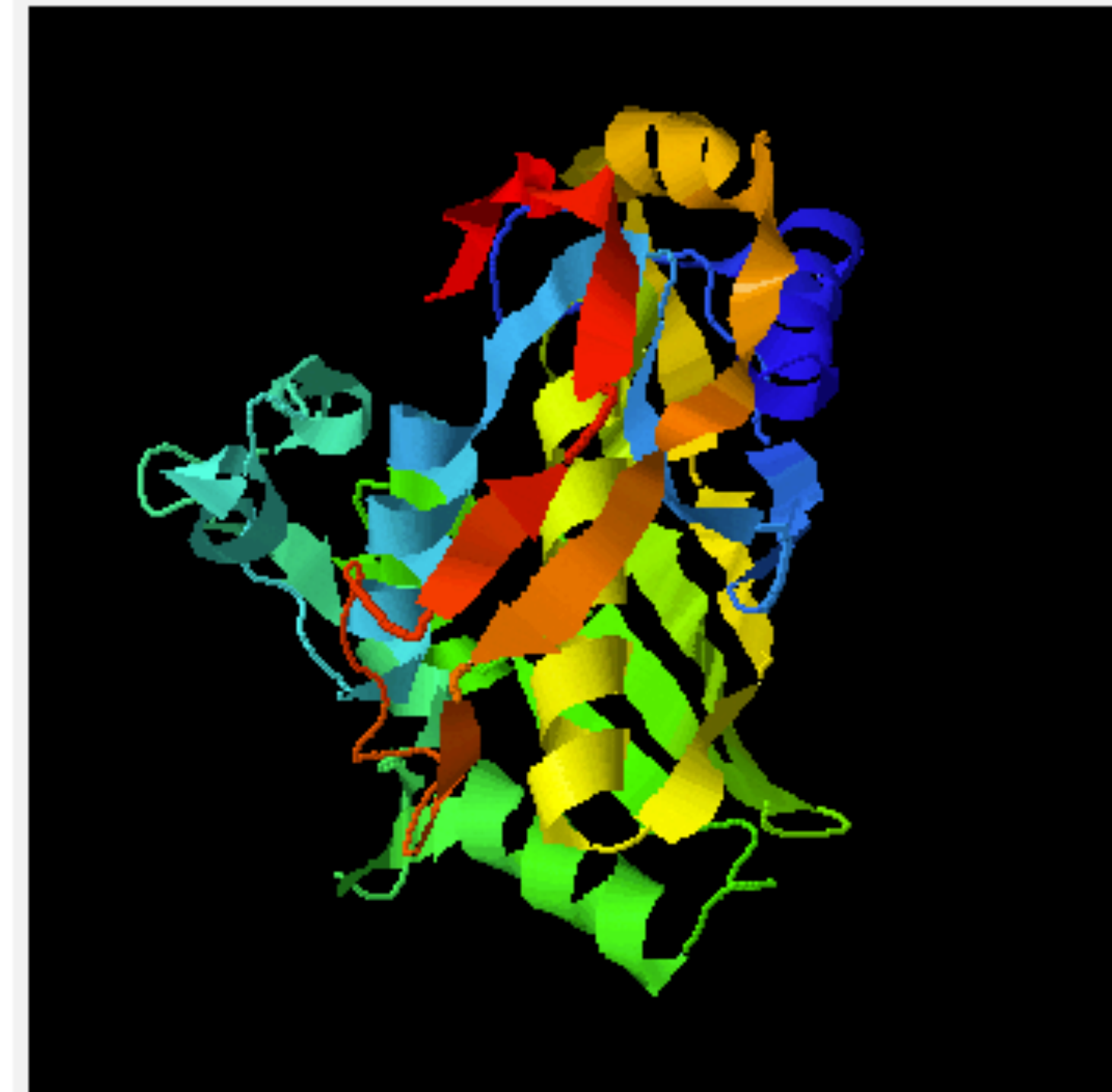
- The confidence of each model is quantitatively measured by C-score that is calculated based on the significance of threading template alignments and the convergence parameters of the structure assembly simulations. C-score is typically in the range of $[-5, 2]$, where a C-score of a higher value signifies a model with a higher confidence and vice-versa. TM-score and RMSD are estimated based on C-score and protein length...
- Is I-TASSER confident about its final model?

Top 5 final models predicted by I-TASSER

(For each target, I-TASSER simulations generate a large ensemble of structural models 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 rank models as seen in our benchmark tests. If the I-TASSER simulations converge, the top 5 models are shown below.)

- [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 orientation)



☐ Spin On/Off

- [Download Model 1](#)
- C-score=1.91 ([Read more about C-score](#))
- Estimated TM-score = 0.99 ± 0.04
- Estimated RMSD = $2.2 \pm 1.7 \text{ \AA}$