

## Supplementary material

## Supplementary Figure S1

[illegible]

Supplementary Figure S2.

### Top 5 final models from C-I-TASSER

Click to view	Rank <sup>a</sup>	Download	C-score <sup>b</sup>	Estimated TM-score <sup>c</sup>	Estimated RMSD <sup>c</sup>
	1	<a href="#">model1.pdb.gz</a>	1.59	0.94±0.05	3.2±2.3Å
	2	<a href="#">model2.pdb.gz</a>	-3.52		
	3	<a href="#">model3.pdb.gz</a>	-4.10		
	4	<a href="#">model4.pdb.gz</a>	-4.99		
	5	<a href="#">model5.pdb.gz</a>	-4.99		

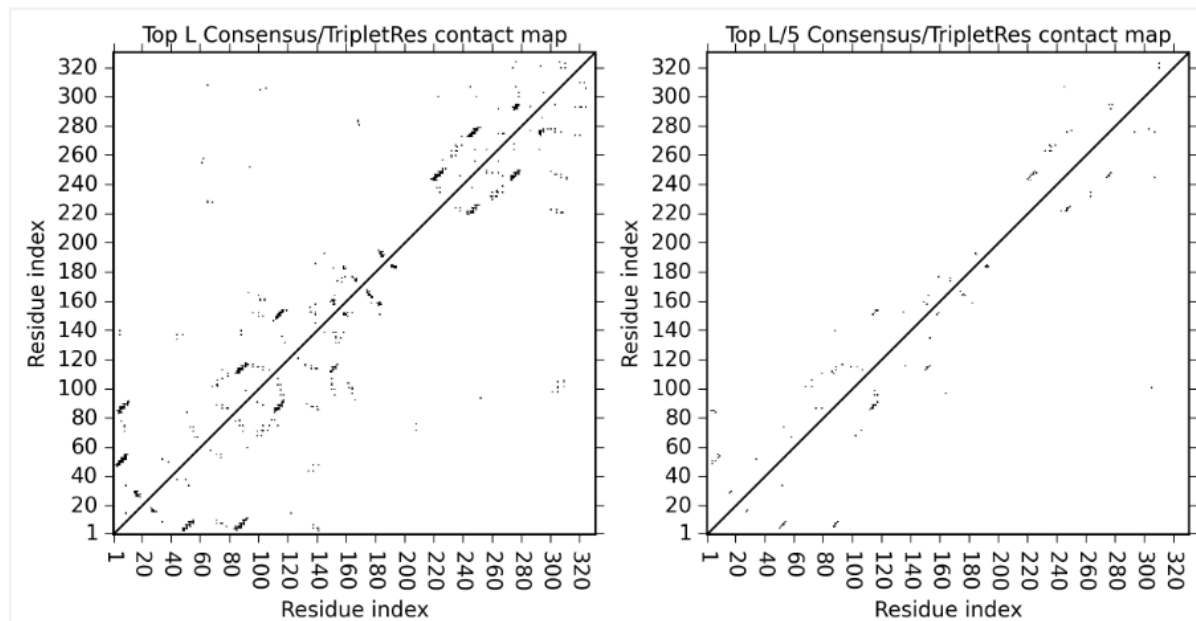
(a) C-I-TASSER simulations generate a large ensemble of structural conformations, i.e. decoys. These decoys are clustered by [SPICKER](#) based on pairwise structure similarity to report up to five final models from the five largest clusters. Models are ranked in descending order of cluster size. If the simulations converge well, it is possible to have less than 5 models generated, which is usually an indication of good model quality.

(b) The model confidence is quantified by C-score, calculated based on significance of threading template alignments, convergence of C-I-TASSER simulations and contact map satisfaction rate. C-score is typically in the range of [-5, 2], with higher C-score signifies higher model confidence.

(c) Model [TM-score](#) and RMSD are estimated based on C-score and protein length for the first model.

Supplementary Figure S3.

Predicted contact map used in C-I-TASSER simulation



C-I-TASSER simulation is guided by consensus contact map (upper left triangle) derived based on confidence scores of [TripletRes](#) (lower right triangle), [ResTriplet](#), [ResPRE](#), and [NeBcon](#). In the contact map, the axes mark the residue indexes along the sequence, while each dot represents a residue pair with predicted contact. No dot is close to the diagonal, because C-I-TASSER does not consider contacts for residue pairs separated by <6 residues.

Supplementary Figure S4.

Ran	PDB	hit	ID	ID	2	Cov	Norm. Zscore	Download alignment	
1	7p9	0.4	0.3	11.					
	CA	0	8	34			3.94	SPARKS-F	
2	1hf	0.4	0.4	13.					
	6	5	17				4.00	EFAS-3D	
3	2jk	0.4	0.4	13.			12.4	5 Hhpred	
	7	6	41				5		
4	2jk	0.4	0.4	13.					
	7	6	42				2.97	MUSTER	
5	514	0.4	0.4	13.					
	6	5	09				4.04	CNFpred	
6	2jk	0.4	0.4	13.					
	7	6	41				1.54	Hsaearc h-2	
7	2jk	0.4	0.4	13.					
	7	6	42				3.70	Heff- PFAS	
8	2jk	0.4	0.4	13.					
	6	5	17				2.46	Hsaearc h	
9	7p9	0.4	0.3	11.					
	CA	1	9	42			3.00	PROSPEC TOR2	
10	2d6	0.2	0.2	7.0					
	FA	4	3	9			4.44	SAM	