Supplementary materials for the following manuscript:

Sheng Wang, Zhen Li, Yizhou Yu and Jinbo Xu. Folding membrane proteins by deep transfer learning.

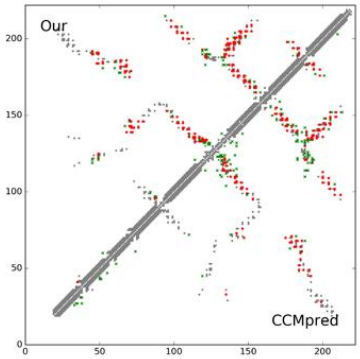
Table S1. A list of 510 non-redundant membrane proteins with solved structures in PDB, related to *Table 1 and STAR Methods section "Data for model parameter optimization and test"*.

1a0sP	1pw4A	2evuA	2lnlA	2wpvB	3cn5A	3kvnA	3udcA	4chvA	4il3A	4or2A	4wgvA	5c8jI
1ar1B	1q16C	2f1cX	2lomA	2wsc1	3cx5C	3l1lA	3ug9A	4cskA	4in5H	4p6vB	4wmzA	5cfbA
1bccE	1q90A	2f93B	2loqA	2wsc3	3d31C	3lnmB	3ukmA	4czbA	4in5L	4p6vC	4x5mA	5ctgA
1bctA	1q90B	2f95B	2lorA	2wscF	3ddlA	3lw54	3um7A	4d5bA	4j05A	4p6vD	4xk83	5d0yA
1bhaA	1qcrD	2fynB	2losA	2wscG	3dhwA	3lw5H	3uq7A	4d6tD	4j72A	4p6vE	4xnkA	5dirA
1c17M	1qd6C	2ge4A	2lotA	2wscH	3dinE	3m71A	3ux4A	4d6tG	4j7cI	4p6vF	4xnvA	5doqA
1e7pC	1qleC	2gfpA	2lp1A	2wscK	3dl8C	3mk7A	3v2wA	4d6tJ	4jkvA	4p79A	4xu4A	5doqB
1ehkB	1rh5B	2gr7A	2m0qA	2wscL	3dl8E	3mk7B	3v5sA	4d6uD	4k1cA	4pgrA	4xxjA	5ee7A
1fftB	1rh5C	2gr8A	2m20A	2wswA	3dwoX	3mk7C	3vmqA	4djiA	4kjrA	4phzA	4xydB	5ek0A
1fftC	1rwtA	2h8aA	2m67A	2wwbB	3dwwA	3mktA	3vouA	4dojA	4knfA	4pirA	4y25A	5ekeA
1fw2A	1s5lB	2h8pC	2m6bA	2wwbC	3dzmA	3mp7A	3vr8C	4dveA	4kppA	4px7A	4y28G	5eulE
1fx8A	1s5lE	2hdfA	2m7gA	2x4mA	3effK	3mp7B	3vr8D	4dxwA	4kt0F	4q2eA	4y28K	5ezmA
1gzmA	1s5lX	2ibzG	2m8rA	2xq2A	3eh3A	3njtA	3vwiA	4e1tA	4kt0K	4qncA	4y28L	5f1cA
1h2sB	1sqqK	2ibzI	2mafA	2xutA	3ejzA	3nymA	3wdoA	4ea3A	4ky0A	4qndA	4y7jA	5fn2B
1h6s1	1t16A	2iubA	2mfrA	2y5yA	3emnX	3o0rB	3wmfA	4ezcA	4l6rA	4qtnA	4ymkA	5gaeh
1izlA	1tlwA	2j58A	2mgyA	2y69D	3emoA	3o7pA	3wmm1	4f35A	4l6v6	4quvA	4ymsC	5gaqA
1izlC	1tqqA	2j7aC	2mm8A	2y69G	3fhhA	3ohnA	3wmmM	4f4lA	4l6v8	4r1iA	4ytpC	5garO
1jb0K	1uunA	2jafA	2mmuA	2y69I	3fidA	3orgA	3wo7A	4fqeA	4ltoA	4rdqA	4ytpD	5hk1A
1k24A	1uynX	2jlnA	2mn6A	2y69J	3g67A	3oufA	3wvfA	4fuvA	4m58A	4rfsS	4z34A	5i1mV
1kf6C	1vclA	2jo1A	2mpnA	2y69K	3gi8C	3p5nA	3wxvA	4g1uA	4m64A	4ri2A	4z3nA	5i20A
1kf6D	1vf5B	2jp3A	2mxbA	2y69L	3hd6A	3pjsK	3x29A	4g7vS	4mbsA	4rjwA	4z7fA	5i32A
1kqfB	1vf5D	2k0lA	2n4xA	2y69M	3hw9A	3pjzA	3x2rA	4g80I	4meeA	4rl8A	4zp0A	5i6cA
1kqfC	1wrgA	2k21A	2n6lA	2yevB	3iyzA	3pwhA	3x3bA	4gbyA	4mndA	4rl9A	4zr0A	5i6zA
1kzuA	1xioA	2k73A	2n7qA	2yevC	3iz1A	3q7kA	3ze3A	4gd3A	4mqsA	4rlcA	4zr1A	5id3A
1lghA	1xl4A	2k9pA	2nmrA	2yiuA	3j08A	3qe7A	3zevA	4gx5A	4mt4A	4rngA	4zw9A	5iofA
1m56B	1yc9A	2kluA	2nq2A	2ynkA	3j1zP	3qnqA	3zjzA	4gycB	4n74A	4rp8A	5a1sA	5irxA
1m56D	1yewC	2kogA	2nr9A	2z73A	3j9tR	3qraA	3zk1A	4h33A	4n75A	4ryiA	5a40A	5ivaA
1m57A	1yq3C	2ks9A	2nrgA	2ziyA	3jbrE	3rbzA	3zuxA	4he8A	4njnA	4s0vA	5a63C	5iwsA
1mm4A	1yq3D	2ksdA	2o01F	2zjsE	3jcuD	3rgwS	4a2nB	4he8C	4nppA	4tkrA	5a63D	5ixmB
1mprA	1zrtE	2kseA	2oarA	2zxeB	3jcuH	3rkoA	4atvA	4he8D	4ntjA	4tq3A	5a6eB	5jagA
1n7lA	1zzaA	2ksfA	2pnoA	2zxeG	3jcuK	3rkoB	4aw6A	4hkrA	4nykA	4tquM	5abbZ	
1nekC	2a0lA	2ksrA	2q67A	3a2sX	3jcuR	3rkoC	4b4aA	4hqjE	4o6mA	4tquN	5araT	
1nekD	2a9hA	2kyhA	2q7mA	3a7kA	3jcuS	3rkoD	4bemJ	4httA	4o6yA	4twkA	5araW	
1o5wA	2akhA	2l35A	2qomA	3anzA	3jcuW	3rkoF	4bgnA	4huqS	4o9pA	4u15A	5awwG	
1occD	2akhB	2l8sA	2r6gF	3b4rA	3jcuX	3rkoG	4bog3	4huqT	4o9pB	4u4tA	5awwY	
1oedC	2bg9A	2lckA	2r6gG	3b5dA	3jcuZ	3s0xA	4bpmA	4hw9A	4o9uB	4u9lA	5awzA	
1orsC	2bl2A	2lhfA	2vpwC	3b9wA	3jycA	3sljA	4bwzA	4hycA	4od4A	4uc1A	5aymA	
1p49A	2cpbA	2lkgA	2w1pA	3bryA	3k3fA	3sybA	4c9jA	4hyoA	4ogqC	4us3A	5azbA	
1p4tA	2d57A	2llyA	2wjqA	3chxB	3kj6A	3tijA	4cadC	4hzuS	4oh3A	4v1fA	5bwkE	
1p7bA	2ervA	2lmeA	2wpdJ	3chxC	3kp9A	3tx3A	4cfgA	4iffA	4oo9A	4wd7A	5c6oA	

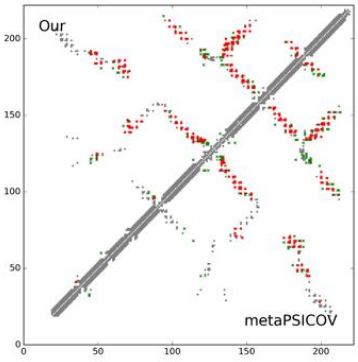
Figure S1. Case study of one CAMEO target 5jkiA, related to section "*Blind test in CAMEO" and Figure 4*. (A) The long- and medium-range contact prediction accuracy of our methods, MetaPSICOV, CCMpred, and EVfold (Web Server). (B-D) The overlap between top L predicted all-range contacts and the native contact map. A grey, red and green dot represents a native contact, a correct prediction and a wrong prediction, respectively. (E) The superimposition between our predicted model (in red) and the native structure (in green).

	Long range accuracy				Medium range accuracy			
	L	L/2	L/5	L/10	L	L/2	L/5	L/10
Our method	0.658	0.883	1.000	1.000	0.185	0.351	0.659	0.864
MetaPSICOV	0.554	0.820	0.977	1.000	0.158	0.279	0.523	0.727
CCMpred	0.495	0.703	0.773	0.818	0.131	0.207	0.477	0.682
EVfold(web)	0.514	0.712	0.773	0.841	0.126	0.207	0.432	0.727

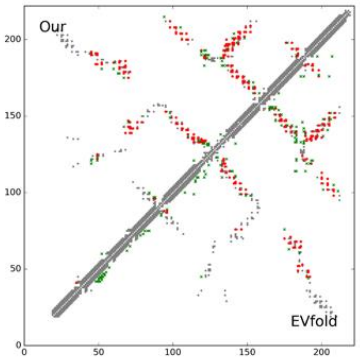
(A)



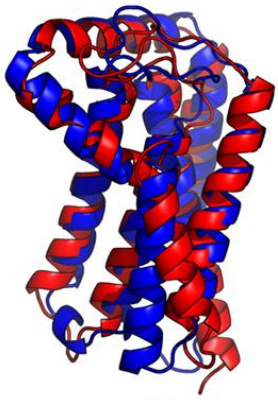
(B)



(C)



(D)

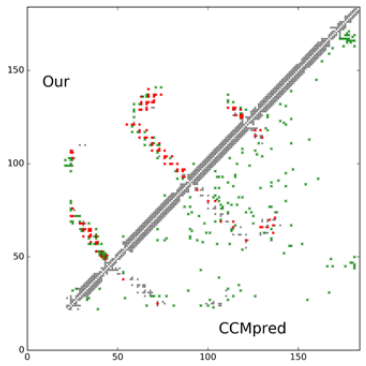


(E)

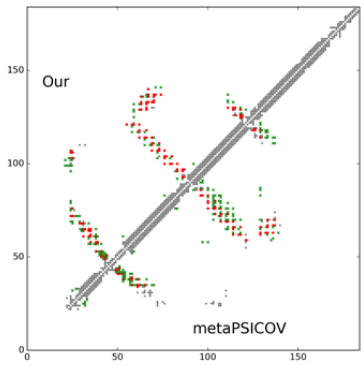
Figure S2. Case study of one CAMEO target 5l0wA, related to section "*Blind test in CAMEO" and Figure 4*. (A) The long- and medium-range contact prediction accuracy of our methods, MetaPSICOV and CCMpred. (B-C) The overlap between top L predicted all-range contacts and the native contact map. A grey, red and green dot represents a native contact, a correct prediction and a wrong prediction, respectively. (D) The superimposition between our predicted model (in red) and the native structure (in green).

	Long range accuracy				Medium range accuracy			
	L	L/2	L/5	L/10	L	L/2	L/5	L/10
Our method	0.397	0.674	0.889	1.000	0.103	0.207	0.444	0.778
metaPSICOV	0.250	0.391	0.528	0.722	0.098	0.163	0.278	0.389
CCMpred	0.087	0.109	0.222	0.333	0.016	0.033	0.056	0.056

(A)



(B)



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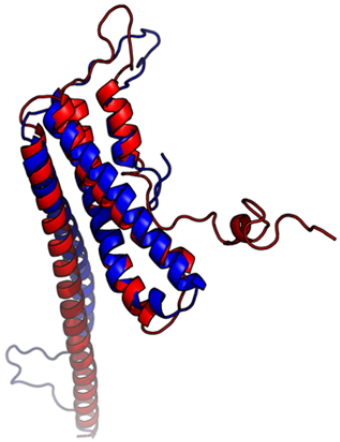

(D)

Supplementary Figure 3. Top 20 long-range 5x5 contact occurrence patterns, related to section "*Why does deep transfer learning work?" and STAR method*.

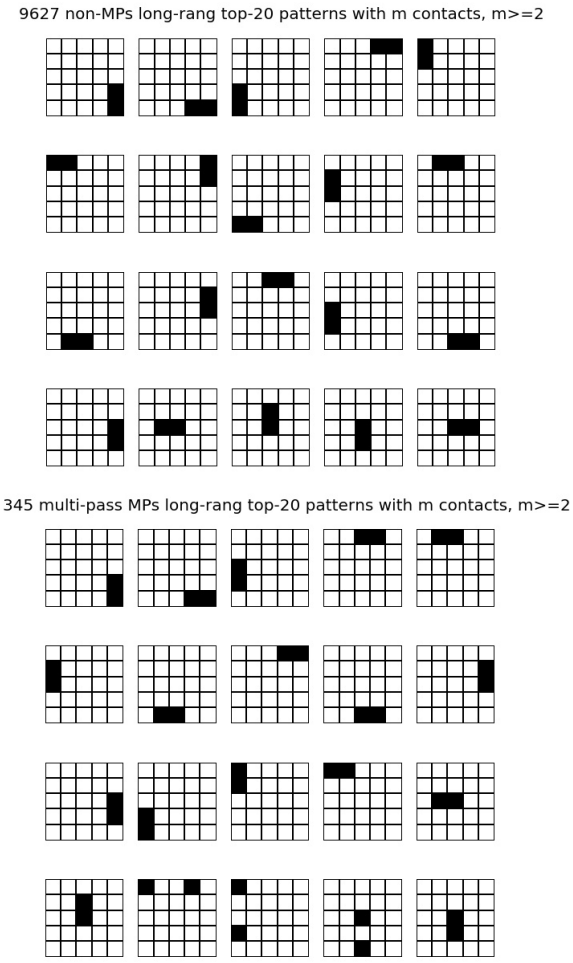

Table S2. Contact prediction accuracy on the 87 COMSAT test proteins, *related to STAR Method and Table 1*. Only contacts between two transmembrane segments are evaluated. Acc, Cov, Sp and Mcc represent accuracy, coverage, specificity and Mathew correlation coefficient, respectively. Note that here our result is based upon the deep model trained without using any membrane proteins while COMSAT was trained by some membrane proteins. The result of COMSAT is taken from its paper. Following the COMSAT paper, the results of the latter three methods are calculated on top L_m predicted contacts where L_m is the length of transmembrane regions in a test protein.

Accuracy of top L_m predicted contacts when a contact is defined by C_α-C_α distance less than14Å.												
Method	**>=6**				**>=12**				**>=24**			
	Acc	**Cov**	**Sp**	**Mcc**	**Acc**	**Cov**	**Sp**	**Mcc**	**Acc**	**Cov**	**Sp**	**Mcc**
CCMpred	0.63	0.07	0.98	0.15	0.61	0.07	0.98	0.15	0.57	0.08	0.97	0.14
MetaPSICOV	0.73	0.08	0.99	0.19	0.72	0.08	0.99	0.19	0.69	0.10	0.98	0.19
Our Method	0.86	0.10	0.99	0.23	0.85	0.10	0.99	0.23	0.82	0.12	0.98	0.24
COMSAT	0.65	0.05	0.99	0.11	0.63	0.054	0.99	0.11	0.61	0.052	0.99	0.10
Accuracy of top L_m predicted contacts when a contact is defined by C_β-C_β distance less than 8Å.												
Method	**>=6**				**>=12**				**>=24**			
	Acc	**Cov**	**Sp**	**Mcc**	**Acc**	**Cov**	**Sp**	**Mcc**	**Acc**	**Cov**	**Sp**	**Mcc**
CCMpred	0.32	0.25	0.98	0.26	0.31	0.26	0.97	0.26	0.29	0.27	0.96	0.25
MetaPSICOV	0.39	0.31	0.98	0.32	0.38	0.31	0.98	0.32	0.35	0.33	0.96	0.31
Our Method	0.59	0.46	0.98	0.48	0.58	0.46	0.98	0.48	0.53	0.49	0.97	0.47
COMSAT	0.43	0.14	0.99	0.21	0.43	0.14	0.99	0.21	0.44	0.14	0.98	0.21