

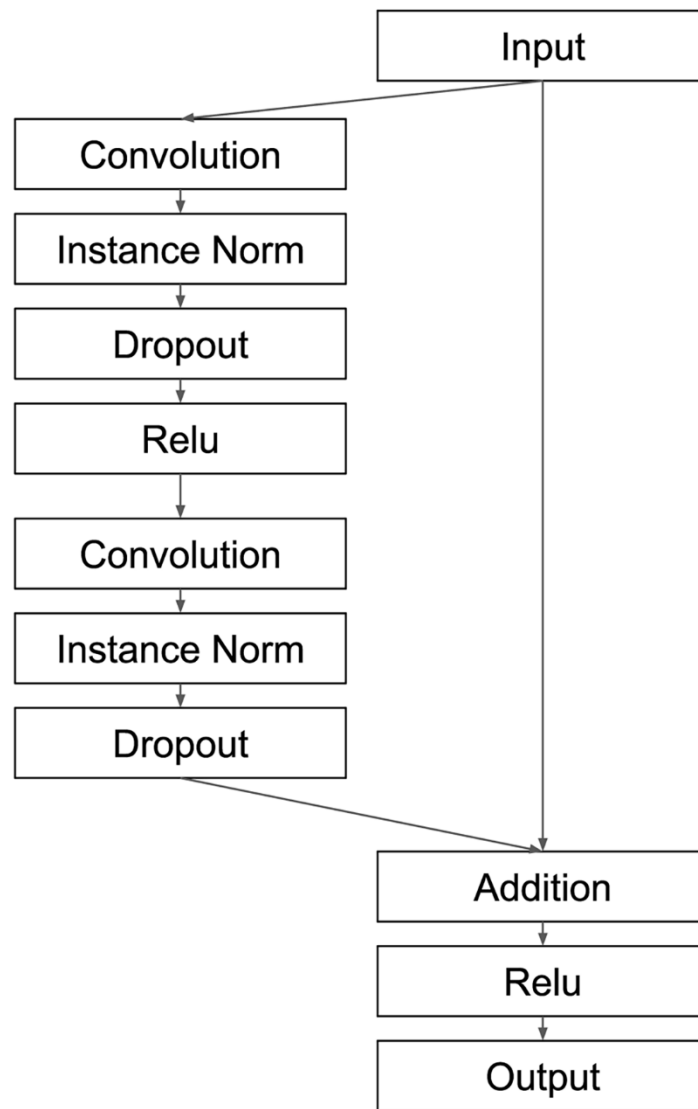
## Supporting Information

### Supporting Texts

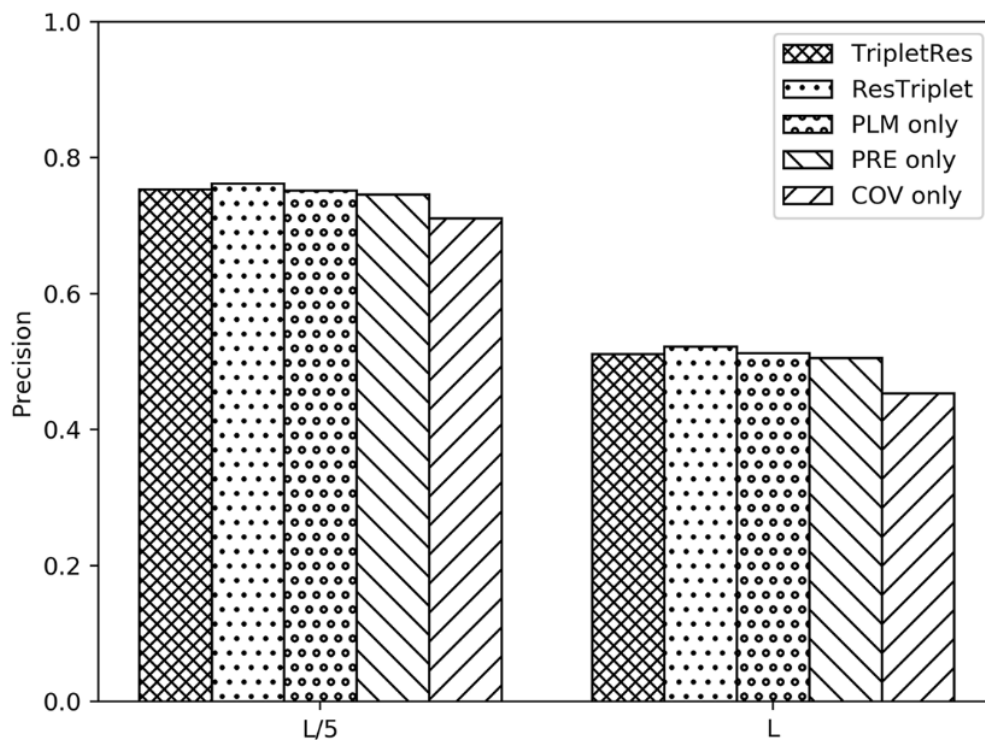
#### **Text S1. The training sets of TripletRes and ResTriplet.**

TripletRes and ResTriplet were trained on a subset of domain sequences from the SCOPe 2.07 database<sup>1</sup>, which was collected using following filters: (1) Sequence length should be in the range of 30-400; (2) Resolution of the corresponding PDB structure should be better than 2.0 Å; (3) Maximum pairwise sequence identity is set to 30%. These resulted in 7,671 non-redundant domains that are used for training our pipelines.

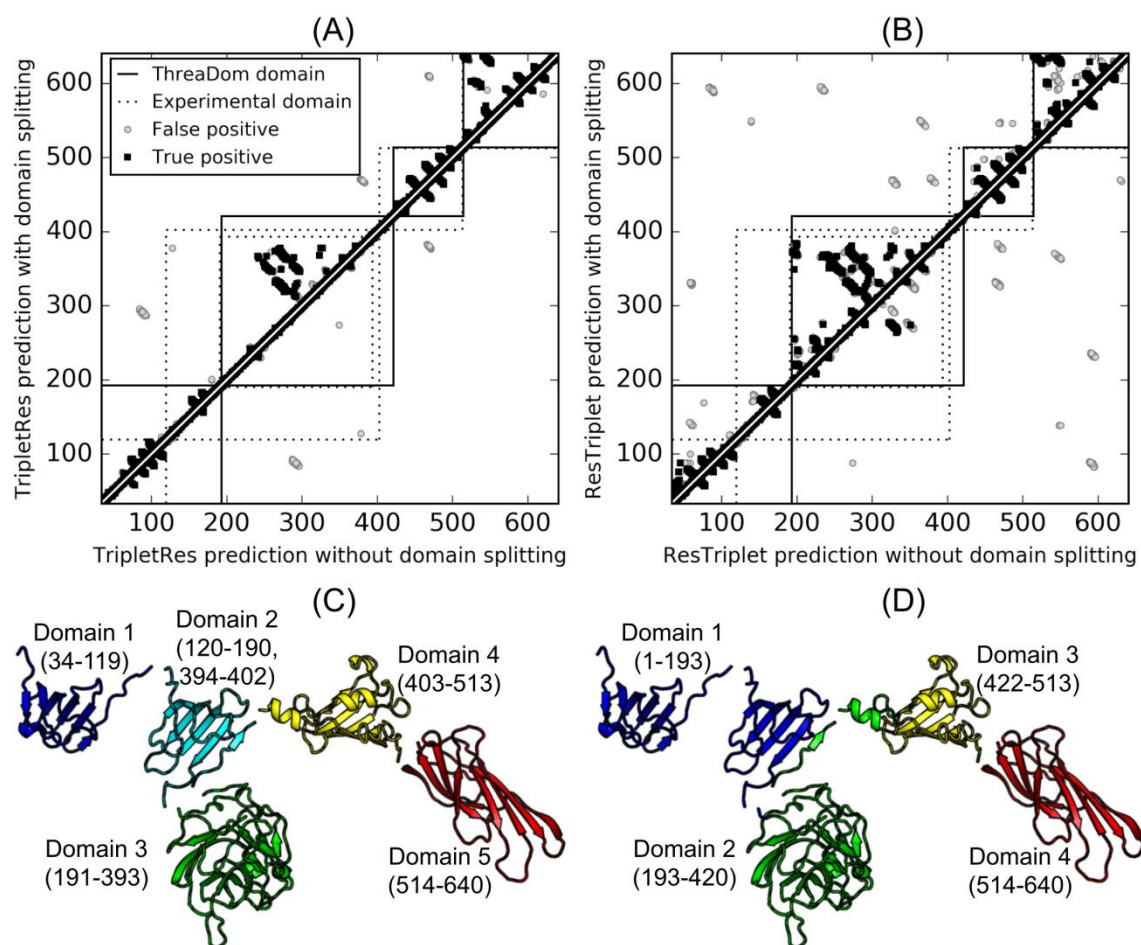
## Supporting Figures



**Figure S1.** The architecture of a basic residual block.



**Figure S2.** Mean precisions of long-range top L and top L/5 contacts of TripletRes and ResTriplet on all CASP13 targets, compared to the predictors trained on the component features from the covariance matrix feature (COV), the precision matrix feature (PRE) and the coupling matrix of the inverse Potts model feature (PLM).



**Figure S3.** Domain partitioning and contact prediction results for T0981 in CASP13. **(A)** Contact prediction by TripletRes with domain partitioning versus those without domain partitioning. Grey and black dots are false and true positive predictions respectively, and solid and dotted lines mark the domain boundaries by ThreaDom and experimental assignments, respectively. **(B)** Same as **(A)** but for ResTriplet. **(C)** Domain partitioning from experimental structure. **(D)** Domain partitioning by ThreaDom prediction.

## Supporting Tables

**Table SI.** Summary of contact-map predictions by ResTriplet and TripletRes on all 122 domains in CASP13.

Method	Target	Type*	Nf	Short			Medium			Long		
				L	L/2	L/5	L	L/2	L/5	L	L/2	L/5
ResTriplet	T0949-D1	FM/TBM	282.0	0.2014	0.3188	0.5926	0.3525	0.5797	0.9630	0.8705	1.0000	1.0000
	T0950-D1	FM	10.2	0.0585	0.0760	0.1765	0.1140	0.1988	0.4559	0.5088	0.7427	0.9412
	T0951-D1	TBM-easy	2104.7	0.3008	0.5038	0.7925	0.2556	0.4887	0.8679	0.8835	0.9624	1.0000
	T0953s1-D1	FM	17.6	0.6418	0.9394	1.0000	0.2985	0.5758	0.9231	0.0000	0.0000	0.0000
	T0953s2-D1	FM/TBM	102.6	0.0909	0.0000	0.0000	0.1136	0.1818	0.2500	0.2500	0.4091	0.5000
	T0953s2-D2	FM	64.6	0.1029	0.1961	0.4250	0.2108	0.3922	0.5500	0.7745	0.8725	0.9750
	T0953s2-D3	FM	70.6	0.6364	0.7895	0.9333	0.5455	0.6579	0.6667	0.6623	0.8421	0.8667
	T0954-D1	TBM-hard	1678.7	0.5322	0.7953	0.8824	0.6696	0.7895	0.8529	0.3743	0.5088	0.5441
	T0955-D1	FM/TBM	0.2	0.5610	0.9000	0.8750	0.5610	0.8000	1.0000	0.0976	0.2000	0.2500
	T0957s1-D1	FM	6.7	0.3148	0.6049	1.0000	0.3333	0.5926	0.9062	0.3025	0.4198	0.5938
	T0957s1-D2	TBM-hard	9.4	0.1296	0.2222	0.3000	0.1296	0.2593	0.7000	0.5185	0.7778	1.0000
	T0957s2-D1	FM	4.7	0.2129	0.3636	0.5484	0.2452	0.4545	0.6774	0.3419	0.4805	0.6129
	T0958-D1	FM/TBM	2.9	0.1948	0.3947	0.7333	0.2727	0.4474	0.6000	0.3636	0.3947	0.5333
	T0959-D1	TBM-hard	418.7	0.2116	0.3511	0.6757	0.3228	0.4894	0.6757	0.5714	0.7553	0.8108
	T0960-D1	NE	6.9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	T0960-D2	FM	4.3	0.2976	0.4048	0.6875	0.4286	0.5714	0.9375	0.0595	0.0714	0.1250
	T0960-D3	TBM-hard	4.1	0.3708	0.6818	1.0000	0.6292	0.8636	1.0000	0.2472	0.3864	0.7059
	T0960-D4	NE	4.9	0.1094	0.1562	0.3333	0.0156	0.0312	0.0833	0.0000	0.0000	0.0000
	T0960-D5	TBM-easy	7.6	0.3333	0.4423	0.7143	0.4000	0.5192	0.6667	0.8381	0.8846	0.9524
	T0961-D1	TBM-easy	514.1	0.2624	0.4622	0.7200	0.2803	0.5259	0.9100	0.8072	0.9124	0.9900
	T0962-D1	TBM-easy	225.1	0.4463	0.6477	0.9429	0.3785	0.5795	0.8286	0.6102	0.8864	0.9143
	T0963-D1	NE	38.1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	T0963-D2	FM	23.4	0.4268	0.7317	0.9375	0.7683	0.9024	0.9375	0.1098	0.1951	0.3125
	T0963-D3	TBM-hard	22.0	0.3978	0.7174	1.0000	0.6882	0.8261	1.0000	0.2581	0.4348	0.7778
	T0963-D4	NE	244.6	0.2656	0.3125	0.4167	0.0469	0.0625	0.0000	0.0000	0.0000	0.0000
	T0963-D5	TBM-easy	201.8	0.2872	0.4894	0.5556	0.2660	0.3830	0.5556	0.7128	0.7872	0.8889
	T0964-D1	TBM-hard	56.6	0.5474	0.8511	1.0000	0.4421	0.7021	0.9474	0.8632	0.9787	0.9474
	T0965-D1	TBM-hard	2469.8	0.2236	0.4231	0.7258	0.3003	0.5513	0.9032	0.8594	0.9231	1.0000
	T0966-D1	TBM-hard	2.0	0.2398	0.4350	0.7755	0.2439	0.4431	0.8061	0.6362	0.8049	0.9388
	T0967-D1	TBM-easy	851.5	0.2405	0.4615	0.8667	0.5190	0.9231	1.0000	0.7215	0.8205	1.0000
	T0968s1-D1	FM	16.0	0.3644	0.6610	0.9565	0.5339	0.8814	1.0000	0.2881	0.3559	0.3913
	T0968s2-D1	FM	33.0	0.6435	0.9298	1.0000	0.7304	0.8070	0.9565	0.2957	0.3333	0.4783
	T0969-D1	FM	87.3	0.2090	0.3503	0.5286	0.2655	0.4407	0.7143	0.7401	0.8701	0.9571
	T0970-D1	FM/TBM	12.9	0.2990	0.4583	0.6316	0.4433	0.6667	0.8947	0.5876	0.8333	0.8947
	T0971-D1	TBM-easy	1280.0	0.4231	0.7231	0.9615	0.7231	0.9846	1.0000	0.7000	0.9538	1.0000
	T0973-D1	TBM-easy	40.7	0.2740	0.5342	0.8621	0.6164	0.8904	1.0000	0.4041	0.6301	0.9655
	T0974s1-D1	TBM-easy	4576.9	0.3043	0.5882	1.0000	0.1594	0.2647	0.6154	0.3768	0.6176	0.8462
	T0974s2-D1	NE	4174.0	0.3500	0.6000	0.8125	0.2375	0.4250	0.8125	0.3750	0.5750	0.8125
	T0975-D1	FM	387.2	0.2150	0.3699	0.7759	0.2150	0.4041	0.7241	0.4539	0.5890	0.7241
	T0976-D1	TBM-easy	2060.0	0.1750	0.3500	0.6667	0.3750	0.7167	0.9583	0.8917	1.0000	1.0000
	T0976-D2	TBM-easy	424.9	0.1935	0.3871	0.7917	0.3790	0.6935	1.0000	0.8629	0.9839	1.0000
	T0977-D1	TBM-easy	24.5	0.5017	0.8533	0.9833	0.7442	0.9533	0.9667	0.4419	0.5800	0.7500
	T0977-D2	TBM-easy	2.3	0.3627	0.6078	0.9500	0.6912	0.9020	0.9750	0.2304	0.3529	0.6500
	T0978-D1	FM/TBM	183.2	0.1671	0.2427	0.3049	0.2228	0.3495	0.5732	0.4843	0.7039	0.8659
	T0979-D1	TBM-hard	631.8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	T0980s1-D1	FM	7.6	0.2952	0.5000	0.7619	0.3524	0.5000	0.7143	0.3619	0.5192	0.9048
	T0980s2-D1	NE	6.0	0.1290	0.2667	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
T0981-D1	TBM-hard	14.1	0.4884	0.6279	0.7647	0.6628	0.6279	0.9412	0.1395	0.2326	0.2941	
T0981-D2	FM	0.6	0.0989	0.1773	0.3929	0.2544	0.3475	0.6071	0.0636	0.0638	0.0714	
T0981-D3	FM/TBM	242.8	0.1823	0.2871	0.4500	0.3547	0.4851	0.6000	0.8177	0.9208	1.0000	
T0981-D4	TBM-hard	0.5	0.4054	0.5455	0.5909	0.5946	0.8545	1.0000	0.2523	0.4182	0.9091	
T0981-D5	TBM-hard	2.8	0.4016	0.6349	0.9200	0.5276	0.7619	0.9200	0.6693	0.8095	0.9600	
T0982-D1	TBM-easy	204.8	0.5111	0.7910	0.9630	0.6889	0.8806	0.9630	0.6815	0.8806	0.9630	









	T1022s1-D1	FM	436.0	0.2756	0.5128	0.7419	0.5064	0.8333	0.9677	0.6090	0.7692	0.8710
	T1022s1-D2	TBM-hard	486.3	0.1343	0.1515	0.3846	0.3582	0.6667	0.7692	0.5224	0.8485	0.8462
	T1022s2-D1	TBM-hard	132.5	0.3181	0.5725	0.8952	0.4514	0.7710	0.9619	0.6552	0.8626	0.9619
	Average			0.2894	0.4808	0.7073	0.3683	0.5597	0.7504	0.5115	0.6454	0.7538

\* Target type as defined by CASP13 assessors ([http://predictioncenter.org/casp13/domains\\_summary.cgi](http://predictioncenter.org/casp13/domains_summary.cgi)). NE stands for “not evaluated”. “FM/TBM”, “TBM-easy”, “TBM-hard” are all considered as TBM by this manuscript.

## Reference

1. Fox NK, Brenner SE, Chandonia J-M. SCOPe: Structural Classification of Proteins—extended, integrating SCOP and ASTRAL data and classification of new structures. *Nucleic acids research* 2013;42(D1):D304-D309.