Supplementary Table I

List of 624 PDB Chains used in the MetaPSICOV Training Set

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1atgA 1bgfA 1bx7A 1c5eA 1dbfA 1e4mM 1e5kA 1e7lA 1eaqA 1eb6A 1f86A 1f8eA 1fsgA 1g61A
1gk8I 1gk9A 1gqvA 1gu2A 1gveA 1gyxA 1h12A 1h4gA 1hbnB 1hbnC 1hyoA 1i27A 1jcdA 1ji7A
1jniA 1k5cA 1k5nA 1ka1A 1kkoA 1kmtA 1kqpA 1kv0A 1kyfA 1l9lA 1lc5A 1lniA 1lq9A 1lwbA
1lyvA 1m1qA 1m2dA 1m55A 1mkkA 1mn8A 1munA 1muwA 1mwqA 1mxrA 1n8vA 1nkdA 1nqjA 1nuyA
1nz0A 1o2dA 1o4yA 1o7qA 1oaiA 1odmA 1oh4A 1ox0A 1p4cA 1pbjA 1q5yA 1q7lA 1q7lB 1qh4A
1qqfA 1qtwA 1qw9A 1r29A 1r85A 1ra0A 1rkuA 1sauA 1sjwA 1svfA 1t2dA 1t6uA 1tt8A 1u07A
1u7iA 1ucrA 1ucsA 1ukuA 1uz3A 1v05A 1vlyA 1vmfA 1vp8A 1vr7A 1vykA 1w0nA 1w1hA 1w66A
1wc2A 1wcwA 1wdpA 1wluA 1wn2A 1wpnA 1wzdA 1x6iA 1x6zA 1xbiA 1xd3A 1xdnA 1xmkA 1xmtA
1xqoA 1xubA 1yfqA 1yiiA 1z0nA 1zgkA 1zzkA 256bA 2aebA 2aibA 2b0aA 2b3hA 2b82A 2b97A
2bcgG 2bkxA 2bmoA 2bmoB 2bt9A 2c0rA 2c1vA 2c2uA 2c4bA 2c60A 2carA 2cb8A 2ccvA 2cg7A
2ciwA 2ckkA 2covD 2cs7A 2dkoB 2dlbA 2ehzA 2endA 2erfA 2f22A 2fb6A 2fbaA 2fcjA 2fcwB
2fmaA 2fsqA 2g7sA 2gkeA 2gkpA 2glzA 2gqtA 2gsoA 2gudA 2h1vA 2h8eA 2halA 2hbaA 2hoxA
2hzcA 2i5vO 2ia7A 2iayA 2ic6A 2imsA 2ivyA 2j5yA 2j6bA 2j8bA 2jekA 2jliA 2lisA 2nlvA
2nr7A 2nszA 2nxvA 2o37A 2o90A 2odiA 2odkA 2ofzA 2oizA 2olmA 2ovgA 2ovjA 2oxgA 2oxgB
2p0nA 2p2sA 2p51A 2p8gA 2p8iA 2pieA 2pneA 2q52A 2qfaB 2qfeA 2qipA 2qjzA 2qngA 2qsbA
2qvkA 2r0xA 2r16A 2r2zA 2r31A 2r5oA 2r751 2ra9A 2rctA 2rdqA 2rffA 2rfrA 2rh2A 2uvoA
2ux9A 2v89A 2v8tA 2v9vA 2ve8A 2vfrA 2vlaA 2vn6B 2vwsA 2w3gA 2w5qA 2w7aA 2wbqA 2wcjA
2wdsA 2wl1A 2wlvA 2wnpF 2wq4A 2x3mA 2x4kA 2x5yA 2xfdA 2xioA 2xjpA 2xmjA 2xolA 2xomA
2xpwA 2xw6A 2y0oA 2y39A 2y5pA 2y6hA 2y9fA 2yh5A 2yhgA 2ylbA 2ylnA 2z4uA 2z5wA 2zexA
2znrA 3a02A 3a09A 3a6rA 3a72A 3a9bA 3achA 3acxA 3agnA 3aiaA 3ak2A 3amrA 3ap9A 3awuA
3b5mA 3b79A 3bbbA 3bfqG 3bjeA 3bmzA 3bnjA 3bo6A 3boeA 3bqpA 3buuA 3bwzA 3bxuA 3chbD
3chvA 3ci3A 3cijA 3cimA 3cjsB 3ckmA 3clmA 3d32A 3d3bJ 3d4eA 3d9xA 3db7A 3e4gA 3e8tA
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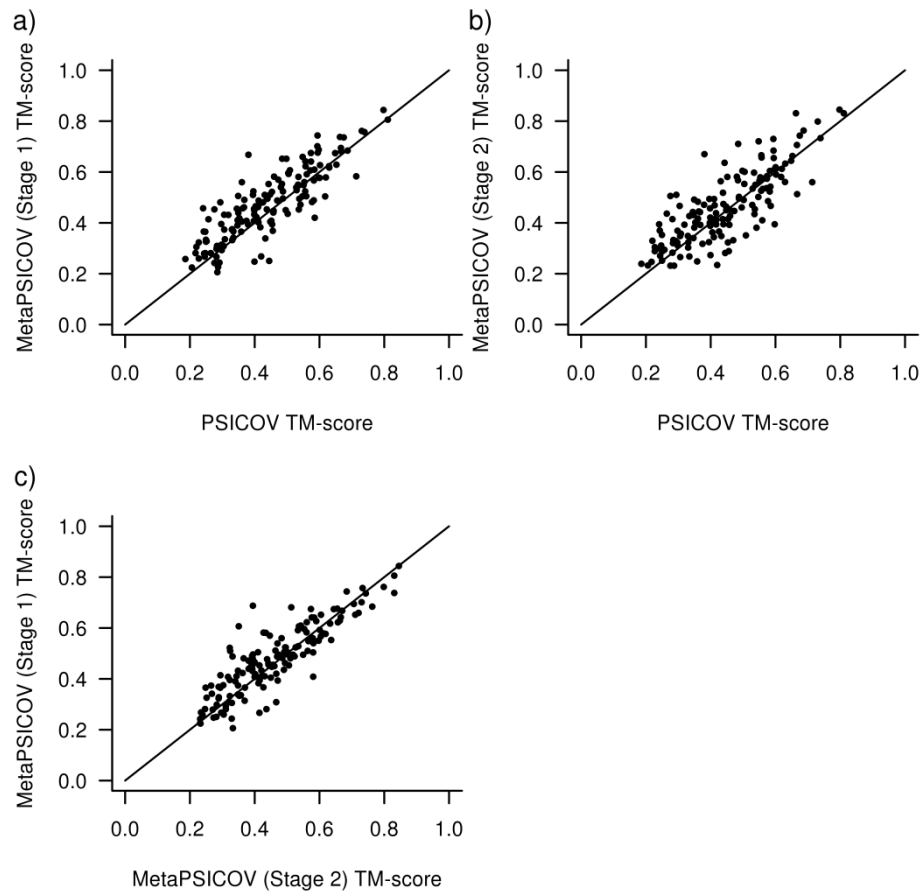
Supplementary Table II

Mean precision values for the top-L, top-L/2, top-L/5 and top-L/10 contacts, L= length of target protein, at different sequence separation ranges i-j ≥ 5 and i-j ≥ 23, where the $C\beta$-$C\beta$ distance < 8 Å. Each row corresponds to the first stage results from a different combination of the three coevolution methods, with all other neural network features included.

	[i-j]≥5				[i-j]≥23			
	L	L/2	L/5	L/10	L	L/2	L/5	L/10
PSICOV	0.39	0.43	0.55	0.7	0.29	0.37	0.45	0.52
DCA	0.45	0.5	0.67	0.81	0.36	0.47	0.6	0.68
PSICOV+DCA	0.49	0.57	0.76	0.87	0.41	0.54	0.7	0.78
CCMpred	0.6	0.75	0.88	0.94	0.44	0.59	0.75	0.82
PSICOV+CCMpred	0.63	0.78	0.89	0.95	0.46	0.61	0.77	0.84
DCA+CCMpred	0.65	0.79	0.9	0.95	0.47	0.62	0.77	0.84
PSICOV+DCA+CCMpred	0.66	0.79	0.9	0.95	0.47	0.63	0.78	0.85

Supplementary Figure 1

Comparison of model TM-score for FRAGFOLD generated models using contacts from a) MetaPSICOV stage 1 and PSICOV b) MetaPSICOV stage 2 and PSICOV c) MetaPSICOV stage 1 and MetaPSICOV stage 2 (line x=y shown for reference).

Supplementary Table III

TM scores for representative models extracted from FRAGFOLD ensembles for each of the 150 benchmark protein chains.

PDB Code & Chain	No contacts	PSICOV contacts	MP Stage1 contacts	MP Stage2 contacts
1a3aA	0.286	0.422	0.549	0.566
1a6mA	0.332	0.391	0.494	0.571
1a70A	0.279	0.353	0.400	0.424
1aapA	0.273	0.408	0.280	0.359
1abaA	0.278	0.477	0.527	0.599
1ag6A	0.224	0.351	0.460	0.453
1aoeA	0.176	0.305	0.244	0.334
1atlA	0.336	0.263	0.297	0.329
1atzA	0.293	0.578	0.381	0.404
1avsA	0.615	0.417	0.435	0.561
1bdoA	0.170	0.306	0.258	0.293
1bebA	0.424	0.248	0.440	0.506
1behA	0.191	0.236	0.278	0.249
1bkrA	0.314	0.415	0.534	0.578
1brfA	0.204	0.237	0.378	0.355
1bsgA	0.184	0.358	0.321	0.313
1c44A	0.265	0.241	0.456	0.434
1c52A	0.338	0.271	0.497	0.327
1c9oA	0.438	0.582	0.641	0.595
1cc8A	0.555	0.687	0.819	0.720
1chdA	0.225	0.530	0.581	0.525
1cjwA	0.242	0.394	0.572	0.502
1ckeA	0.247	0.394	0.402	0.400
1ctfA	0.402	0.561	0.509	0.636
1cxyA	0.278	0.463	0.451	0.473
1cznA	0.254	0.436	0.496	0.448
1d0qA	0.240	0.437	0.497	0.415
1d1qA	0.233	0.374	0.453	0.340
1d4oA	0.263	0.311	0.205	0.302
1dbxA	0.229	0.275	0.482	0.278
1dixA	0.291	0.204	0.260	0.304
1dlwA	0.588	0.614	0.519	0.625
1dmgA	0.225	0.285	0.316	0.336
1dqgA	0.186	0.206	0.243	0.251
1dsxA	0.269	0.353	0.437	0.379
1eazA	0.382	0.394	0.589	0.623
1ej0A	0.274	0.394	0.556	0.605
1ej8A	0.269	0.206	0.341	0.278
1ek0A	0.234	0.541	0.552	0.455
1f6bA	0.288	0.395	0.473	0.405
1fcyA	0.302	0.438	0.256	0.350
1fk5A	0.375	0.441	0.502	0.446
1fl0A	0.253	0.229	0.313	0.370
1fnaA	0.719	0.687	0.757	0.744
1fqtA	0.309	0.524	0.488	0.515
1fvgA	0.229	0.391	0.501	0.400
1fvkA	0.213	0.585	0.559	0.441
1fx2A	0.255	0.559	0.501	0.508
1g2rA	0.387	0.515	0.423	0.454
1g9oA	0.369	0.565	0.677	0.474
1gbsA	0.223	0.321	0.492	0.497
1gmiA	0.177	0.254	0.330	0.404
1gmxA	0.375	0.583	0.631	0.604
1guuA	0.405	0.645	0.510	0.522
1gz2A	0.246	0.303	0.278	0.287
1gzcA	0.211	0.200	0.298	0.263
1h0pA	0.213	0.264	0.287	0.252
1h2eA	0.227	0.436	0.465	0.410

PDB Code & Chain	No contacts	PSICOV contacts	MP Stage1 contacts	MP Stage2 contacts
1h4xA	0.340	0.559	0.653	0.733
1h98A	0.227	0.284	0.325	0.367
1hdoA	0.210	0.572	0.624	0.655
1hfcA	0.250	0.312	0.246	0.346
1hh8A	0.282	0.496	0.448	0.394
1htwA	0.272	0.511	0.671	0.583
1hxnA	0.261	0.189	0.261	0.297
1i1jA	0.220	0.178	0.261	0.353
1i1nA	0.322	0.538	0.438	0.467
1i4jA	0.358	0.413	0.621	0.487
1i58A	0.224	0.399	0.435	0.460
1i5gA	0.401	0.475	0.541	0.573
1i71A	0.246	0.257	0.184	0.322
1ihzA	0.291	0.535	0.493	0.441
1iibA	0.606	0.567	0.639	0.622
1im5A	0.278	0.506	0.530	0.464
1iwdA	0.213	0.438	0.470	0.398
1j3aA	0.287	0.345	0.504	0.460
1jbeA	0.639	0.811	0.798	0.811
1jbkA	0.219	0.222	0.293	0.250
1jfuA	0.294	0.416	0.578	0.464
1jfxA	0.211	0.534	0.585	0.548
1jkxA	0.305	0.413	0.578	0.461
1jl1A	0.278	0.408	0.385	0.414
1jo0A	0.421	0.562	0.612	0.486
1jo8A	0.814	0.796	0.839	0.799
1josA	0.295	0.426	0.632	0.611
1jvwA	0.206	0.332	0.400	0.428
1jwqA	0.292	0.486	0.459	0.528
1jyhA	0.233	0.292	0.369	0.294
1k6kA	0.280	0.531	0.604	0.605
1k7cA	0.200	0.448	0.402	0.419
1k7jA	0.185	0.286	0.260	0.307
1kidA	0.265	0.417	0.377	0.299
1kq6A	0.281	0.377	0.516	0.400
1kqrA	0.205	0.186	0.190	0.232
1ktgA	0.270	0.304	0.360	0.250
1ku3A	0.514	0.607	0.546	0.469
1kw4A	0.538	0.505	0.652	0.645
1lm4A	0.203	0.368	0.407	0.259
1lo7A	0.229	0.458	0.570	0.498
1lpyA	0.224	0.483	0.368	0.297
1m4jA	0.260	0.251	0.502	0.338
1m8aA	0.432	0.475	0.305	0.491
1mk0A	0.301	0.266	0.315	0.373
1mugA	0.286	0.310	0.301	0.303
1nb9A	0.214	0.359	0.408	0.335
1ne2A	0.309	0.392	0.536	0.401
1npsA	0.291	0.362	0.330	0.366
1nrvA	0.467	0.550	0.461	0.580
1ny1A	0.236	0.314	0.437	0.379
1o1zA	0.383	0.498	0.597	0.597
1p90A	0.264	0.269	0.498	0.435
1pchA	0.303	0.504	0.617	0.663
1pkoA	0.267	0.322	0.349	0.295
1qf9A	0.263	0.447	0.385	0.415
1qjpA	0.189	0.276	0.279	0.282
1ql0A	0.194	0.243	0.306	0.288
1r26A	0.474	0.687	0.698	0.634
1roaA	0.395	0.425	0.453	0.418
1rw1A	0.292	0.419	0.578	0.448
1rw7A	0.206	0.355	0.461	0.442
1rybA	0.290	0.369	0.369	0.262
1smxA	0.316	0.395	0.375	0.375
1svyA	0.426	0.527	0.524	0.599
1t8kA	0.441	0.675	0.728	0.673
1tifA	0.325	0.480	0.541	0.416

PDB Code & Chain	No contacts	PSICOV contacts	MP Stage1 contacts	MP Stage2 contacts
1tqgA	0.389	0.663	0.738	0.822
1tqhA	0.207	0.358	0.471	0.531
1tzvA	0.314	0.693	0.739	0.731
1vfyA	0.284	0.218	0.358	0.287
1vhuA	0.412	0.589	0.653	0.628
1vjkA	0.338	0.510	0.524	0.502
1vmbA	0.263	0.439	0.524	0.290
1vp6A	0.295	0.251	0.470	0.385
1w0hA	0.211	0.334	0.405	0.581
1whiA	0.241	0.335	0.373	0.359
1wjxA	0.208	0.269	0.371	0.414
1wkcA	0.244	0.470	0.536	0.566
1xdzA	0.267	0.574	0.641	0.513
1xffA	0.221	0.622	0.442	0.379
1xkrA	0.258	0.268	0.249	0.270
2arcA	0.203	0.320	0.264	0.298
2cuaA	0.264	0.440	0.410	0.442
2hs1A	0.224	0.218	0.220	0.231
2mhrA	0.416	0.586	0.643	0.675
2phyA	0.337	0.411	0.570	0.323
2tpsA	0.312	0.521	0.540	0.479
2vxnA	0.225	0.648	0.661	0.570
3borA	0.247	0.620	0.610	0.561
3dqgA	0.249	0.247	0.359	0.415
5ptpA	0.205	0.350	0.462	0.516