SUPPLEMENTARY TABLES:

Table S1: Details of the decoy / modelled structures and their corresponding native structures, selected for the present study.

(A) Critical Assessment of Techniques for Protein (CASP) - CASP 3, 7, 8, 9 and 10 STRUCTURE PREDICTION DATA SET [CASP 3, 7, 8, 9 and 10] (http://predictioncenter.org/download_area/); The datasets in this table are selected on the basis of Resolution ≤ 3Å, R-factor 0.25, length ≥ 100 and the modeled structure sequence length = native ± 10.

Serial number	***Protein name(PDB ID)***	***Number of residues in the native and the decoy/ modelled structure***	***Resolution of the native structure (in Å)***	***R-Factor***	***Number of decoy structures***
		CASP 10			
01.	Mimivirus sulfhydryl oxidase R596 (3TD7)	295	2.21	0.227	260
02.	Hypothetical protein from Bacteroides ovatus (4E6F)	181	1.49	0.161	251
03.	Transcription anti-terminator antagonist UpxZ (4EPZ)	162	1.68	0.169	260
04.	Hypothetical protein from Ruminococcus gnavus (4ESN)	104	2.20	0.183	253
05.	Putative lipoprotein (4EXR)	174	1.85	0.186	244
06.	Leucine rich hypothetical protein (4EZG)	197	1.50	0.172	256
07.	Hypothetical protein from Legionella pneumophila (4EZI)	377	1.15	0.137	250
08.	Probable hydrolytic enzyme (4F0J)	315	1.50	0.161	250

09.	Susd homolog from Bacteroides vulgates (4F7A)	511	1.85	0.142	228
10.	Susd homolog from Bacteroides ovatus (4F53)	520	2.25	0.150	239
11.	Hypothetical protein from Bacteroides thetaiotaomicron (4F54)	197	1.60	0.169	242
12.	Double mutant of UPF0176 protein lpg2838 from Legionella pneumophila (4F67)	265	1.79	0.170	257
13.	leucine rich hypothetical protein (4FDO)	404	2.07	0.178	239
14.	Lipoprotein (4FDY)	313	2.23	0.201	252
15.	Aminopeptidase N family protein (4FGM)	597	2.39	0.191	240
16.	Glycoside hydrolase (4FJ6)	523	1.90	0.209	254
17.	Putative Thioredoxin Reductase TrxB from Bacillus anthracis (4FK1)	304	2.40	0.174	260
18.	Esterase YqiA (YE3661) from Yersinia enterocolitica (4FLE)	202	2.10	0.194	259
19.	(4FM3)				268
20.	Hypothetical protein (BVU_2165) from Bacteroides vulgatus (4FMR)	265	2.25	0.171	249
21.	ChpT protein (4FMT)	228	2.30	0.185	256
22.	Internalin (inlF) from Listeria monocytogenes str. (4FMZ)	347	1.91	0.178	241
23.	Thioredoxin-like protein from Parabacteroides distasonis (4FO5)	143	2.02	0.177	262
24.	Hypothetical protein (BACEGG_03550) from Bacteroides eggerthii (4FTD)	453	1.91	0.155	233
25.	Putative lipoprotein from Parabacteroides distasonis (4FVS)	215	2.70	0.189	240
26.	Hypothetical protein (4FXT)	202	2.77	0.184	254
27.	Hypothetical protein (lpg2210) from Legionella	322	2.33	0.170	256

	pneumophila (4G2A)				
28.	Hypothetical protein (BACUNI_01323) from Bacteroides (4GHB)	272	2.32	0.175	238
29.	Putative glucoamylase (BACUNI_03963) from Bacteroides (4GL3)	424	2.01	0.143	254
CASP 9					
30.	Hypothetical protein pa0856 (2X3O)	146	2.90	0.265	314
31.	Sensory Box Histidine Kinase (3MR0)	142	1.49	0.165	402
32.	Adenylate (3MR7)	189	2.60	0.184	600
33.	putative carboxynorspermidine decarboxylase protein (3MT1)	365	2.50	0.194	540
34.	Putative galactose mutarotase (3MWX)	325	1.45	0.149	365
35.	SusD homolog (3MX3)	506	2.00	0.167	370
36.	Nh3-Dependent Nad+ Synthetase (3N05)	590	2.35	0.233	362
37.	Putative immunoglobulin A1 protease (3N6Z)	381	1.30	0.137	614
38.	Imelysin peptida (3N8U)	384	1.44	0.168	643
39.	Structural genomics (3N91)	344	2.40	0.183	645
40.	Protein of Unknown Function (3NA2)	172	2.29	0.190	628
41.	Conserved Protein of Unknown Function EF_1977 (3NAT)	164	2.92	0.206	626
42.	Histidyl-tRNA synthetase (3NET)	465	2.70	0.219	401
43.	Functionally-unknown protein lin1836 (3NEU)	125	1.58	0.195	601
44.	Putative Polyprenyl Synthetase (3NF2)	352	2.20	0.233	596
45.	Alginate lyase (3NFV)	400	1.95	0.158	566
46.	BH2092 protein (3NHV)	144	2.50	0.199	601
47.	TetR transcriptional regulator (3NI7)	213	2.78	0.250	602

48.	PFC0360w, an HSP90 activator (3NI8)	140	2.50	0.226	593
49.	PAS domain of a GGDEF family protein (3NJA)	125	2.37	0.212	315
50.	CRISP-associated protein Cas1 (3NKD)	305	1.95	0.220	401
51.	GEBA250068378 (3NKG)	172	2.00	0.172	649
52.	Integrase (3NKH)	220	2.50	0.158	386
53.	UDP-D-Quinovosamine 4-Dehydrogenase (3NKL)	138	1.90	0.169	620
54.	Putative sugar hydrolase (3NMB)	288	2.40	0.172	378
55.	N-terminal domain of Moloney murine leukemia virus integrase (3NNQ)	106	2.69	0.234	413
56.	Protein of unknown function (3NO2)	294	1.35	0.147	587
57.	Glycerophosphodiester phosphodiesterase (3NO3)	258	1.89	0.151	411
58.	Putative thiaminase II (3NO6)	229	1.65	0.167	390
59.	Putative peptide binding protein (3NOH)	169	1.60	0.161	613
60.	Putative secreted protein (3NPD)	136	1.60	0.162	625
61.	Putative dipeptidyl-peptidase VI (3NPF)	326	1.72	0.142	391
62.	Structural genomics, unknown function (3NQK)	339	2.61	0.200	618
63.	A metazoan ortholog of SpoT hydrolyzes ppGpp (3NQW)	179	2.90	0.213	377
64.	Aspartate aminotransferase (3NRA)	406	2.15	0.156	393
65.	Histidine triad protein (3NRD)	134	2.06	0.170	371
66.	Putative aldose 1-epimerase (3NRE)	290	1.59	0.162	557
67.	ApaG protein (3NRF)	126	1.50	0.186	589
68.	TetR family transcriptional regulator (3NRG)	216	2.56	0.209	399
69.	Protein BF1032 (3NRH)	182	1.80	0.198	602
70.	MarR/EmrR family transcriptional regulator (3NRV)	148	2.00	0.198	410

71.	N-terminal domain of Phage integrase/site-specific recombinase (3NRW)	111	1.70	0.187	614
72.	2-oxo-3-deoxygalactonate kinase (3NUW)	295	2.09	0.174	586
73.	BH2602 protein (3NWZ)	168	2.57	0.233	414
74.	Fat acid (stearic acid)-binding protein (3NYI)	296	1.90	0.171	403
75.	Putative glycyl-glycine endopeptidase lytM (3NYY)	279	1.60	0.150	621
76.	Pfam DUF1425 family member (3O0L)	129	1.81	0.205	304
77.	Formyltetrahydrofolate deformylase (3O1L)	283	2.20	0.175	385
78.	Formyltetrahydrofolate deformylase (3OBI)	287	1.95	0.236	383
79.	TenA homolog (3OQL)	261	2.54	0.178	602
80.	DUF1989 family protein (3ORU)	233	1.11	0.127	582
81.	Galactose mutarotase-like protein (3OS7)	340	1.08	0.145	384
82.	Putative nuclease belonging to DUF820 (3OT2)	186	1.96	0.217	582
83.	Putative aminotransferase (3P1T)	336	2.60	0.202	388
CASP 8					
84.	The structure of the rhodanese domain of the human dual specificity phosphatase 16 (2VSW)	153	2.2	0.227	550
85.	Human haspin kinase domain (2VUW)	336	1.80	0.148	289
86.	Human ribonucleotide reductase, subunit m2 b (2VUX)	326	2.80	0.213	279
87.	Human enoyl coenzyme a hydratase domain-containing protein (2VX2)	287	2.30	0.172	295
88.	Human dual specificity tyrosine-phosphorylation-regulated kinase 1a (2VX3)	382	2.40	0.186	294
89.	The structure of human GPX8 (3CYN)	189	2	0.199	381
90.	Putative polyphosphate kinase 2 (3CZP)	500	2	0.231	515

91.	Putative polyphosphate kinase 2 from Sinorhizobium meliloti (3CZQ)	304	2.23	0.24	510
92.	The human ephrin A2- ephrin A1 complex (3CZU)	207	2.65	0.195	398
93.	Putative N-acetylmuramoyl-L-alanine amidase (3CZX)	182	1.6	0.218	500
94.	BIG_1156.2 domain of putative penicillin-binding protein mrca (3D0F)	106	1.64	0.217	544
95.	Conserved protein of unknown function CA_C3497 from Clostridium acetobutylicum ATCC 824 (3D0J)	140	1.53	0.184	377
96.	Poly(3-hydroxybutyrate) depolymerase from Bordetella parapertussis (3D0K)	304	1.83	0.209	488
97.	Protein Atu1372 (3D01)	165	1.7	0.214	496
98.	Putative NADP oxidoreductase BF3122 from Bacteroides fragilis (3D1L)	266	2.19	0.239	512
99.	Uncharacterized protein from Saccharomyces cerevisiae (3D1P)	139	0.98	0.124	540
100.	Effector domain of the putative transcriptional regulator iclr (3D3O)	178	2.46	0.269	393
101.	L-2,4-diaminobutyric acid acetyltransferase (3D3S)	189	1.87	0.21	514
102.	4-hydroxybutyrate coa-transferase (3D3U)	439	2.80	0.202	291
103.	Conserved protein from Enterococcus faecalis (3D3Y)	425	1.95	0.174	288
104.	Putative beta-lactamase inhibitor protein (3D4E)	179	1.4	0.201	549
105.	Dipicolinate synthase subunit A (3D4O)	293	2.1	0.24	372
106.	DUF2118 family protein (3D4R)	169	2.2	0.236	571
107.	Putative glucan synthesis regulator of smi1/knr4 family (3D5P)	144	1.45	0.175	545
108.	Putative haloacid dehalogenase-like hydrolase (3D6J)	225	2	0.235	389

109.	Putative aminotransferase from Corynebacterium diphtheriae (3D6K)	422	2.00	0.192	300
110.	Lyttr DNA-binding domain of putative methyl-accepting/DNA (3D6W)	111	2.4	0.209	522
111.	Carboxymuconolactone decarboxylase family protein (3D7I)	105	1.75	0.197	412
112.	Protein lin1944 from Listeria innocua (3D7L)	202	2.06	0.165	300
113.	Human fidgetin-like protein 1 in complex with ADP (3D8B)	357	2	0.237	408
114.	Phosphoglycerate mutase (3D8H)	267	2.01	0.233	309
115.	Acetyltransferase of GNAT family (3D8P)	163	2.2	0.218	379
116.	Purr family transcriptional regulator (3D8U)	275	2.88	0.217	291
117.	Conserved metalloprotein from Bacillus cereus (3D19)	283	2.30	0.210	292
118.	Tail protein from Neisseria meningitidis MC58 (3D37)	381	2.1	0.273	379
119.	Soluble Rieske Ferredoxin from Mus musculus (3D89)	157	2.07	0.228	527
120.	Glycerol-3-phosphate dehydrogenase from Bacillus halodurans (3DA1)	561	2.70	0.222	285
121.	Human carbonic anhydrase 13 (3DA2)	262	2.05	0.221	385
122.	Bromodomain of the human ATAD2 (3DAI)	130	1.95	0.203	314
123.	Methyltransferase domain of human PR domain-containing protein 1 (3DAL)	196	1.65	0.197	288
124.	Putative phosphate (3DAO)	283	1.80	0.170	301
125.	Human CYP7A1 (3DAX)	491	2.15	0.190	291
126.	Putative Pyridoxamine 5'-phosphate oxidase (3DB0)	128	2	0.239	394
127.	E3 ubiquitin-protein ligase (3DB3)	161	2.40	0.215	285

128.	Methyltransferase domain of human PR domain-containing protein 4 (3DB5)	151	2.15	0.226	308
129.	UPF0317 protein Atu3911 from Agrobacterium tumefaciens (3DB9)	269	2.80	0.229	293
130.	Protein Q88SR8 from Lactobacillus plantarum (3DC7)	232	2.12	0.186	277
131.	Galactose mutarotase related enzyme (3DCD)	307	1.90	0.179	283
132.	Putative histidinol phosphatase hisk from Listeria monocytogenes (3DCP)	283	2.10	0.193	299
133.	Duf1696 family protein with a pleckstrin-homology domain (3DCX)	117	2.00	0.186	303
134.	TP53-induced glycolysis and apoptosis regulator protein from Homo sapiens (3DCY)	275	1.75	0.229	375
135.	Transcriptional regulator (gntr family) from Enterococcus faecalis (3DDV)	145	2.65	0.208	308
136.	C-terminal domain of Probable hemolysin (3DED)	113	2.14	0.188	311
137.	Putative regulatory protein (3DEE)	249	2.10	0.225	280
138.	SH1221 protein from Staphylococcus haemolyticus (3DEV)	320	3.00	0.193	275
139.	Putative tetr family transcriptional regulator (3DEW)	206	1.75	0.173	301
140.	SAV_2001 protein from Streptomyces avermitilis (3DEX)	107	2.70	0.230	305
141.	Possible hxlr family transcriptional factor from Thermoplasma volcanium GSS1 (3DF8)	111	1.65	0.173	310
142.	Calcium-dependent protein kinase (3DFA)	286	2.45	0.234	303
143.	Human trna-specific adenosine-34 deaminase subunit ADAT2 (3DH1)	189	2.80	0.205	302
144.	Putative epimerase Q89Z24_BACTN from Bacteroides thetaiotaomicron (3DHN)	227	2.00	0.232	298

145.	HD-superfamily hydrolase (3DJB)	223	2.90	0.246	304
146.	Dinb-like protein from bacillus subtilis (3DKA)	155	2.30	0.219	301
147.	Human DEAD-box RNA-helicase DDX52 (3DKP)	245	2.10	0.185	304
148.	Q7W9W5_BORPA protein from Bordetella parapertussis (3DKZ)	142	2.40	0.238	310
149.	Putative Metal-dependent Hydrolase (3DL1)	267	2.20	0.172	283
150.	Guide-strand-containing Argonaute protein silencing complex (3DLB)	685	2.70	0.254	270
151.	Putative s-adenosyl-l-methionine-dependent methyltransferase (3DLC)	219	1.15	0.121	298
152.	Tudor domain of human Histone-lysine N-methyltransferase SETDB1 (3DLM)	213	1.77	0.210	293
153.	Human PAS kinase bound to ADP (3DLS)	335	2.30	0.244	291
154.	Domain of a Replication factor A protein, from Methanocaldococcus jannaschii (3DM3)	105	2.40	0.225	290
155.	Primosomal replication protein n (3DM4)	115	2.00	0.252	309
156.	Exopolyphosphatase-related protein (3DMA)	343	2.25	0.223	295
157.	Putative general stress family protein (3DMB)	147	2.30	0.213	304
158.	Ntf2-like protein from anabaena variabilis (3DMC)	134	1.65	0.177	295
159.	Conserved exported protein from Bordetella pertussis (3DME)	369	1.70	: 0.190	296
160.	C-terminal domain of a possilbe DNA helicase (3DMN)	174	1.66	0.193	290
161.	Cyclic nucleotide binding regulatory protein (3DN7)	194	1.80	0.173	300
162.	Protein Atu2129 (3DNH)	258	1.94	0.189	295
163.	Stress response protein yhax (3DNP)	290	1.85	0.16	304
164.	SPO1766 protein (3DNX)	153	1.94	: 0.174	292

165.	Putative Homoserine Dehydrogenase (3DO5)	327	2.20	0.189	299
166.	Putative Formyltetrahydrofolate Synthetase (3DO6)	543	1.85	0.164	282
167.	Protein with unknown function from Archaeoglobus fulgidus (3DO8)	148	1.60	0.169	297
168.	Protein ba1542 (3DO9)	188	2.75	0.265	293
169.	Fibrinogen binding protein from Staphylococcus aureus (3DOA)	288	2.81	0.191	286
170.	Methyltransferase (3DOU)	191	1.45	0.167	300
171.	Q8NRD3_CORGL protein from Corynebacterium glutamicum (3DR5)	221	2.25	0.211	294
172.	Surface layer protein BACUNI_02894 from Bacteroides uniformis(3DSM)	328	1.90	0.168	274
173.	Protein b from bartonella henselae (3DTD)	175	2.35	0.236	289
174.	Mutt/nudix family hydrolase from rhodospirillum rubrum (3DUP)	300	1.80	0.171	291
175.	Putative dehydrogenase from Xanthomonas campestris (3E03)	274	1.69	0.162	300
176.	Two-domain protein from bacteroides vulgatus (3E38)	343	2.2	0.225	513
177.	Candida glabrata FMN Adenylyltransferase in complex with FMN and ATP analog AMPCPP (3G5A)	308	1.95	0.236	526
178.	Protein yqbn (3KLU)	157	2.20	0.225	299
CASP 7					
179.	CagS (HP0534, Cag13) from Helicobacter pylori (2G3V)	208	2.3	0.219	458
180.	PDZ domain of human PICK1 (2GZV)	114	1.12	0.15	531
181.	Homoserine O-succinyltransferase (2H2W)	312	2.52	0.19	476

182.	BH3980 (10176605) from BACILLUS HALODURANS (2HH6)	113	2.04	0.225	541
183.	Protein of Unknown Function SP1558 from Streptococcus pneumoniae (2HNG)	127	1.63	0.193	608
184.	Hypothetical protein, rv2844, from Mycobacterium tuberculosis (2IB0)	170	2.00	0.204	526
	CASP 3				
185.	Multiple Antibiotic Resistance Protein (MARA) / DNA Complex (1BL0)	99	2.30	0.225	973

(B) ROSETTA PROTEIN DECOY DATA SET [Rosetta] (http://depts.washington.edu/bakerpg/decoys/)

186.	Acanthamoeba Castellanii Profilin (1ACF)	125	2.00	0.179	140
187.	Human Thioredoxin (1AIU)	105	2.00	0.179	140
188.	Calponin Homology (1BKR)	108	1.10	0.141	140
189.	Deoxy Form Hemoglobin (1CG5)	141	1.60	0.191	140
190.	Dihydroneopterin Aldolase (1DHN)	121	1.65	0.197	140
191.	Bromodomain (1E6I)	110	1.87	0.187	140
192.	TPRI Domain Of HOP (1ELW)	117	1.60	0.180	140
193.	Escherichia Coli Cyay Protein (1EW4)	106	1.40	0.188	140
194.	Mycobacterium Tuberculosis (1EYV)	131	1.60	0.190	140
195.	Rapamycin Human Immunophilin (1FKB)	107	1.70	0.165	140
196.	Iibcellobiose (1IIB)	103	1.80	0.187	140
197.	PKCI (1KPE)	108	1.80	0.195	140
198.	Bovine Calbindin D9K Binding MG2 (1LOU)	92	1.95	0.197	140
199.	Barnase-D Complex (1RNB)	109	1.90	0.214	140

200.	TLP20 (1TUL)	102	2.20	0.181	140
201.	Aspartate Receptor (1VLS)	146	1.85	0.197	140
202.	MG2 (2CHF)	128	1.80	0.180	140
203.	Bacillus Pasteurii Urease (4UBP)	100	1.55	0.151	140
204.	Cytochrome b562 (256B)	106	1.40	0.164	140

(C) STANDARD AND COMPLETE COLLECTION OF PROTEIN DECOY DATA SET [Std and Comp] (http://babylone.ulb.ac.be/decoys)

205.	Human Thioredoxin (1ERV)	105	1.65	0.21	999
206.	Immunosuppressant Complex (1FKF)	107	1.7	0.17	200
207.	Human Lyzozyme (1LHM)	130	1.8	0.160	200
208.	Bence-Jones Protein (2RHE)	114	1.6	0.149	200
209.	Ribonuclease T1 (2RNT)	104	1.8	0.149	200

(D) DECOY R US DATA SET (http://dd.compbio.washington.edu/download.shtml)

(i) Single decoy sets [Single] ➔

210.	Bovine Pancreatic Phospholipase (1BP2)	123	1.70	0.171	1
211.	Leghemoglobin (1LH1)	153	2.00	0.00	1
212.	Porcine Pancreatic Phospholipase (1P2P)	124	2.60	0.241	1
213.	Bence-Jones protein (1REI)	212	2.00	0.00	1
214.	Bovine Liver Rhodanese (1RHD)	293	2.50	0.00	1
215.	Bovine Ribonuclease A (1RN3)	124	1.45	0.233	1
216.	Cytochrome (2CDV)	107	1.80	0.176	1

217.	Yeast Cytochrome C Peroxidase (2CYP)	293	1.70	0.202	1
218.	3-D structure of 2-crystal forms of FAB R19.9 (2F19)	214	2.80	0.182	1
219.	Interleukin-1 Beta (2I1B)	153	2.00	0.172	1
220.	Tetracenomycin Polyketide Synthesis Protein (2ILB)	153	1.6	0.184	1
221.	Pseudoazurin (2PAZ)	123	1.60	0.178	1
222.	Proteinase Inhibitor Streptomyces Subtilisin Inhibitor (2SSI)	107	2.30	0.185	1
223.	Phosphoramidates (2TMN)	316	1.60	0.179	1
224.	Tyrosyl-T/RNA Synthetase (2TS1)	317	2.30	0.228	1
225.	Ribonuclease A (3RN3)	124	1.45	0.223	1
226.	Azotobacter Vinelandii Ferredoxin (5FD1)	106	1.90	0.215	1

(ii) HG structural decoy sets [HG Struct] ➔

227.	Ascaris Hemoglobin (1ASH)	147	2.15	0.179	29
228.	Hemoglobin Thionville (1BAB-B)	146	1.50	0.157	29
229.	Colicin (1COL-A)	197	2.40	0.180	29
230.	C-Phycocyanin (1CPC-A)	162	1.66	0.181	29
231.	Cyano-Met Myoglobin (1EMY)	153	1.78	0.153	29
232.	Sulfide Reactive Hemoglobin (1FLP)	142	1.50	0.170	29
233.	Leghemoglobin (1GDM)	153	1.70	0.158	29
234.	Glycera Dibranchiata Hemoglobin (1HBG)	147	1.50	0.146	29
235.	Caudina Arenicola (1HLB)	157	2.50	0.150	29
236.	Globin (1HLM)	158	2.90	0.190	29

237.	Metmyoglobin (1HSY)	153	1.90	0.163	29
238.	Homotetrameric Hemoglobin (1ITH-A)	141	2.50	0.147	29
239.	Loggerhead Sea Turtle Myoglobin (1LHT)	153	2.00	0.178	29
240.	Aplysia Limacina Myoglobin (1MBA)	146	1.60	0.193	29
241.	Pig Metmyoglobin (1MYG-A)	153	1.75	0.198	29
242.	Threonine68(E11) Mutant (1MYJ-A)	153	1.90	0.207	29
243.	Metmyoglobin Lacking The D – Helix (1MYT)	146	1.74	0.1777	29
244.	Lamprey hemoglobin (2LHB)	149	2.00	0.142	29
245.	aquomet porcine hemoglobin (2PGH-A)	141	2.80	0.154	29
246.	Aquomet porcine hemoglobin (2PGH-B)	146	2.80	0.154	29
247.	Dimeric Hemoglobin (4SDH-A)	145	1.60	0.158	29

(iii) IG structural decoy sets [IG Struct] ➔ The resolution range is for this set is 1.7-3.1 Å

248.	principal neutralizing site of hiv-1 (1ACY)	232	3.00	0.210	60
249.	Anti-dinitrophenyl-spin-label monoclonal antibody (1BAF)	222	2.90	0.195	60
250.	neutralizing antibody to human rhinovirus serotype 2 (1BBD)	231	2.80	0.190	60
251.	chimeric fab' fragment of an antibody binding tumour cells (1BBJ)	221	3.10	0.176	60
252.	Anti-steroid fab' and progesterone-fab' complex (1DBB)	231	2.70	0.210	60
253.	Human antibody (1DFB)	231	2.70	0.177	60
254.	Antiidiotopic Antibody (1DVF)	223	1.90	0.194	60
255.	Serine Protease (1EAP)	225	2.40	0.186	60

256.	fab r19.9 (1FAI)	231	2.70	0.189	60
257.	complex between fab f9.13.7 and guinea-fowl lysozyme (1FBI)	229	3.00	0.190	60
258.	Humanized Anti-CD18 Antibody (1FGV)	227	1.90	0.180	60
259.	Ctalytic Antibody (1FIG)	227	3.00	0.220	60
260.	Fab Fragment (1FLR)	228	1.85	0.188	60
261.	Fab fragment (1FOR)	225	2.75	0.174	60
262.	Neutralizing antibody for type 1 poliovirus and its viral epitope (1FPT)	231	3.00	0.230	60
263.	Anti-Influenza Ha Peptide Antibody (1FRG)	233	2.80	0.190	60
264.	Antigen Binding Domains (1FVC)	229	2.20	0.183	60
265.	Humanized Anti-P185-HER2 Antibody (1FVD)	227	2.50	0.179	60
266.	48G7 Hybridoma Line Fab Complex (1GAF)	221	1.95	0.244	60
267.	HIV-1 Neutralizing Antibody (1GGI)	226	2.80	0.188	60
268.	Fab Fragment Of A Murine (1GIG)	231	2.30	0.195	60
269.	Induced FIT For Antigen-Antibody Recognition (1HIL)	233	2.00	0.195	60
270.	Esterolytic Catalytic Antibody (1HKL)	221	2.68	0.184	60
271.	Idiotype-Anti-Idiotype FAB Complex (1IAI)	228	2.90	0.210	60
272.	Anti-Digoxin Antibody (1IBG)	232	2.70	0.209	60
273.	IGG1 FAB Fragment (1IGC)	227	2.60	0.168	60
274.	Antibody To A Peptide (1IGF)	231	2.80	0.180	60
275.	Digoxin Complex (1IGI)	231	2.70	0.177	60
276.	FV from Human Immunoglobulin(1IGM)	227	2.30	0.201	60
277.	Cyclosporin (1IKF)	233	2.50	0.164	60

278.	FAB Hapten Complexes (1IND)	222	2.20	0.188	60
279.	HPR Complex (1JEL)	230	2.50	0.210	60
280.	Heteroclitic Antigen-Antibody (1JHL)	224	2.40	0.214	60
281.	Catalytic Antibody 28B4 FAB Fragment (1KEM)	231	2.20	0.183	60
282.	Brucella A Cell Wall (1MAM)	227	2.45	0.215	60
283.	Phosphocholine Binding Immunoglobulin FAB (1MCP)	235	2.70	0.225	60
284.	FV Complexed With Carbohydrate Antigen (1MFA)	229	1.70	0.166	60
285.	Monoclonal Antibody FAB (1MLB)	223	2.10	0.181	60
286.	Antibody FAB Fragment (1MRD)	225	2.30	0.195	60
287.	Autoantibody To Single Stranded DNA (1NBV)	232	2.00	0.246	60
288.	Neuraminidase Antibody Compplexes (1NCB)	227	2.50	0.165	60
289.	N1G9 Fab Fragment (1NGQ)	229	2.40	0.194	60
290.	NC10 Antibody (1NMB)	231	2.20	0.210	60
291.	Antibody N10-Staphylococal Nuclease Complex (1NSN)	224	2.80	0.195	60
292.	OPG2 Fab Fragment (1OPG)	232	2.00	0.160	60
293.	Polysaccharide Epitopes (1PLG)	228	2.80	0.164	60
294.	Monoclonal Anti-Icam-1 Antibody (1RMF)	231	2.80	0.188	60
295.	Anticholera Toxin Peptide Complex (1TET)	228	2.30	0.148	60
296.	Uncomplexed FAB (1UCB)	228	2.50	0.200	60
297.	Bound Water Molecules (1VFA)	224	1.80	0.158	60
298.	Human IGG1 Kappa Autoantibody (1VGE)	231	2.00	0.180	60
299.	FAB Fragment (1YUH)	225	3.00	0.190	60
300.	Anti-Sweetener (2CGR)	228	2.20	0.214	60

301.	Monoklonalen Immunoglobulins (2FB4)	236	1.90	0.189	60
302.	Galactan Binding Immunoglobulin (2FBJ)	224	1.95	0.194	60
303.	Catalytic FAB (2GFB)	227	3.00	0.213	60
304.	Fab HyHEL5 (3HFL)	223	1.70	0.195	60
305.	Antibody-Antigen Complex (3HFM)	220	3.00	0.246	60
306.	Murine Anti-P-Azophenylarsonate (6FAB)	228	1.90	0.209	60
307.	Human Immunoglobulin (7FAB)	219	2.00	0.169	60
308.	Human Myeloma Immunoglobulin (8FAB)	228	1.80	0.173	60

(iv) IG structural hires decoy sets [IG Struct Hires] ➔ this is a subset of immunoglobulin decoy set with resolution between 1.7-2.2 Å.

309.	Antiidiotopic Antibody (1DVF)	223	1.90	0.194	19
310.	Humanized Anti-CD18 Antibody (1FGV)	227	1.90	0.180	19
311.	Fab Fragment (1FLR)	228	1.85	0.188	19
312.	Antigen Binding Domains (1FVC)	229	2.20	0.183	19
313.	48G7 Hybridoma Line Fab Complex (1GAF)	221	1.95	0.244	19
314.	Induced FIT For Antigen-Antibody Recognition (1HIL)	233	2.00	0.195	19
315.	FAB Hapten Complexes (1IND)	222	2.20	0.188	19
316.	Catalytic Antibody 28B4 FAB Fragment (1KEM)	231	2.20	0.183	19
317.	FV Complexed With Carbohydrate Antigen (1MFA)	229	1.70	0.166	19
318.	Monoclonal Antibody FAB (1MLB)	223	2.10	0.181	19
319.	Autoantibody To Single Stranded DNA (1NBV)	232	2.00	0.246	19
320.	OPG2 Fab Fragment (1OPG)	232	2.00	0.160	19

321.	Bound Water Molecules (1VFA)	224	1.80	0.158	19
322.	Human IGG1 Kappa Autoantibody (1VGE)	231	2.00	0.180	19
323.	Anti-Sweetener (2CGR)	228	2.20	0.214	19
324.	Monoklonalen Immunoglobulin (2FB4)	236	1.90	0.189	19
325.	Galactan Binding Immunoglobulin (2FBJ)	224	1.95	0.194	19
326.	Murine Anti-P-Azophenylarsonate(6FAB)	228	1.90	0.209	19
327.	Human Immunoglobulin (7FAB)	219	2.00	0.169	19
328.	Human Myeloma Immunoglobulin (8FAB)	228	1.80	0.173	19

Table S2: Scores for F select and ReliefF for all the features used in the SVM model (for the dataset d2). (Please note that the values of ReliefF scores are scaled to match the values of F-score – the parameters are sorted based on F-score results).

P. Id.	***P.description***	***F-score***	***ReliefF***
01.	difference between Ncov (non-covalent interactions) between Imin =2% and Imin =3%	0.380943	0.011437853
02.	Main chain hydrogen bond	0.255801	0.015251426
03.	difference between Ncov (non-covalent interactions) between Imin =3% and Imin =4%	0.203179	0.003607793
04.	difference between the size of the largest k-2 community between Imin = 1% and Imin= 2%	0.202492	0.00212212
05.	size of the largest cluster at Imin = 5%	0.15296	-0.002238445
06.	CCoe of the protein at Imin=6%	0.150572	-0.003970773
07.	CCoe of the protein at Imin=7%	0.150297	-0.006303096
08.	size of the largest cluster at Imin = 6%	0.148246	-0.004288293
09.	CCoe of the protein at Imin=5%	0.138256	-0.001858441
10.	Size of the largest cluster at Imin= 7%	0.134712	-0.005881021
11.	CCoe of the largest cluster at Imin = 6%	0.133285	-0.004451838
12.	NCov at Imin = 7%	0.131566	0.0006873

13.	CCoe of the largest cluster at Imin = 5%	0.12991	-0.004473293
14.	CCoe of the largest cluster at Imin = 7%	0.127564	-0.004727989
15.	NCov at Imin = 6%	0.123091	0.000881472
16.	difference between the size of the largest cluster between Imin = 3% and Imin= 4%	0.118192	0.007548283
17.	size of the top2 largest k-1 community at Imin = 4%	0.111406	-0.003627042
18.	CCoe of the protein at Imin=4%	0.111386	0.001190685
19.	size of the top2 largest k-1 community at Imin = 3%	0.109637	-0.003918638
20.	CCoe of the largest k-2 community at Imin = 4%	0.109392	-0.004117449
21.	size of the top2 largest k-1 community at Imin = 5%	0.10786	-0.003314213
22.	CCoe of the largest cluster at Imin = 4%	0.107665	-0.003641361
23.	NCov at Imin = 5%	0.104514	0.000963003
24.	size of the largest k-2 community at Imin = 4%	0.103288	-0.005139254
25.	size of the top2 largest k-1 community at Imin = 6%	0.102499	-0.002618381
26.	size of the top3 largest k-1 community at Imin = 7%	0.098521	-0.003554102
27.	CCoe of the largest k-2 community at Imin = 7%	0.098315	-0.004693102
28.	size of the top2 largest k-1 community at Imin = 7%	0.097578	-0.003228213
29.	CCoe of the largest k-2 community at Imin = 5%	0.097576	-0.004570994
30.	CCoe of the largest k-2 community at Imin = 3%	0.096996	-0.00358305
31.	CCoe of the largest k-2 community at Imin = 6%	0.095785	-0.004912421
32.	size of the largest k-2 community at Imin = 3%	0.095533	-0.004341449
33.	size of the top3 largest k-1 community at Imin = 4%	0.095091	-0.003387986
34.	size of the top3 largest k-1 community at Imin = 6%	0.093634	-0.003319176
35.	size of the top3 largest k-1 community at Imin = 3%	0.091536	-0.003682235
36.	size of the largest k-2 community at Imin = 5%	0.091106	-0.005552565
37.	size of the largest k-2 community at Imin = 6%	0.087453	-0.00592716
38.	size of the largest k-2 community at Imin = 7%	0.087299	-0.006125938

39.	size of the largest cluster at Imin = 4%	0.084418	0.00153203
40.	size of the top1 largest k-1 community at Imin = 7%	0.083856	-0.004069676
41.	size of the top1 largest k-1 community at Imin = 4%	0.082921	-0.004499402
42.	difference between the size of the largest cluster between Imin = 2% and Imin= 3%	0.08268	0.009320567
43.	size of the top1 largest k-1 community at Imin = 3%	0.081748	-0.004839216
44.	size of the top1 largest k-1 community at Imin = 6%	0.079475	-0.004309323
45.	size of the top3 largest k-1 community at Imin = 5%	0.079423	-0.00495913
46.	size of the top2 largest k-1 community at Imin = 2%	0.078677	-0.00161203
47.	size of the top1 largest k-1 community at Imin = 5%	0.077913	-0.00450442
48.	NCov at Imin = 4%	0.070309	0.001035916
49.	difference between Ncov (non-covalent interactions) between Imin =4% and Imin =5%	0.069355	0.002342673
50.	size of the top3 largest k-1 community at Imin = 2%	0.06455	-0.001718724
51.	CCoe of the largest cluster at Imin = 3%	0.063881	-0.002521659
52.	size of the top1 largest k-1 community at Imin = 2%	0.058993	-0.003297809
53.	CCoe of the protein at Imin=3%	0.043487	0.001860548
54.	CCoe of the largest k-2 community at Imin = 2%	0.042008	-0.001324448
55.	difference between the size of the largest k-2 community between Imin = 4% and Imin= 5%	0.041637	-0.009461873
56.	size of the largest k-2 community at Imin = 2%	0.041302	-0.002074712
57.	difference between the size of the largest k-2 community between Imin = 2% and Imin= 3%	0.038696	0.00001908
58.	size of the largest k-2 community at Imin = 0%	0.032848	0.002466718
59.	size of the largest k-2 community at Imin = 1%	0.032758	0.002421482
60.	NCov at Imin = 3%	0.031286	0.000725629
61.	CCoe of the protein at Imin=0%	0.030808	0.005463941
62.	CCoe of the protein at Imin=1%	0.030772	0.005410968
63.	CCoe of the largest cluster at Imin = 2%	0.029812	-0.002160284
64.	CCoe of the largest k-2 community at Imin = 0%	0.026858	0.000113601

65.	CCoe of the largest k-2 community at Imin = 1%	0.026719	0.000056265
66.	difference between the size of the largest k-2 community between Imin = 5% and Imin= 6%	0.021867	-0.009977731
67.	difference between the size of the largest k-2 community between Imin = 6% and Imin= 7%	0.020155	-0.010592884
68.	difference between the size of the largest cluster between Imin = 6% and Imin= 7%	0.01746	-0.009085017
69.	difference between Ncov (non-covalent interactions) between Imin =5% and Imin =6%	0.017357	0.000512447
70.	difference between the size of the largest cluster between Imin = 4% and Imin= 5%	0.016972	0.001637244
71.	difference between Ncov (non-covalent interactions) between Imin =1% and Imin =2%	0.014996	0.002343104
72.	CCoe of the largest cluster at Imin = 0%	0.008508	-0.000744212
73.	CCoe of the largest cluster at Imin = 1%	0.008499	-0.00075063
74.	size of the largest cluster at Imin = 3%	0.008117	0.003275702
75.	NCov at Imin = 2%	0.004473	0.000545307
76.	difference between the size of the largest cluster between Imin = 5% and Imin= 6%	0.003837	-0.005236466
77.	difference between Ncov (non-covalent interactions) between Imin =0% and Imin =1%	0.002829	0.000914811
78.	difference between the size of the largest k-2 community between Imin = 3% and Imin= 4%	0.001903	-0.006547925
79.	size of the largest cluster at Imin = 2%	0.001617	0.004158636
80.	difference between the size of the largest cluster between Imin = 0% and Imin= 1%	0.00136	-0.000487444
81.	NCov at Imin = 1%	0.001237	0.002122264
82.	NCov at Imin = 0%	0.001204	0.002134273
83.	difference between the size of the largest cluster between Imin = 1% and Imin= 2%	0.000889	0.007412963
84.	size of the largest cluster at Imin = 1%	0.00071	0.006996162
85.	size of the largest cluster at Imin = 0%	0.000692	0.007007433
86.	CCoe of the protein at Imin=2%	0.000688	0.003641855
87.	size of the top1 largest k-1 community at Imin = 1%	0.000449	0.002051029
88.	size of the top1 largest k-1 community at Imin = 0%	0.000417	0.002085514

89.	difference between Ncov (non-covalent interactions) between Imin =6% and Imin =7%	0.000113	-0.00002480
90.	difference between the size of the largest k-2 community between Imin = 0% and Imin= 1%	0.000056	0.000545156
91.	size of the top2 largest k-1 community at Imin = 0%	0.00005	0.003185745
92.	size of the top2 largest k-1 community at Imin = 1%	0.000043	0.003143881
93.	size of the top3 largest k-1 community at Imin = 0%	0	0.003627682
94.	size of the top3 largest k-1 community at Imin = 1%	0	0.003578665

SUPPLEMENTARY FIGURES:

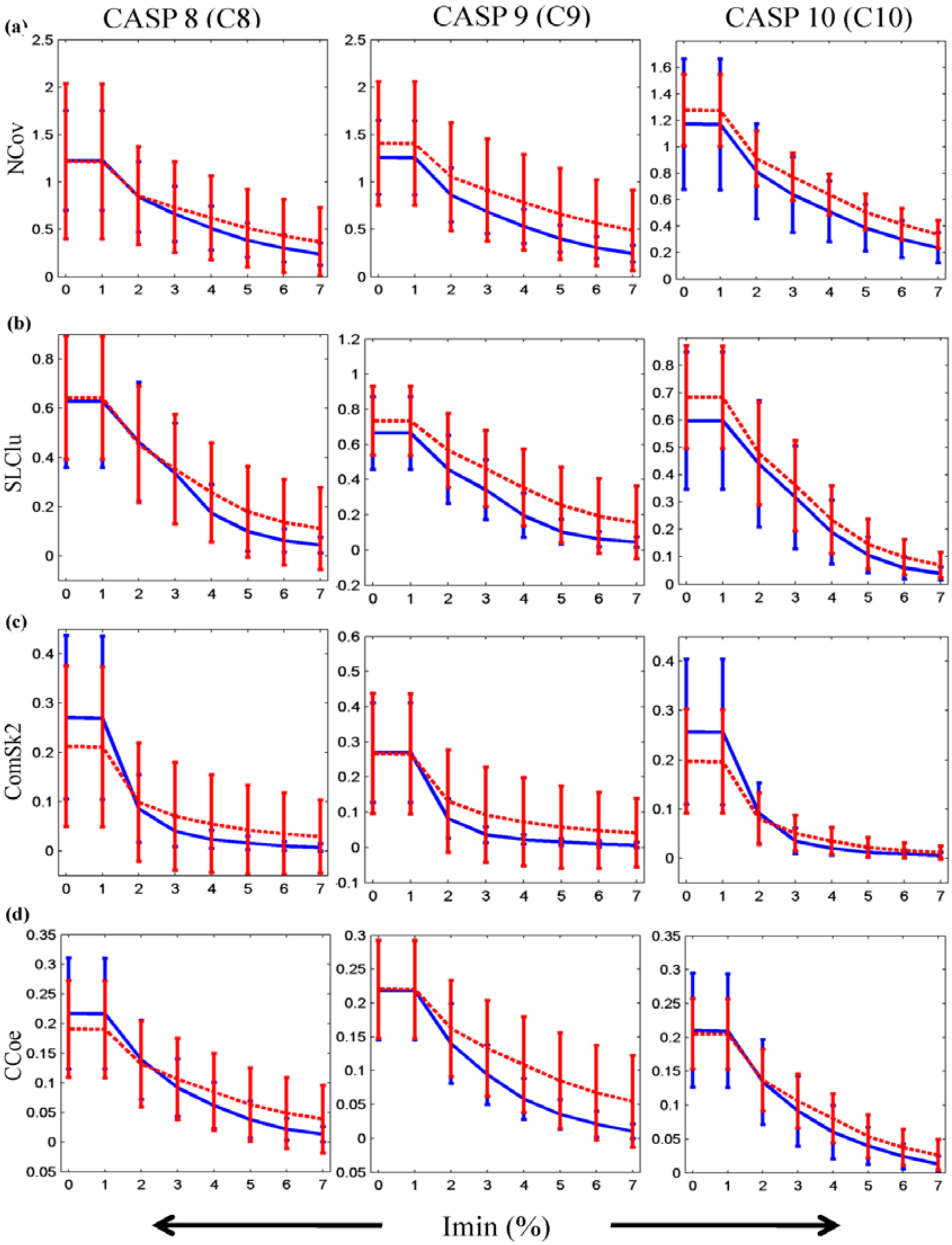


Figure S1: Profiles of the network parameters [NCov, SLClu, ComSk2, CCoe] are shown for CASP8 [C8], CASP9 [C9] and CASP10 [C10]. Blue line represents native structures while red line represents decoy / modeled structures. I_{min} is shown on the X-axis and the average values of the network properties are represented on the Y-axis, along with standard deviation.

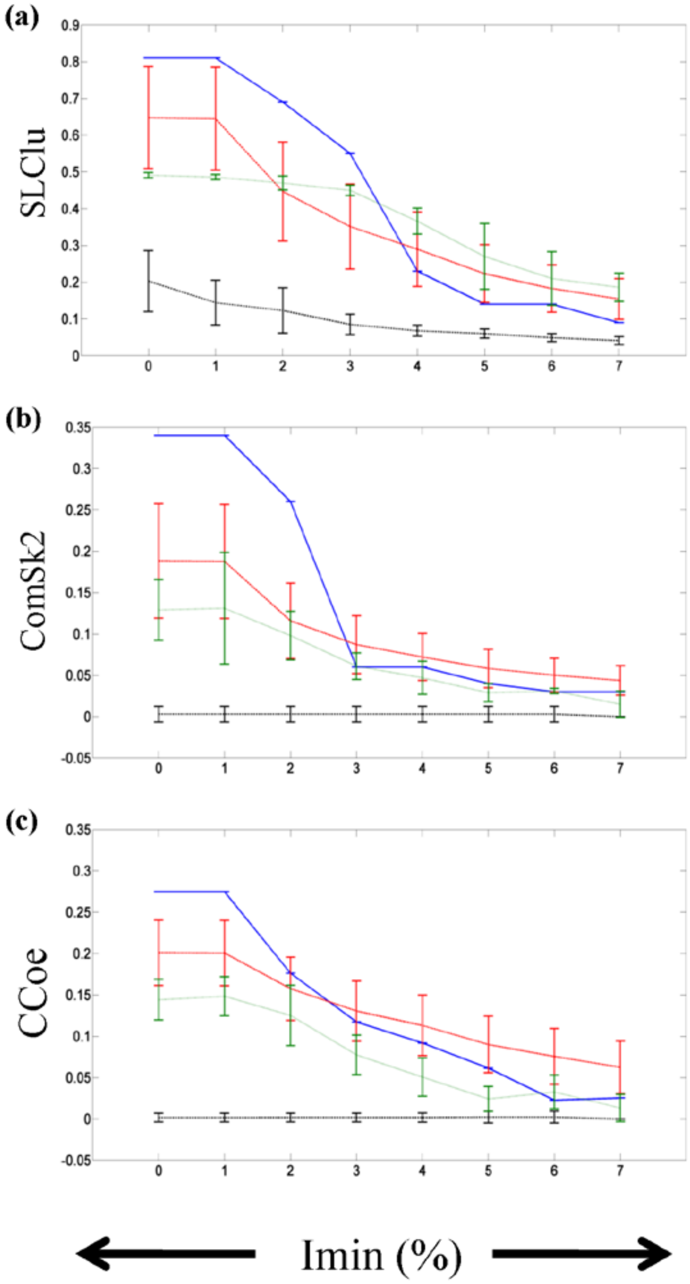
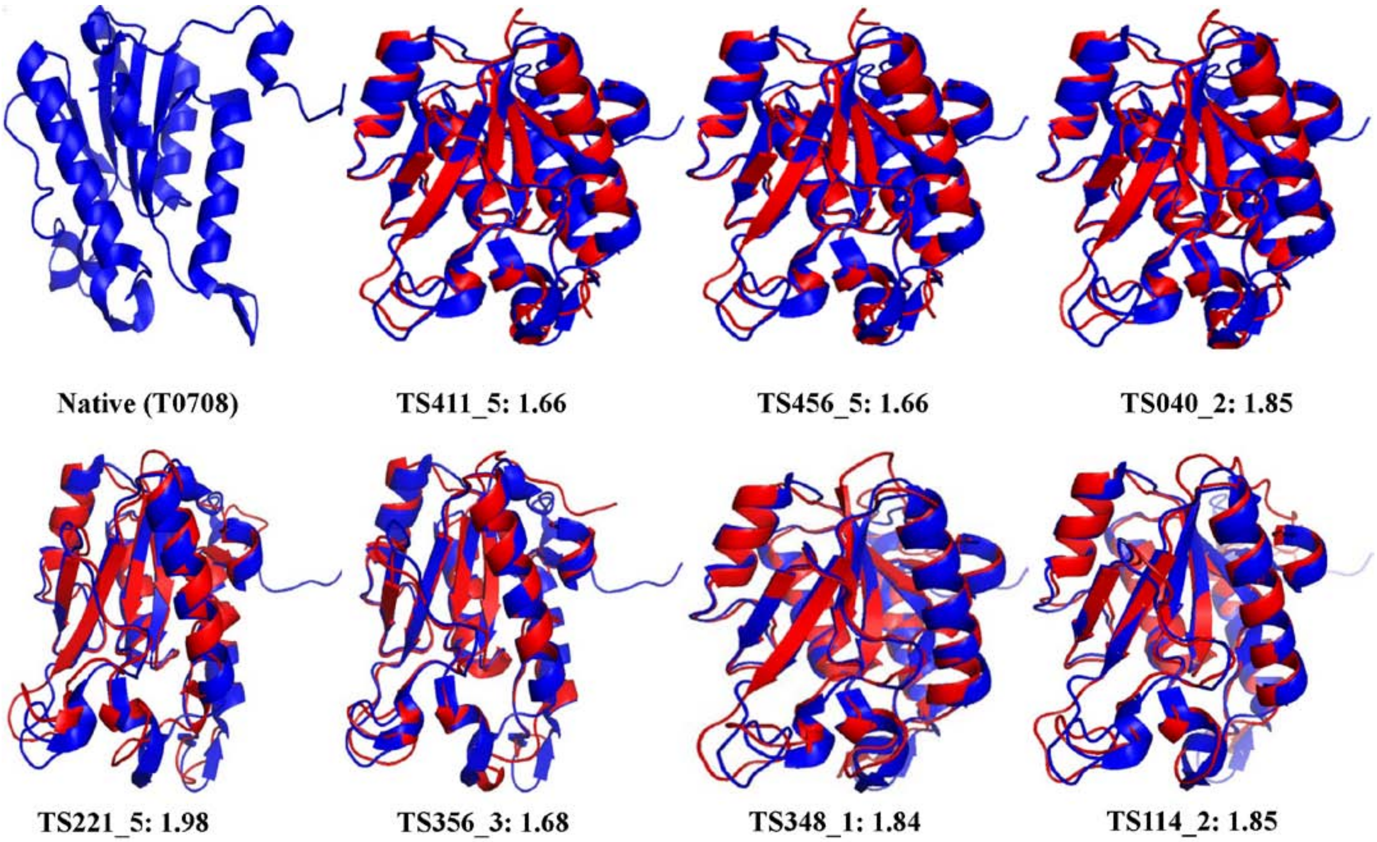


Figure S2: Transition profiles for three network features [SLClu, ComSk2 and CCoe] corresponding to CASP3 native structure [1BL0] and its decoy models. X-axis represents Imin values ranging from 0% to 7% and Y-axis shows the average values with standard deviation. Blue line corresponds to the native structure, while red corresponds to decoy models. Corresponding profiles of the random models, RM1 (Erdos-Renyi) and RM3 (described in Results section) are shown in black and green respectively. The RM1 model fails to exhibit any transition as a function of Imin, however, the RM3 models shows a transition profile closer to the decoy models.



Native (T0708) TS411_5: 1.66 TS456_5: 1.66 TS040_2: 1.85

TS221_5: 1.98 TS356_3: 1.68 TS348_1: 1.84 TS114_2: 1.85

Figure S3: Comparison of model structures predicted by SVM as well as by GDT-TS scores and the native structure for target Id T0708 (4H17). The native structure in these figures is shown in blue while the SVM predicted models are shown, aligned with the native structure. The names of the modelled structures as provided in CASP10 are used. RMSD value for each structure is also provided.