

Table S1: PDB codes of the protein-nucleic acid structures used in this study. *

ID	PDB	R/D	Id% **	Cov% **	Models	Method	Protein
P1d	1a02F	DNA	36	100	1	Xray	Structure of the dna binding domains of nfat, fos and jun bound to dna
P2r	1a1tA	RNA	93	100	5	NMR	Hiv-1 nucleocapsid protein bound to the sl3 psi-rna recognition element
P3d	1a31A	DNA	47	47	5	Xray	Human reconstituted dna topoisomerase i in covalent complex with a 22 base pair dna duplex
P4d	1a3qA	DNA	62	100	2	Xray	Human nf-kappa-b p52 bound to dna
P5d	1a73A	DNA	31	95	5	Xray	Intron-encoded endonuclease i-ppoi complexed with dna
P6r	1a9nB	RNA	76	100	5	Xray	Spliceosomal u2b''-u2a' protein complex bound to a fragment of u2 small nuclear rna
P7d	1aayA	DNA	65	100	5	Xray	Zif268 zinc finger-dna complex
P8d	1am9A	DNA	33	100	2	Xray	Human srebp-1a bound to ldl receptor promoter
P9r	1aq3A	RNA	86	98	1	Xray	Bacteriophage ms2 capsid protein/rna complex
P10r	1asyA	RNA	50	94	5	Xray	Aspartyl-trna synthetase complexed with trna asp
P11r	1b23P	RNA	56	96	5	Xray	CysteinyI-trna and T. Aquaticus elongation factor EF-TU:GTP ternary complex
P12r	1b34A	RNA	28	95	5	Xray	D1d2 sub-complex
P13d	1b3tA	DNA	94	95	5	Xray	Ebna-1 nuclear protein/dna complex
P14d	1bdtA	DNA	90	92	5	Xray	Wild type gene-regulating protein arc/dna complex
P15d	1bnkA	DNA	24	94	5	Xray	Human 3-methyladenine dna glycosylase complexed to dna
P16d	1cktA	DNA	80	99	1	Xray	Hmg1 domain a bound to a cisplatin-modified dna duplex
P17d	1cmaA	DNA	39	95	5	Xray	Met repressor/dna complex + s-adenosyl-methionine
P18r	1cx0A	RNA	76	100	5	Xray	Hepatitis delta virus ribozyme

P19d	1d66A	DNA	37	100	5	Xray	Dna recognition by gal4: structure of a protein/dna complex
P20r	1ddlA	RNA	43	100	5	Xray	Desmodium yellow mottle tymovirus
P21d	1ddnA	DNA	80	100	1	Xray	Diphtheria tox repressor (c102d mutant)/tox dna operator complex
P22r	1e8oB	RNA	36	96	5	Xray	Core of the alu domain of the mammalian srp
P23r	1ec6A	RNA	84	85	5	Xray	Nova-2 kh3 k-homology rna-binding domain bound to 20-mer rna hairpin
P24d	1ecrA	DNA	24	98	5	Xray	E. Coli replication terminator protein (tus) complexed with dna
P25r	1f7uA	RNA	30	93	5	Xray	Arginyl-trna synthetase complexed with the trna(arg) and l-arg
P26r	1fjgB	RNA	41	95	5	Xray	T. Thermophilus 30s ribosomal subunit
P27r	1fjgC	RNA	52	100	5	Xray	T. Thermophilus 30s ribosomal subunit
P28r	1fjgF	RNA	30	99	1	Xray	T. Thermophilus 30s ribosomal subunit
P29r	1fjgG	RNA	90	90	5	Xray	T. Thermophilus 30s ribosomal subunit
P30r	1fjgI	RNA	54	100	5	Xray	T. Thermophilus 30s ribosomal subunit
P31r	1fjgJ	RNA	51	100	5	Xray	T. Thermophilus 30s ribosomal subunit
P32r	1fjgK	RNA	53	98	5	Xray	T. Thermophilus 30s ribosomal subunit
P33r	1fjgL	RNA	72	98	5	Xray	T. Thermophilus 30s ribosomal subunit
P34r	1fjgM	RNA	54	92	5	Xray	T. Thermophilus 30s ribosomal subunit
P35r	1fjgN	RNA	47	100	5	Xray	T. Thermophilus 30s ribosomal subunit
P36r	1fjgO	RNA	59	100	2	Xray	T. Thermophilus 30s ribosomal subunit
P37r	1fjgP	RNA	39	90	5	Xray	T. Thermophilus 30s ribosomal subunit
P38r	1fjgR	RNA	41	79	5	Xray	T. Thermophilus 30s ribosomal subunit
P39r	1fjgS	RNA	92	92	5	Xray	T. Thermophilus 30s ribosomal subunit
P40r	1fjgT	RNA	40	88	5	Xray	T. Thermophilus 30s ribosomal subunit
P41d	1fokA	DNA	21	85	5	Xray	Restriction endonuclease

							foki bound to dna
P42r	1gtfA	RNA	81	99	5	Xray	Trp rna-binding attenuation protein (trap) bound to a 53-nucleotide rna molecule
P43r	1h2cA	RNA	94	94	5	Xray	Ebola virus matrix protein vp40 n-terminal domain in complex with rna
P44d	1hmiA	DNA	95	96	2	Xray	Hiv-1 reverse transcriptase complexed with double-stranded dna
P45r	1hq1A	RNA	51	91	5	Xray	Universally conserved protein from the signal recognition particle
P46r	1i6uA	RNA	50	98	2	Xray	Ribosomal protein s8/rrna complex from m. Jannaschii
P47d	1ignA	DNA	24	100	5	Xray	Dna-binding domain of rap1 in complex with telomeric dna site
P48d	1ihfA	DNA	38	99	1	Xray	Integration host factor/dna complex
P49r	1jidA	RNA	25	80	5	Xray	Human SRP19 in complex with RNA
P50r	1k8wA	RNA	32	95	5	Xray	Pseudouridine synthase trub bound to a T stem-loop RNA
P51r	1kq2A	RNA	53	100	1	Xray	Hfq-rna complex
P52d	1lmb3	DNA	85	92	5	Xray	The lambda repressor-operator complex
P53r	1m8wA	RNA	95	95	5	Xray	Human pumilio1 homology domain in complex with nre1-19 rna
P54r	1mmsA	RNA	64	100	3	Xray	Ribosomal protein l11-rna complex
P55d	1mnmA	DNA	66	99	5	Xray	Yeast matalpha2/mcm1/dna ternary transcription complex
P56r	1mzpA	RNA	38	97	2	Xray	L1 protuberance in the ribosome
P57d	1pdnC	DNA	67	98	5	Xray	Paired domain-dna complex
P58d	1pnrA	DNA	34	97	5	Xray	Purine repressor-hypoxanthine-purf-operator complex
P59r	1rgoA	RNA	36	53	5	NMR	Structural Basis for Recognition of the mrna Class II AU-Rich Element by the Tandem Zinc Finger Domain of TIS11d
P60r	1ropA	RNA	82	98	5	Xray	Col e1 rop protein

P61d	1sknP	DNA	35	99	5	Xray	Skn-1 in complex with dna
P62d	1tc3C	DNA	22	90	5	Xray	Transposase tc3a1-65 from c. Elegans
P63d	1trrA	DNA	92	94	5	Xray	Trp repressor/operator half-site complex
P64d	1tupA	DNA	91	91	5	Xray	Tumor suppressor p53 dna complex
P65d	1wetA	DNA	34	97	5	Xray	Purr-guanine-purf operator complex
P66d	1xbrA	DNA	51	97	1	Xray	T domain from xenopus laevis bound to dna
P67d	2bopA	DNA	31	94	1	Xray	Bovine papillomavirus-1 e2 dna-binding domain bound to its dna target
P68d	2dgcA	DNA	69	100	5	Xray	Gcn4 basic domain, leucine zipper complexed with atf/creb site dna
P69r	2fmtA	RNA	33	92	5	Xray	Methionyl-trnafmet formyltransferase complexed with formyl-methionyl-trnafmet
P70d	2irfG	DNA	73	94	1	Xray	Irf-2/dna complex.
P71d	2nllA	DNA	67	100	1	Xray	Retinoid x receptor-thyroid hormone receptor dna-binding domain heterodimer bound to thyroid response element dna
P72d	3croL	DNA	50	97	1	Xray	The phage 434 cro/or1 complex
P73d	3mhtA	DNA	38	88	5	Xray	Hhai methyltransferase with unmodified dna and adohcy
P74d	3pviA	DNA	69	69	5	Xray	Pviii endonuclease mutant complexed with cognate dna

* The 55 proteins for which I-TASSER produced 5 models are marked in bold.

** Highest id% and coverage of the whole template chains with the query sequence homologue used by I-TASSER, (see manuscript and [http://zhanglab.ccmb.med.umich.edu/RNA_project/\\$pdbchain](http://zhanglab.ccmb.med.umich.edu/RNA_project/$pdbchain) links)