

## A Appendix

Table A1: Mappings from DeepSequence alignments to PDB structures.

Alignment	PDB	chain_idx	aln_s	aln_e	pdb_s	pdb_e
AMIE_PSEAE_1_b0	2uxy	0	0	341	0	341
B3VI55_LIPSTSTABLE_1_b0	4zfv	1	9	439	0	430
B3VI55_LIPST_1_b0	4zfv	1	9	439	0	430
BG_STRSQ_1_b0	1gnx	0	14	478	0	464
BLAT_ECOLX_1_b0	1s0w	0	0	263	0	263
BRCA1_HUMAN_1_b0	1jm7	0	0	103	0	103
BRCA1_HUMAN_BRCT_1_b0	4u4a	0	21	235	0	214
CALM1_HUMAN_1_b0	3sjq	0	1	148	0	147
DLG4_RAT_2_b0	2xkx	0	0	101	296	397
DYR_ECOLI_1_b0	5uio	0	0	159	1	160
F7YBW7_MESOW_1_b0	5ceg	1	0	103	0	103
FYN_HUMAN_1_b0	3uf4	0	5	66	0	61
GAL4_YEAST_1_b0	3coq	0	7	75	0	68
HG_FLU_1_b0	6mya	4	16	508	0	493
HIS7_YEAST_1_b0	6ezm	0	2	219	0	217
HSP82_YEAST_1_b0	2cg9	0	1	216	0	215
IF1_ECOLI_1_b0	1ah9	0	1	72	0	71
KKA2_KLEPN_1_b0	1nd4	0	9	264	0	255
MK01_HUMAN_1_b0	7opm	0	0	360	2	362
MTH3_HAEAESTABILIZED_1_b0	3ubt	0	0	328	0	328
P84126_THETH_1_b0	1vc4	0	0	254	0	254
PABP_YEAST_1_b0	6r5k	1	0	96	77	173
PA_FLU_1_b0	7nj7	0	0	716	0	716
POLG_HCVJF_1_b0	3fqq	0	32	114	1	83
POL_HV1N5-CA_1_b0	6wap	0	0	231	0	231
PTEN_HUMAN_1_b0	7jvx	0	6	351	0	345
PYP_HALHA_1_b0	4bbv	0	0	125	0	125
RASH_HUMAN_1_b0	4q2l	0	0	169	0	169
RL401_YEAST_1_b0	6zqh	1	0	76	0	76
SUMO1_HUMAN_1_b0	1a5r	0	0	101	2	103
TPK1_HUMAN_1_b0	3s4y	0	15	242	0	227
TPMT_HUMAN_1_b0	2h1l	0	16	245	0	229
TRPC_SULSO_1_b0	1igs	0	1	248	0	247
TRPC_THEMA_1_b0	1i4n	0	1	252	0	251
TRY2_RAT_1_b0	3fp6	0	0	223	0	233
UBC9_HUMAN_1_b0	2xwu	0	0	158	0	158
UBE4B_MOUSE_1_b0	2kre	0	8	104	4	100
YAP1_HUMAN_1_b0	2ltw	0	0	36	0	36

Table A2: Zero-shot performance on *de novo* miniproteins from Rocklin et al. [2017], broken out by fold.

Fold	Pearson correlation		
	CARP-640M	MIF	MIF-ST
HHH <sub>138</sub>	0.41	0.46	0.52
HHH <sub>134</sub>	0.36	0.45	0.48
HEEH <sub>872</sub>	0.23	0.37	0.41
HEEH <sub>726</sub>	0.21	0.26	0.25
HEEH <sub>223</sub>	0.22	0.53	0.56
HEEH <sub>779</sub>	0.50	0.55	0.62
EEHEE <sub>1498</sub>	0.10	0.36	0.32
EEHEE <sub>37</sub>	0.41	0.65	0.68
EEHEE <sub>1716</sub>	0.22	0.60	0.60
EEHEE <sub>1702</sub>	0.03	0.26	0.24

Table A3: Zero-shot Spearman rank correlation on GB1 broken out by number of mutations.

Model	PDB				AF2			
	1	2	3	4	1	2	3	4
CARP-640M	0.19	0.12	-0.01	-0.01	0.19	0.12	-0.01	-0.01
MIF	0.83	0.64	0.42	0.11	0.84	0.66	0.44	0.15
MIF-ST	0.76	0.62	0.41	0.11	0.83	0.67	0.44	0.15