

EvoDesign: *de novo* protein design based on structural and evolutionary profiles

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Table S1. Structure folding results on seven designed sequences by EvoDesign using three independent methods of I-TASSER, SPARKS-X, and Rosetta.

PDB ID	Physics-based included?	I-TASSER				SPARK-X						Rosetta			
		First Model		Best in Top ten		First Model			Best in Top ten			First Model		Best in Top ten	
		TM-score	RMSD (Å)	TM-score	RMSD(Å)	TM-score	RMSD(Å)	Alignment coverage	TM-score	RMSD(Å)	Alignment coverage	TM-score	RMSD(Å)	TM-score	RMSD(Å)
1GUTA	No	0.90	0.8	0.92	0.7	0.86	1.2	98%	0.92	0.7	100%	0.63	2.9	0.63	2.9
	Yes	0.95	0.5	0.92	0.6	0.85	1.1	98%	0.93	0.5	100%	0.46	5.2	0.54	4.0
1V5IB	No	0.60	3.3	0.62	3.2	0.57	3.4	97%	0.98	0.3	100%	0.38	9.5	0.58	3.3
	Yes	0.86	1.5	0.86	1.4	0.43	4.7	94%	0.99	0.2	100%	0.33	8.2	0.47	3.7
1BKRA	No	0.98	0.4	0.99	0.3	0.91	1.9	99%	0.95	1.2	99%	0.47	5.3	0.47	5.3
	Yes	0.99	0.3	0.99	0.3	0.95	1.2	99%	0.95	1.2	99%	0.73	2.7	0.73	2.7
1T3YA	No	0.86	1.9	0.86	1.9	0.85	2.0	93%	0.95	1.1	98%	0.57	4.9	0.57	4.9
	Yes	0.85	1.8	0.88	1.7	0.82	2.4	94%	0.85	1.9	93%	0.52	5.5	0.52	5.5
2GMYA	No	0.97	1.0	0.97	1.0	0.95	1.8	100%	0.95	1.8	100%	0.33	12.4	0.39	9.3
	Yes	0.99	0.3	0.99	0.3	0.82	3.1	97%	0.99	0.5	100%	0.37	9.9	0.38	8.8
1Y25A	No	0.88	2.3	0.92	1.4	0.81	6.7	88%	0.95	1.2	99%	0.48	10.8	0.48	10.8
	Yes	0.95	1.2	0.95	1.0	0.93	1.6	98%	0.93	1.6	98%	0.29	14.0	0.38	11.9
2PTHA	No	0.93	1.7	0.93	1.7	0.22	17.1	79%	0.76	4.5	91%	0.23	16.7	0.24	14.8
	Yes	0.98	0.9	0.98	0.9	0.9	2.1	97%	0.99	0.2	100%	0.28	15.4	0.36	9.9
Average	No	0.87	1.6	0.89	1.4	0.74	4.9	93%	0.92	1.5	98%	0.44	8.9	0.48	7.3
	Yes	0.94	0.9	0.94	0.9	0.81	2.3	96%	0.95	0.9	98%	0.43	8.7	0.48	6.6