

Supplementary Materials for

Template-guided method for protein-ligand complex structure prediction: Application to CASP15 protein-ligand studies

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Table S1 Performance of our modeling methods in CASP15 ligand predictions. The results were based on the top 5 submitted models for each target.

Target	Ligands	IDDT_pli	RMSD (Å)	Template
H1114	3NI/F3S/FCO/MG/MQ7	0.86/0.82/0.95/0.93/0.05	0.70/1.06/0.43/0.50/20.15	1e3d
H1135	K	0.99	0.06	6r15
T1124	SAH/TYR	0.62/0.39	3.07/5.23	4a6e
T1127v2	COA	0.66	4.19	3bj7
T1146	NAG	0.97	0.46	4q68
T1152	NAG	0.79	1.48	4b8v
T1158v1	XPG	0.73	3.06	-
T1158v2	P2E	0.63	3.1	-
T1158v3	XH0	0.00	20.61	6uy0
T1158v4	ATP/MG	0.80/0.95	1.26/2.31	6uy0
T1170	ADP/AGS/MG	0.90/0.86/0.92	0.88/1.12/1.27	6oax
H1171	ADP/AGS/MG	0.91/0.86/0.97	0.72/1.35/0.54	6oax
H1172	ADP/AGS/MG	0.88/0.82/1.00	0.83/1.13/0.39	6oax
T1181	CA/OAA/ZN	0.00/0.31/0.45	138.32/9.47/3.80	-
T1186	LIG	0.65	3.76	6cyq
T1187	NAG	0.05	16.02	-
T1188	CD/CO/DW0	0.75/0.18/0.66	1.55/9.76/4.16	2ybt