

Table 1: For the dataset T0784 and T0769, the tables show the computed contact energies and the RMSD counterparts sorted by energies (left) and by RMSD (right).

T0784	Energy in $\frac{kcal}{mol}$	RMSD	T0784	Energy in $\frac{kcal}{mol}$	RMSD
T0784TS156_1	-130.48	1.15	T0784TS117_1	-230.12	1.73
T0784TS420_1	-127.74	1.17	T0784TS008_1	-203.16	1.86
T0784TS499_1	-149.46	1.18	T0784TS251_1	-193.6	1.63
T0784TS237_1	-139.99	1.22	T0784TS038_1	-162.31	1.38
T0784TS268_1	-160.82	1.28	T0784TS268_1	-160.82	1.28

T0769	Energy in $\frac{kcal}{mol}$	RMSD	T0769	Energy in $\frac{kcal}{mol}$	RMSD
T0769TS241_1	-59.34	2.67	T0769TS442_1	-90.73	16.72
T0769TS368_1	-66.75	3.16	T0769TS155_1	-90.62	17.12
T0769TS258_1	-74.39	4.37	T0769TS044_1	-84.32	10.38
T0769TS361_1	-79.04	4.41	T0769TS169_1	-81.02	10.39
T0769TS186_1	-79.97	4.51	T0769TS317_1	-80.61	6.89