

Table S12. Affinity and RMSD values for the co-crystallized ligands.

	Affinity Average (kcal/mol)±SD	RMSD Average±SD
1P8D	-12.57±0.15	1.68±0.11
3NMQ	-8.93±0.06	1.19±0.10
3O96	-11.20±0.10	2.10±0.10
4ACG	-9.87±0.06	1.96±0.33
5J20	-10.17±0.06	1.02±0.54