

ID	RMSE [kcal/mol]	MAE [kcal/mol]	ME [kcal/mol]
TEMOA-G6	1.59 [1.02, 2.11]	1.31 [0.86, 1.82]	0.40 [-0.41, 1.25]
OA-G6	1.80 [0.81, 2.53]	1.33 [0.70, 2.06]	0.72 [-0.15, 1.70]
OA-G0	1.86 [0.96, 2.54]	1.39 [0.74, 2.12]	1.00 [0.15, 1.91]
TEMOA-G0	1.80 [1.03, 2.46]	1.42 [0.86, 2.06]	0.32 [-0.57, 1.34]
OA-G7	1.69 [1.05, 2.31]	1.42 [0.96, 1.99]	-0.02 [-0.91, 0.99]
OA-G3	1.75 [1.06, 2.40]	1.45 [0.96, 2.05]	0.18 [-0.75, 1.22]
OA-G5	2.03 [1.18, 2.79]	1.55 [0.85, 2.33]	0.68 [-0.39, 1.78]
TEMOA-G1	1.99 [1.26, 2.70]	1.62 [1.04, 2.29]	0.40 [-0.61, 1.51]
TEMOA-G3	1.83 [1.33, 2.35]	1.63 [1.19, 2.11]	0.02 [-0.95, 1.04]
OA-G1	2.10 [1.19, 2.84]	1.65 [0.96, 2.43]	0.98 [-0.04, 2.05]
OA-G4	2.65 [1.30, 3.78]	1.84 [0.84, 3.00]	1.26 [-0.01, 2.62]
TEMOA-G5	2.35 [1.47, 3.23]	1.89 [1.19, 2.70]	0.80 [-0.35, 2.04]
OA-G2	2.43 [1.45, 3.25]	1.90 [1.09, 2.79]	0.44 [-0.96, 1.74]
CB8-G6	2.67 [1.70, 3.46]	2.15 [1.24, 3.10]	0.37 [-1.19, 1.95]
TEMOA-G7	3.04 [1.75, 4.14]	2.35 [1.38, 3.45]	1.44 [0.04, 2.93]
TEMOA-G4	3.06 [1.96, 4.06]	2.45 [1.51, 3.49]	1.69 [0.32, 3.09]
CB8-G10	3.04 [1.99, 3.85]	2.46 [1.42, 3.52]	1.39 [-0.26, 2.94]
CB8-G9	3.31 [1.67, 4.67]	2.52 [1.36, 3.88]	1.62 [-0.01, 3.38]
TEMOA-G2	3.22 [2.17, 4.08]	2.56 [1.51, 3.62]	1.80 [0.30, 3.19]
CB8-G7	3.01 [2.08, 3.81]	2.61 [1.74, 3.51]	-0.82 [-2.49, 0.92]
CB8-G1	3.43 [2.28, 4.39]	2.85 [1.74, 3.99]	-0.78 [-2.70, 1.24]
CB8-G8	3.58 [2.22, 4.71]	2.91 [1.73, 4.18]	-0.44 [-2.53, 1.66]
CB8-G0	3.75 [2.35, 4.90]	3.09 [1.88, 4.38]	2.45 [0.77, 4.11]
CB8-G2	4.27 [2.89, 5.51]	3.63 [2.35, 4.98]	2.85 [0.94, 4.69]
CB8-G5	4.70 [3.02, 6.09]	3.78 [2.18, 5.44]	3.71 [2.03, 5.41]
CB8-G3	4.76 [3.05, 6.19]	3.94 [2.42, 5.56]	1.89 [-0.84, 4.33]
CB8-G4	4.64 [3.15, 5.99]	3.98 [2.60, 5.42]	1.54 [-1.03, 4.12]