

ID	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)
TEMOA-G0	6.22 [2.21, 10.18]	2.85 [1.68, 4.75]	1.88 [0.52, 3.92]
TEMOA-G1	6.01 [2.28, 9.76]	2.96 [1.86, 4.74]	1.90 [0.57, 3.83]
TEMOA-G3	6.27 [2.16, 10.28]	2.97 [1.83, 4.84]	1.94 [0.57, 3.94]
OA-G0	6.17 [2.33, 9.97]	3.03 [1.84, 4.92]	2.44 [1.10, 4.40]
OA-G7	7.12 [2.03, 11.62]	3.04 [1.58, 5.27]	2.12 [0.51, 4.43]
OA-G3	7.09 [2.13, 11.71]	3.09 [1.76, 5.28]	2.33 [0.82, 4.64]
TEMOA-G5	5.66 [2.53, 9.03]	3.11 [2.10, 4.74]	2.42 [1.21, 4.15]
TEMOA-G6	6.12 [2.37, 9.87]	3.12 [1.97, 4.94]	2.33 [1.02, 4.26]
OA-G5	5.99 [2.49, 9.56]	3.26 [2.13, 5.03]	2.78 [1.51, 4.64]
OA-G6	6.93 [2.41, 11.09]	3.33 [1.92, 5.45]	2.60 [1.04, 4.84]
OA-G1	6.39 [2.62, 10.23]	3.40 [2.19, 5.30]	2.92 [1.58, 4.89]
OA-G4	7.26 [3.06, 11.57]	3.70 [2.25, 5.92]	3.11 [1.52, 5.42]
OA-G2	8.92 [3.02, 14.62]	3.99 [2.26, 6.79]	-0.20 [-3.31, 1.88]
TEMOA-G4	7.75 [3.41, 12.26]	4.15 [2.70, 6.35]	3.03 [1.29, 5.38]
TEMOA-G7	7.40 [3.62, 11.57]	4.37 [3.08, 6.37]	3.58 [2.04, 5.73]
TEMOA-G2	7.93 [3.79, 12.39]	4.68 [3.28, 6.83]	3.52 [1.78, 5.85]
CB8-G9	6.86 [4.32, 9.74]	4.83 [3.47, 6.58]	2.60 [0.67, 4.79]
CB8-G7	6.76 [4.20, 9.69]	4.86 [3.57, 6.58]	-1.59 [-3.86, 0.36]
CB8-G6	6.44 [4.45, 8.70]	4.96 [3.77, 6.39]	0.87 [-1.13, 3.02]
CB8-G10	7.60 [4.90, 10.81]	5.61 [4.16, 7.53]	1.52 [-0.80, 4.16]
CB8-G5	7.60 [5.42, 10.23]	5.85 [4.43, 7.61]	3.61 [1.50, 5.88]
CB8-G2	8.31 [5.45, 11.19]	6.09 [4.41, 8.08]	3.16 [0.69, 5.73]
CB8-G1	10.68 [4.51, 16.43]	6.12 [3.73, 9.44]	0.50 [-2.57, 4.48]
CB8-G8	9.09 [5.44, 12.94]	6.27 [4.42, 8.64]	0.25 [-2.55, 3.36]
CB8-G0	9.91 [5.34, 14.67]	6.47 [4.40, 9.25]	3.12 [0.25, 6.44]
CB8-G11	8.74 [4.02, 12.88]	6.63 [2.67, 11.20]	1.54 [-4.20, 8.35]
CB8-G4	12.41 [5.74, 19.35]	7.49 [4.95, 11.30]	2.95 [-0.46, 7.42]
CB8-G3	11.31 [6.34, 15.57]	7.77 [5.41, 10.78]	1.49 [-2.10, 5.27]
CB8-G13	16.13 [4.38, 25.45]	11.02 [3.75, 20.85]	4.74 [-4.95, 17.35]
CB8-G12	23.92 [9.61, 36.55]	17.56 [7.05, 30.94]	4.70 [-10.66, 23.51]