

ID	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)
TEMOA-G0	6.22 [2.22, 10.16]	2.85 [1.68, 4.71]	1.88 [0.51, 3.87]
TEMOA-G1	6.01 [2.28, 9.77]	2.96 [1.86, 4.75]	1.90 [0.58, 3.85]
TEMOA-G3	6.27 [2.14, 10.27]	2.97 [1.83, 4.84]	1.94 [0.57, 3.96]
OA-G0	6.17 [2.32, 9.95]	3.03 [1.83, 4.89]	2.44 [1.11, 4.39]
OA-G7	7.12 [2.03, 11.61]	3.04 [1.59, 5.26]	2.12 [0.52, 4.43]
OA-G3	7.09 [2.10, 11.70]	3.09 [1.74, 5.26]	2.33 [0.81, 4.61]
TEMOA-G5	5.66 [2.53, 9.02]	3.11 [2.10, 4.72]	2.42 [1.21, 4.15]
TEMOA-G6	6.12 [2.37, 9.86]	3.12 [1.97, 4.92]	2.33 [1.00, 4.24]
OA-G5	5.99 [2.50, 9.54]	3.26 [2.14, 4.98]	2.78 [1.53, 4.59]
OA-G6	6.93 [2.40, 11.07]	3.33 [1.92, 5.41]	2.60 [1.04, 4.76]
OA-G1	6.39 [2.62, 10.19]	3.40 [2.18, 5.27]	2.92 [1.57, 4.86]
OA-G4	7.26 [3.10, 11.54]	3.70 [2.26, 5.85]	3.11 [1.52, 5.35]
OA-G2	8.92 [2.96, 14.57]	3.99 [2.24, 6.73]	-0.20 [-3.25, 1.86]
TEMOA-G4	7.75 [3.39, 12.29]	4.15 [2.69, 6.38]	3.03 [1.29, 5.40]
TEMOA-G7	7.40 [3.63, 11.58]	4.37 [3.09, 6.39]	3.58 [2.04, 5.74]
TEMOA-G2	7.93 [3.79, 12.40]	4.68 [3.29, 6.84]	3.52 [1.79, 5.89]
CB8-G9	6.86 [4.33, 9.78]	4.83 [3.47, 6.61]	2.60 [0.68, 4.81]
CB8-G7	6.76 [4.19, 9.65]	4.86 [3.57, 6.58]	-1.59 [-3.88, 0.39]
CB8-G6	6.44 [4.44, 8.74]	4.96 [3.77, 6.44]	0.87 [-1.13, 3.04]
CB8-G10	7.60 [4.91, 10.76]	5.61 [4.19, 7.51]	1.52 [-0.77, 4.08]
CB8-G5	7.60 [5.41, 10.22]	5.85 [4.43, 7.59]	3.61 [1.50, 5.88]
CB8-G2	8.31 [5.44, 11.23]	6.09 [4.43, 8.11]	3.16 [0.70, 5.73]
CB8-G1	10.68 [4.53, 16.40]	6.12 [3.77, 9.37]	0.50 [-2.58, 4.36]
CB8-G8	9.09 [5.44, 13.01]	6.27 [4.41, 8.67]	0.25 [-2.54, 3.41]
CB8-G0	9.91 [5.34, 14.73]	6.47 [4.40, 9.27]	3.12 [0.31, 6.46]
CB8-G11	8.74 [4.10, 12.80]	6.63 [2.77, 11.10]	1.54 [-4.32, 8.26]
CB8-G4	12.41 [5.73, 19.27]	7.49 [4.97, 11.24]	2.95 [-0.48, 7.34]
CB8-G3	11.31 [6.31, 15.53]	7.77 [5.37, 10.72]	1.49 [-2.13, 5.23]
CB8-G13	16.13 [4.42, 25.43]	11.02 [3.84, 20.69]	4.74 [-5.00, 17.17]
CB8-G12	23.92 [9.71, 36.55]	17.56 [7.13, 30.84]	4.70 [-10.81, 23.52]