ID	receipt_id	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)	R^2	m	τ
US/PMF/MT/MD_19	finzb	0.50 [0.29, 0.66]	0.40 [0.21, 0.61]	-0.24 [-0.54, 0.06]	0.93 [0.61, 0.99]	1.15 [0.72, 1.43]	0.57 [-0.12, 1.00]
US/PMF/MT/MD_2	mknyd	0.60 [0.35, 0.81]	0.51 [0.29, 0.74]	-0.24 [-0.63, 0.14]	0.88 [0.23, 0.99]	1.15 [0.43, 1.43]	0.69 [0.08, 1.00]
US/PMF/MT/MD_22	iyo2o	0.80 [0.45, 1.14]	0.67 [0.41, 1.01]	0.57 [0.19, 0.97]	0.83 [0.24, 0.99]	0.66 [0.24, 0.86]	0.71 [0.05, 1.00]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/D	ttmwo	0.94 [0.55, 1.44]	0.79 [0.41, 1.28]	0.11 [-0.62, 0.81]	0.75 [0.03, 0.98]	1.24 [0.09, 1.80]	0.57 [-0.15, 1.00]
US/PMF/MT/MD_20	uui3y	1.06 [0.45, 1.51]	0.80 [0.37, 1.31]	0.77 [0.31, 1.30]	0.83 [0.24, 0.99]	1.20 [0.42, 1.56]	0.69 [0.04, 1.00]
US/PMF/MT/MD_9	rkitq	1.15 [0.49, 1.79]	0.86 [0.44, 1.46]	-0.09 [-0.96, 0.60]	0.15 [0.00, 0.87]	0.15 [-0.08, 0.59]	0.36 [-0.36, 1.00]
US/PMF/MT/MD_26	o3aiv	1.24 [0.75, 1.67]	1.05 [0.62, 1.52]	0.88 [0.26, 1.48]	0.65 [0.09, 0.95]	0.97 [-0.81, 1.43]	0.14 [-0.83, 0.84]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	8jxan	1.31 [0.68, 1.95]	1.09 [0.60, 1.69]	0.68 [-0.10, 1.50]	0.72 [0.03, 0.95]	1.33 [0.04, 2.17]	0.50 [-0.17, 1.00]
US/PMF/MT/MD_7	4ndha	1.46 [1.03, 1.85]	1.32 [0.88, 1.75]	1.27 [0.74, 1.74]	0.75 [0.13, 0.95]	0.49 [0.18, 0.82]	0.55 [-0.04, 1.00]
FEP-MM	w2q3q	1.48 [1.06, 1.86]	1.36 [0.94, 1.79]	-1.23 [-1.77, -0.57]	0.74 [0.46, 0.98]	1.09 [0.68, 2.08]	0.79 [0.33, 1.00]
US/PMF/MT/MD_12	emfe8	1.50 [1.03, 1.87]	1.31 [0.78, 1.80]	1.21 [0.55, 1.79]	0.70 [0.08, 0.95]	0.31 [0.08, 0.46]	0.57 [0.05, 1.00]
US/PMF/MT/MD_23	7uted	1.54 [1.09, 1.88]	1.38 [0.90, 1.83]	-1.32 [-1.82, -0.76]	0.72 [0.01, 0.99]	0.99 [-0.30, 1.42]	0.43 [-0.39, 1.00]
US/PMF/MT/MD_25	vgqcz	1.55 [1.01, 2.06]	1.40 [1.00, 1.90]	1.40 [1.00, 1.90]	0.72 [0.01, 0.99]	0.72 [-0.22, 1.04]	0.43 [-0.39, 1.00]
US/PMF/MT/MD_21	ftout	1.64 [1.10, 2.11]	1.49 [1.04, 1.99]	1.49 [1.04, 1.99]	0.83 [0.25, 0.99]	1.16 [0.41, 1.51]	0.69 [0.04, 1.00]
FEP-QM/MM	ahtcq	1.74 [1.31, 2.12]	1.59 [1.13, 2.07]	-1.59 [-2.06, -0.99]	0.81 [0.46, 0.99]	1.14 [0.73, 2.00]	0.79 [0.25, 1.00]
US/PMF/MT/MD_24	aai8i	1.76 [1.23, 2.30]	1.62 [1.20, 2.14]	1.62 [1.20, 2.14]	0.72 [0.01, 0.99]	0.83 [-0.25, 1.19]	0.43 [-0.39, 1.00]
SQM-opt	c8jfq	1.92 [0.99, 2.66]	1.57 [0.86, 2.37]	-0.29 [-1.53, 1.10]	0.18 [0.00, 0.93]	0.70 [-0.21, 2.82]	0.40 [-0.33, 0.98]
US/PMF/MT/MD_11	7fk2x	1.94 [1.42, 2.35]	1.77 [1.20, 2.29]	1.77 [1.20, 2.29]	0.70 [0.08, 0.95]	0.43 [0.11, 0.64]	0.57 [0.05, 1.00]
US/PMF/MT/MD_6	egmst	1.96 [1.51, 2.36]	1.85 [1.41, 2.29]	1.85 [1.41, 2.29]	0.75 [0.14, 0.95]	0.68 [0.26, 1.13]	0.55 [-0.04, 1.00]
US/PMF/MT/MD_4	gt5n0	1.98 [1.38, 2.48]	1.77 [1.15, 2.37]	1.77 [1.15, 2.37]	0.58 [0.02, 0.92]	0.81 [-0.21, 1.28]	0.50 [-0.18, 1.00]
FS-DAM/GAFF2/TIP3P	gemch	2.00 [0.90, 2.85]	1.55 [0.76, 2.48]	1.55 [0.76, 2.48]	0.84 [0.29, 0.98]	1.69 [0.39, 2.41]	0.71 [0.24, 1.00]
US/PMF/MT/MD_27	8pxph	2.05 [1.50, 2.56]	1.91 [1.42, 2.44]	1.91 [1.42, 2.44]	0.65 [0.10, 0.95]	0.71 [-0.60, 1.06]	0.14 [-0.83, 0.84]
US/PMF/MT/MD_17	iaz7f	2.19 [1.70, 2.57]	2.04 [1.44, 2.53]	2.04 [1.44, 2.53]	0.91 [0.81, 1.00]	0.37 [0.28, 0.54]	0.76 [0.22, 1.00]
AMOEBA/BAR/Tinker	8fcb6	2.23 [1.02, 3.26]	1.77 [0.97, 2.80]	-0.77 [-2.29, 0.57]	0.23 [0.00, 0.96]	-0.46 [-0.98, 1.35]	-0.29 [-1.00, 0.48]
DFT-opt	bjyua	2.23 [1.26, 3.08]	1.91 [1.19, 2.78]	-0.29 [-1.69, 1.36]	0.66 [0.01, 0.94]	2.03 [-0.24, 3.65]	0.43 [-0.28, 1.00]
US/PMF/MT/MD_14	rc4qr	2.29 [1.93, 2.62]	2.22 [1.85, 2.58]	2.22 [1.85, 2.58]	0.86 [0.11, 0.99]	1.06 [0.07, 1.32]	0.57 [-0.20, 1.00]
US/PMF/MT/MD_10	s78rs	2.40 [1.92, 2.81]	2.30 [1.81, 2.76]	2.30 [1.81, 2.76]	0.70 [0.08, 0.95]	0.63 [0.15, 0.94]	0.57 [0.05, 1.00]
US/PMF/MT/MD_5	nb8jk	2.51 [2.00, 2.97]	2.41 [1.91, 2.90]	2.41 [1.91, 2.90]	0.75 [0.13, 0.95]	0.99 [0.36, 1.66]	0.55 [-0.04, 1.00]
US/PMF/MT/MD_13	gkdce	2.68 [2.26, 3.07]	2.61 [2.19, 3.02]	2.61 [2.19, 3.02]	0.86 [0.11, 0.99]	1.16 [0.09, 1.44]	0.57 [-0.18, 1.00]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	iv75a	2.70 [1.73, 3.62]	2.34 [1.43, 3.38]	2.30 [1.24, 3.37]	0.75 [0.03, 0.98]	1.65 [0.11, 2.39]	0.57 [-0.17, 1.00]
DDM/GAFF/AM1-BCC/TIP3P	yedi3	2.77 [1.47, 3.82]	2.21 [1.11, 3.41]	1.79 [0.35, 3.26]	0.41 [0.00, 0.89]	1.37 [-0.70, 2.50]	0.18 [-0.64, 0.92]
US/PMF/MT/MD_18	xcuey	2.82 [2.51, 3.08]	2.78 [2.48, 3.06]	2.78 [2.48, 3.06]	0.93 [0.61, 0.99]	0.72 [0.45, 0.90]	0.57 [-0.12, 1.00]
US/PMF/MT/MD_16	ogd0g	2.99 [2.56, 3.33]	2.93 [2.45, 3.31]	2.93 [2.45, 3.31]	0.91 [0.82, 1.00]	0.52 [0.39, 0.75]	0.82 [0.33, 1.00]
US/PMF/MT/MD_1	4ysuf	3.01 [2.25, 3.68]	2.83 [2.15, 3.55]	2.83 [2.15, 3.55]	0.88 [0.23, 0.99]	1.58 [0.60, 1.97]	0.69 [0.08, 1.00]
US/PMF/MT/MD_3	widya	3.17 [2.55, 3.71]	3.05 [2.43, 3.64]	3.05 [2.43, 3.64]	0.58 [0.02, 0.92]	0.80 [-0.19, 1.26]	0.50 [-0.18, 1.00]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	ibhca	3.48 [2.19, 4.66]	3.05 [1.91, 4.29]	3.05 [1.91, 4.29]	0.72 [0.03, 0.95]	1.76 [0.03, 2.87]	0.50 [-0.17, 1.00]
US/PMF/MT/MD_15	m0qdw	4.00 [3.70, 4.25]	3.98 [3.67, 4.24]	3.98 [3.67, 4.24]	0.91 [0.82, 1.00]	0.76 [0.57, 1.09]	0.79 [0.24, 1.00]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	bhns3	4.64 [3.58, 5.64]	4.41 [3.36, 5.48]	4.41 [3.36, 5.48]	0.77 [0.03, 0.98]	1.67 [0.12, 2.39]	0.57 [-0.15, 1.00]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/A	mdqkg	5.41 [4.17, 6.62]	5.14 [4.03, 6.37]	5.14 [4.03, 6.37]	0.74 [0.05, 0.95]	1.81 [0.21, 2.89]	0.57 [-0.04, 1.00]
NULL1	null3	5.98 [5.09, 6.92]	5.85 [5.06, 6.77]	-5.85 [-6.77, -5.06]	0.00 [0.00, 0.00]	0.00 [0.00, 0.00]	nan [nan, nan]
US/PMF/MT/MD_8	e032m	6.26 [4.16, 7.97]	5.57 [3.64, 7.55]	5.57 [3.64, 7.55]	0.15 [0.00, 0.87]	0.96 [-0.46, 3.68]	0.36 [-0.36, 1.00]
EKEN-DIAZ/MD/MMPBSA	8brzp	7.07 [5.62, 8.44]	6.80 [5.51, 8.21]	6.80 [5.51, 8.21]	0.84 [0.12, 0.97]	2.22 [0.56, 3.01]	0.64 [0.00, 1.00]
BSSE-corrected RI-B3PW91 (SMD)/CBS	5r5n7	22.51 [11.40, 34.38]	17.86 [10.92, 28.70]	4.63 [-12.45, 14.84]	0.60 [0.00, 0.96]	-13.14 [-19.90, 3.58]	-0.21 [-1.00, 0.73]
BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	kuovg	36.41 [31.07, 40.10]	35.46 [29.00, 40.01]	31.73 [17.81, 40.01]	0.44 [0.15, 0.94]	-9.02 [-15.68, 4.56]	0.29 [-0.50, 1.00]