ID	receipt_id	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)	R^2	m	τ
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/D	d4twv	1.92 [1.20, 2.68]	1.51 [0.88, 2.34]	-0.24 [-1.39, 0.97]	0.13 [0.00, 0.70]	0.29 [-0.81, 0.72]	0.09 [-0.62, 0.64]
US/PMF/MT/MD_15	wtm6p	1.99 [1.32, 2.55]	1.69 [1.08, 2.32]	-0.38 [-1.53, 0.77]	0.36 [0.08, 0.72]	0.78 [0.38, 2.64]	0.49 [0.09, 0.88]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	j37ec	2.58 [1.43, 3.78]	2.02 [1.10, 3.17]	-1.83 [-3.06, -0.67]	0.13 [0.00, 0.76]	0.24 [-0.91, 0.70]	0.09 [-0.56, 0.68]
US/PMF/MT/MD_19	xdmpa	2.88 [1.67, 3.83]	2.28 [1.29, 3.35]	1.61 [0.23, 3.03]	0.08 [0.00, 0.50]	0.32 [-0.90, 1.62]	0.13 [-0.44, 0.65]
US/PMF/MT/MD_5	ubz3m	3.19 [2.23, 4.02]	2.72 [1.74, 3.70]	-2.72 [-3.70, -1.74]	0.39 [0.00, 0.79]	0.67 [-0.35, 1.68]	0.31 [-0.22, 0.76]
US/PMF/MT/MD_13	cco6p	3.23 [2.01, 4.34]	2.68 [1.69, 3.81]	-2.27 [-3.64, -0.93]	0.24 [0.02, 0.74]	0.69 [0.15, 3.50]	0.31 [-0.17, 0.72]
US/PMF/MT/MD_2	2mgw5	3.51 [1.42, 5.24]	2.44 [1.14, 4.07]	1.61 [-0.09, 3.57]	0.05 [0.00, 0.64]	0.34 [-2.08, 0.81]	-0.09 [-0.65, 0.48]
US/PMF/MT/MD_10	8wns3	3.67 [2.56, 4.55]	3.02 [1.77, 4.22]	-2.93 [-4.20, -1.60]	0.23 [0.00, 0.66]	0.62 [-0.57, 1.75]	0.27 [-0.29, 0.76]
US/PMF/MT/MD_8	cekua	3.73 [2.68, 4.61]	3.24 [2.14, 4.32]	-3.24 [-4.32, -2.14]	0.34 [0.00, 0.76]	0.69 [-0.37, 1.75]	0.31 [-0.23, 0.80]
AMOEBA/BAR/Tinker	tqhg4	3.73 [1.92, 5.23]	2.72 [1.50, 4.16]	1.18 [-0.56, 3.13]	0.14 [0.00, 0.74]	0.83 [-1.63, 1.67]	0.14 [-0.33, 0.60]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	f7duk	3.79 [2.69, 5.45]	3.48 [2.34, 4.88]	2.84 [1.00, 4.58]	0.13 [0.00, 0.77]	0.48 [-1.77, 1.38]	0.09 [-0.56, 0.68]
HREM/BAR/RESP/Force-Matching/TIP3P	3z83m	4.32 [3.14, 5.65]	3.82 [2.66, 5.09]	2.20 [0.04, 4.15]	0.49 [0.10, 0.80]	1.92 [1.11, 3.85]	0.52 [0.18, 0.81]
US/PMF/MT/MD_12	j8yon	4.39 [3.36, 5.26]	4.04 [3.02, 5.04]	4.04 [3.02, 5.04]	0.23 [0.00, 0.67]	0.38 [-0.35, 1.07]	0.27 [-0.30, 0.76]
US/PMF/MT/MD_7	dv8mj	4.41 [3.60, 5.08]	4.17 [3.28, 4.97]	4.17 [3.28, 4.97]	0.39 [0.00, 0.79]	0.41 [-0.21, 1.03]	0.31 [-0.22, 0.76]
US/PMF/MT/MD_20	j6oi0	4.72 [3.49, 5.84]	4.16 [2.85, 5.46]	-4.16 [-5.46, -2.85]	0.30 [0.06, 0.79]	0.78 [0.31, 3.61]	0.49 [0.09, 0.83]
US/PMF/MT/MD_18	vrsfp	4.79 [3.86, 5.57]	4.43 [3.28, 5.42]	4.43 [3.28, 5.42]	0.08 [0.00, 0.51]	0.14 [-0.39, 0.69]	0.13 [-0.44, 0.65]
US/PMF/MT/MD_4	2vfcf	5.05 [3.91, 6.06]	4.68 [3.56, 5.80]	4.68 [3.56, 5.80]	0.29 [0.05, 0.75]	0.61 [0.18, 2.52]	0.45 [0.00, 0.84]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/A	46vw8	5.07 [3.76, 6.77]	4.47 [3.14, 6.20]	4.41 [2.58, 6.14]	0.13 [0.00, 0.77]	0.48 [-1.81, 1.35]	0.05 [-0.57, 0.67]
US/PMF/MT/MD_22	qfqyx	5.31 [4.18, 6.33]	4.96 [3.86, 6.07]	4.96 [3.86, 6.07]	0.30 [0.06, 0.79]	0.63 [0.24, 2.93]	0.49 [0.09, 0.83]
DDM/Force-Matching/FEP/HREM/MBAR	6jsye	5.43 [3.85, 7.28]	4.77 [3.30, 6.44]	1.13 [-1.96, 3.80]	0.26 [0.00, 0.70]	1.76 [-1.39, 4.83]	0.47 [-0.02, 0.81]
US/PMF/MT/MD_16	50jkg	5.44 [4.14, 6.61]	5.00 [3.73, 6.28]	-5.00 [-6.28, -3.73]	0.36 [0.08, 0.72]	0.88 [0.43, 2.98]	0.49 [0.09, 0.88]
US/PMF/MT/MD_9	pz24v	5.45 [4.39, 6.40]	5.17 [4.15, 6.20]	5.17 [4.15, 6.20]	0.34 [0.00, 0.75]	0.62 [-0.34, 1.58]	0.31 [-0.23, 0.80]
US/PMF/MT/MD_3	jb047	5.61 [4.30, 6.71]	5.14 [3.79, 6.44]	-5.14 [-6.44, -3.79]	0.29 [0.05, 0.75]	0.77 [0.23, 3.15]	0.45 [0.00, 0.84]
US/PMF/MT/MD_21	tcy06	5.81 [4.51, 7.03]	5.39 [4.12, 6.69]	5.39 [4.12, 6.69]	0.30 [0.06, 0.79]	0.76 [0.30, 3.55]	0.49 [0.10, 0.83]
US/PMF/MT/MD_17	k6f5g	5.82 [4.94, 6.58]	5.62 [4.69, 6.48]	5.62 [4.69, 6.48]	0.36 [0.08, 0.72]	0.48 [-0.24, 1.65]	0.49 [0.08, 0.88]
US/PMF/MT/MD_14	fy660	6.49 [5.07, 7.80]	6.05 [4.68, 7.44]	-6.05 [-7.44, -4.68]	0.24 [0.02, 0.75]	0.70 [0.15, 3.61]	0.31 [-0.17, 0.72]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	3g2hu	6.61 [4.94, 8.41]	5.99 [4.23, 7.81]	5.96 [4.14, 7.80]	0.13 [0.00, 0.71]	0.58 [-1.60, 1.40]	0.09 [-0.62, 0.65]
DDM/GAFF/AM1-BCC/TIP3P	juz8u	7.21 [5.63, 8.53]	6.65 [4.95, 8.24]	6.44 [4.40, 8.22]	0.29 [0.00, 0.71]	1.14 [-0.42, 2.60]	0.33 [-0.21, 0.76]
US/PMF/MT/MD_6	u6tnc	7.83 [6.75, 8.82]	7.63 [6.56, 8.67]	-7.63 [-8.67, -6.56]	0.39 [0.00, 0.79]	0.75 [-0.39, 1.87]	0.31 [-0.22, 0.76]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	xv5oo	7.87 [6.16, 9.70]	7.33 [5.51, 9.17]	7.33 [5.51, 9.17]	0.13 [0.00, 0.70]	0.57 [-1.62, 1.41]	0.09 [-0.62, 0.64]
US/PMF/MT/MD_1	cbfnz	8.04 [4.88, 10.99]	6.70 [4.31, 9.51]	6.70 [4.31, 9.51]	0.05 [0.00, 0.64]	0.52 [-3.21, 1.23]	-0.09 [-0.65, 0.48]
US/PMF/MT/MD_11	6ux0a	8.23 [6.80, 9.45]	7.86 [6.41, 9.26]	-7.86 [-9.26, -6.41]	0.23 [0.00, 0.67]	0.69 [-0.64, 1.95]	0.27 [-0.30, 0.76]
NULL1	null1	8.59 [7.68, 9.71]	8.42 [7.64, 9.42]	-8.42 [-9.42, -7.64]	0.00 [0.00, 0.00]	0.00 [0.00, 0.00]	nan [nan, nan]
BSSE-corrected RI-B3PW91 (SMD)/CBS	sguyt	17.26 [12.13, 21.81]	14.88 [10.49, 19.63]	-14.41 [-19.45, -9.52]	0.00 [0.00, 0.47]	0.07 [-5.14, 7.01]	0.05 [-0.44, 0.54]
EKEN-DIAZ/MD/MMPBSA	6bwq3	17.80 [14.45, 20.80]	16.69 [13.50, 19.95]	16.69 [13.50, 19.95]	0.00 [0.00, 0.66]	-0.09 [-5.87, 1.34]	-0.19 [-0.67, 0.24]
BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	tb3ck	36.99 [29.89, 43.51]	34.29 [26.97, 41.41]	34.29 [26.97, 41.41]	0.00 [0.00, 0.55]	-0.12 [-10.22, 3.66]	-0.14 [-0.58, 0.24]