

ID	receipt_id	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)	R <sup>2</sup>	m	$\tau$
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/D	d4twv	1.92 [1.18, 2.52]	1.51 [0.82, 2.23]	-0.24 [-1.36, 0.86]	0.13 [0.00, 0.71]	0.29 [-0.71, 0.68]	0.09 [-0.56, 0.67]
US/PMF/MT/MD_15	wtm6p	1.99 [1.31, 2.56]	1.69 [1.07, 2.32]	-0.38 [-1.52, 0.79]	0.36 [0.08, 0.72]	0.78 [0.38, 2.64]	0.49 [0.08, 0.88]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	j37ec	2.58 [1.40, 3.52]	2.02 [1.14, 3.03]	-1.83 [-2.94, -0.79]	0.13 [0.00, 0.75]	0.24 [-0.61, 0.57]	0.09 [-0.54, 0.65]
US/PMF/MT/MD_19	xdmpa	2.88 [1.69, 3.83]	2.28 [1.30, 3.36]	1.61 [0.26, 3.06]	0.08 [0.00, 0.51]	0.32 [-0.92, 1.67]	0.13 [-0.45, 0.65]
US/PMF/MT/MD_5	ubz3m	3.19 [2.26, 4.00]	2.72 [1.75, 3.70]	-2.72 [-3.70, -1.75]	0.39 [0.00, 0.79]	0.67 [-0.33, 1.68]	0.31 [-0.20, 0.76]
US/PMF/MT/MD_13	cco6p	3.23 [2.02, 4.37]	2.68 [1.69, 3.83]	-2.27 [-3.66, -0.92]	0.24 [0.02, 0.74]	0.69 [0.15, 3.50]	0.31 [-0.16, 0.72]
US/PMF/MT/MD_2	2mgw5	3.51 [1.41, 5.20]	2.44 [1.15, 4.03]	1.61 [-0.08, 3.53]	0.05 [0.00, 0.63]	0.34 [-2.16, 0.80]	-0.09 [-0.65, 0.46]
US/PMF/MT/MD_10	8wns3	3.67 [2.56, 4.54]	3.02 [1.76, 4.21]	-2.93 [-4.18, -1.59]	0.23 [0.00, 0.67]	0.62 [-0.57, 1.75]	0.27 [-0.29, 0.76]
US/PMF/MT/MD_8	cekua	3.73 [2.67, 4.63]	3.24 [2.14, 4.34]	-3.24 [-4.34, -2.14]	0.34 [0.00, 0.76]	0.69 [-0.37, 1.78]	0.31 [-0.23, 0.80]
AMOEBA/BAR/Tinker	tqhg4	3.73 [1.94, 5.25]	2.72 [1.51, 4.17]	1.18 [-0.56, 3.11]	0.14 [0.00, 0.73]	0.83 [-1.62, 1.66]	0.14 [-0.33, 0.60]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	f7duk	3.79 [2.83, 4.68]	3.48 [2.64, 4.41]	2.84 [1.28, 4.23]	0.13 [0.00, 0.73]	0.48 [-1.23, 1.09]	0.09 [-0.56, 0.66]
HREM/BAR/RESP/Force-Matching/TIP3P	3z83m	4.32 [3.23, 5.34]	3.82 [2.78, 4.88]	2.20 [0.18, 4.01]	0.49 [0.13, 0.81]	1.92 [1.30, 3.58]	0.52 [0.19, 0.79]
US/PMF/MT/MD_12	j8yon	4.39 [3.35, 5.27]	4.04 [3.01, 5.05]	4.04 [3.01, 5.05]	0.23 [0.00, 0.67]	0.38 [-0.36, 1.07]	0.27 [-0.29, 0.76]
US/PMF/MT/MD_7	dv8mj	4.41 [3.61, 5.09]	4.17 [3.29, 4.98]	4.17 [3.29, 4.98]	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, 5.83]	4.16 [2.85, 5.45]	-4.16 [-5.45, -2.84]	0.30 [0.06, 0.80]	0.78 [0.31, 3.67]	0.49 [0.08, 0.83]
US/PMF/MT/MD_18	vrsfp	4.79 [3.88, 5.57]	4.43 [3.30, 5.43]	4.43 [3.30, 5.43]	0.08 [0.00, 0.51]	0.14 [-0.39, 0.68]	0.13 [-0.43, 0.66]
US/PMF/MT/MD_4	2vfcf	5.05 [3.87, 6.06]	4.68 [3.54, 5.79]	4.68 [3.54, 5.79]	0.29 [0.05, 0.75]	0.61 [0.18, 2.53]	0.45 [0.00, 0.84]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/A	46vw8	5.07 [3.89, 6.10]	4.47 [3.03, 5.81]	4.41 [2.87, 5.81]	0.13 [0.00, 0.74]	0.48 [-1.22, 1.07]	0.05 [-0.57, 0.63]
US/PMF/MT/MD_22	qfqyx	5.31 [4.15, 6.32]	4.96 [3.83, 6.06]	4.96 [3.83, 6.06]	0.30 [0.05, 0.78]	0.63 [0.24, 2.92]	0.49 [0.08, 0.83]
DDM/Force-Matching/FEP/HREM/MBAR	6jsye	5.43 [3.93, 6.75]	4.77 [3.44, 6.17]	1.13 [-1.77, 3.75]	0.26 [0.00, 0.70]	1.76 [-1.29, 4.92]	0.47 [0.02, 0.82]
US/PMF/MT/MD_16	50jkg	5.44 [4.14, 6.60]	5.00 [3.73, 6.28]	-5.00 [-6.28, -3.73]	0.36 [0.08, 0.73]	0.88 [0.42, 2.95]	0.49 [0.10, 0.88]
US/PMF/MT/MD_9	pz24v	5.45 [4.42, 6.41]	5.17 [4.18, 6.21]	5.17 [4.18, 6.21]	0.34 [0.00, 0.75]	0.62 [-0.35, 1.59]	0.31 [-0.23, 0.80]
US/PMF/MT/MD_3	jb047	5.61 [4.30, 6.70]	5.14 [3.79, 6.43]	-5.14 [-6.43, -3.78]	0.29 [0.05, 0.75]	0.77 [0.23, 3.14]	0.45 [-0.02, 0.84]
US/PMF/MT/MD_21	tcy06	5.81 [4.50, 7.06]	5.39 [4.11, 6.71]	5.39 [4.11, 6.71]	0.30 [0.06, 0.78]	0.76 [0.30, 3.56]	0.49 [0.08, 0.83]
US/PMF/MT/MD_17	k6f5g	5.82 [4.93, 6.58]	5.62 [4.69, 6.46]	5.62 [4.69, 6.46]	0.36 [0.08, 0.73]	0.48 [0.23, 1.65]	0.49 [0.09, 0.88]
US/PMF/MT/MD_14	fy660	6.49 [5.07, 7.81]	6.05 [4.67, 7.47]	-6.05 [-7.46, -4.67]	0.24 [0.02, 0.75]	0.70 [0.14, 3.69]	0.31 [-0.18, 0.74]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	3g2hu	6.61 [5.05, 8.15]	5.99 [4.31, 7.67]	5.96 [4.25, 7.66]	0.13 [0.00, 0.70]	0.58 [-1.42, 1.33]	0.09 [-0.58, 0.66]
DDM/GAFF/AM1-BCC/TIP3P	juz8u	7.21 [5.64, 8.49]	6.65 [4.96, 8.21]	6.44 [4.41, 8.19]	0.29 [0.00, 0.72]	1.14 [-0.41, 2.58]	0.33 [-0.21, 0.76]
US/PMF/MT/MD_6	u6tnc	7.83 [6.73, 8.81]	7.63 [6.55, 8.66]	-7.63 [-8.66, -6.54]	0.39 [0.00, 0.79]	0.75 [-0.43, 1.88]	0.31 [-0.22, 0.76]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	xv5oo	7.87 [6.27, 9.39]	7.33 [5.61, 8.99]	7.33 [5.61, 8.99]	0.13 [0.00, 0.71]	0.57 [-1.47, 1.32]	0.09 [-0.57, 0.67]
US/PMF/MT/MD_1	cbfnz	8.04 [4.89, 11.02]	6.70 [4.33, 9.49]	6.70 [4.33, 9.49]	0.05 [0.00, 0.66]	0.52 [-3.16, 1.24]	-0.09 [-0.65, 0.48]
US/PMF/MT/MD_11	6ux0a	8.23 [6.82, 9.43]	7.86 [6.43, 9.24]	-7.86 [-9.24, -6.43]	0.23 [0.00, 0.67]	0.69 [-0.64, 1.93]	0.27 [-0.29, 0.76]
NULL1	null1	8.59 [7.69, 9.71]	8.42 [7.64, 9.43]	-8.42 [-9.43, -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 [12.07, 21.84]	14.88 [10.50, 19.60]	-14.41 [-19.41, -9.48]	0.00 [0.00, 0.47]	0.07 [-5.24, 7.17]	0.05 [-0.44, 0.54]
EKEN-DIAZ/MD/MMPBSA	6bwq3	17.80 [14.51, 20.75]	16.69 [13.54, 19.93]	16.69 [13.54, 19.93]	0.00 [0.00, 0.66]	-0.09 [-5.73, 1.31]	-0.19 [-0.62, 0.28]
BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	tb3ck	36.99 [29.85, 43.57]	34.29 [26.98, 41.46]	34.29 [26.98, 41.46]	0.00 [0.00, 0.54]	-0.12 [-10.20, 3.76]	-0.14 [-0.57, 0.24]