

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, 0.71]	0.09 [-0.63, 0.64]
US/PMF/MT/MD_15	wtm6p	1.99 [1.32, 2.55]	1.69 [1.08, 2.33]	-0.38 [-1.54, 0.78]	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 [1.44, 3.78]	2.02 [1.10, 3.17]	-1.83 [-3.06, -0.67]	0.13 [0.00, 0.76]	0.24 [-0.91, 0.71]	0.09 [-0.56, 0.68]
US/PMF/MT/MD_19	xdmpa	2.88 [1.68, 3.84]	2.28 [1.29, 3.36]	1.61 [0.24, 3.04]	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 [2.24, 4.00]	2.72 [1.74, 3.70]	-2.72 [-3.70, -1.74]	0.39 [0.00, 0.79]	0.67 [-0.34, 1.67]	0.31 [-0.22, 0.76]
US/PMF/MT/MD_13	cco6p	3.23 [2.01, 4.34]	2.68 [1.69, 3.80]	-2.27 [-3.64, -0.93]	0.24 [0.02, 0.75]	0.69 [0.14, 3.55]	0.31 [-0.17, 0.72]
US/PMF/MT/MD_2	2mgw5	3.51 [1.42, 5.25]	2.44 [1.14, 4.09]	1.61 [-0.07, 3.59]	0.05 [0.00, 0.64]	0.34 [-2.13, 0.81]	-0.09 [-0.65, 0.48]
US/PMF/MT/MD_10	8wns3	3.67 [2.57, 4.55]	3.02 [1.78, 4.22]	-2.93 [-4.19, -1.61]	0.23 [0.00, 0.66]	0.62 [-0.57, 1.77]	0.27 [-0.29, 0.76]
US/PMF/MT/MD_8	cekua	3.73 [2.68, 4.61]	3.24 [2.14, 4.31]	-3.24 [-4.31, -2.14]	0.34 [0.00, 0.75]	0.69 [-0.37, 1.75]	0.31 [-0.23, 0.80]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	f7duk	3.79 [2.68, 5.47]	3.48 [2.33, 4.88]	2.84 [0.99, 4.59]	0.13 [0.00, 0.76]	0.48 [-1.77, 1.38]	0.09 [-0.56, 0.68]
AMOEBA/BAR/Tinker	tqhg4	3.92 [1.55, 5.71]	2.70 [1.18, 4.52]	2.26 [0.52, 4.29]	0.13 [0.00, 0.82]	0.66 [-2.68, 1.39]	0.05 [-0.49, 0.59]
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, 1.06]	0.27 [-0.30, 0.76]
US/PMF/MT/MD_7	dv8mj	4.41 [3.60, 5.08]	4.17 [3.28, 4.98]	4.17 [3.28, 4.98]	0.39 [0.00, 0.79]	0.41 [-0.22, 1.03]	0.31 [-0.22, 0.76]
HREM/BAR/RESP/Force-Matching/TIP3P	3z83m	4.65 [3.39, 5.97]	4.24 [3.07, 5.54]	2.68 [0.17, 4.77]	0.44 [0.05, 0.86]	1.73 [0.84, 3.91]	0.53 [0.14, 0.88]
US/PMF/MT/MD_20	j6oi0	4.72 [3.49, 5.83]	4.16 [2.84, 5.44]	-4.16 [-5.44, -2.84]	0.30 [0.06, 0.79]	0.78 [0.30, 3.61]	0.49 [0.08, 0.83]
US/PMF/MT/MD_18	vrsfp	4.79 [3.87, 5.57]	4.43 [3.29, 5.42]	4.43 [3.29, 5.42]	0.08 [0.00, 0.50]	0.14 [-0.39, 0.69]	0.13 [-0.44, 0.64]
US/PMF/MT/MD_4	2vfcf	5.05 [3.92, 6.06]	4.68 [3.57, 5.80]	4.68 [3.57, 5.80]	0.29 [0.05, 0.75]	0.61 [0.18, 2.51]	0.45 [0.00, 0.84]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/A	46vw8	5.07 [3.78, 6.78]	4.47 [3.16, 6.22]	4.41 [2.59, 6.14]	0.13 [0.00, 0.77]	0.48 [-1.80, 1.35]	0.05 [-0.57, 0.67]
US/PMF/MT/MD_22	qfqyx	5.31 [4.18, 6.34]	4.96 [3.86, 6.08]	4.96 [3.86, 6.08]	0.30 [0.06, 0.79]	0.63 [0.24, 2.90]	0.49 [0.09, 0.83]
US/PMF/MT/MD_16	50jkg	5.44 [4.13, 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 [0.08, 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, 1.60]	0.31 [-0.23, 0.80]
DDM/Force-Matching/FEP/HREM/MBAR	6jsye	5.50 [3.97, 7.25]	5.06 [3.67, 6.65]	2.28 [-1.10, 4.97]	0.42 [0.06, 0.83]	2.12 [0.78, 7.64]	0.64 [0.08, 0.92]
US/PMF/MT/MD_3	jb047	5.61 [4.31, 6.71]	5.14 [3.79, 6.44]	-5.14 [-6.44, -3.79]	0.29 [0.05, 0.75]	0.77 [0.23, 3.16]	0.45 [0.00, 0.84]
US/PMF/MT/MD_21	tcy06	5.81 [4.49, 7.04]	5.39 [4.12, 6.69]	5.39 [4.12, 6.69]	0.30 [0.06, 0.79]	0.76 [0.30, 3.54]	0.49 [0.09, 0.83]
US/PMF/MT/MD_17	k6f5g	5.82 [4.94, 6.59]	5.62 [4.69, 6.48]	5.62 [4.69, 6.48]	0.36 [0.08, 0.72]	0.48 [0.24, 1.63]	0.49 [0.09, 0.88]
US/PMF/MT/MD_14	fy660	6.49 [5.08, 7.82]	6.05 [4.68, 7.45]	-6.05 [-7.45, -4.68]	0.24 [0.02, 0.75]	0.70 [0.15, 3.57]	0.31 [-0.17, 0.72]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	3g2hu	6.61 [4.93, 8.41]	5.99 [4.22, 7.81]	5.96 [4.14, 7.80]	0.13 [0.00, 0.70]	0.58 [-1.58, 1.41]	0.09 [-0.62, 0.65]
DDM/GAFF/AM1-BCC/TIP3P	juz8u	7.21 [5.63, 8.52]	6.65 [4.95, 8.22]	6.44 [4.41, 8.20]	0.29 [0.00, 0.71]	1.14 [-0.42, 2.61]	0.33 [-0.21, 0.76]
US/PMF/MT/MD_6	u6tnc	7.83 [6.76, 8.82]	7.63 [6.57, 8.68]	-7.63 [-8.68, -6.57]	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 [6.15, 9.70]	7.33 [5.49, 9.17]	7.33 [5.49, 9.17]	0.13 [0.00, 0.70]	0.57 [-1.61, 1.40]	0.09 [-0.62, 0.64]
US/PMF/MT/MD_1	cbfnz	8.04 [4.88, 11.02]	6.70 [4.32, 9.54]	6.70 [4.32, 9.54]	0.05 [0.00, 0.64]	0.52 [-3.20, 1.23]	-0.09 [-0.65, 0.48]
US/PMF/MT/MD_11	6ux0a	8.23 [6.81, 9.44]	7.86 [6.43, 9.25]	-7.86 [-9.25, -6.43]	0.23 [0.00, 0.67]	0.69 [-0.64, 1.94]	0.27 [-0.29, 0.76]
NULL	null1	17.65 [14.16, 21.21]	16.82 [13.98, 20.21]	14.88 [8.67, 19.87]	0.01 [0.00, 0.46]	0.52 [-3.88, 3.61]	-0.05 [-0.63, 0.52]
BSSE-corrected RI-B3PW91 (SMD)/CBS	sguyt	17.72 [11.92, 22.89]	15.41 [10.50, 20.77]	-14.80 [-20.60, -9.14]	0.02 [0.00, 0.67]	0.77 [-4.30, 12.69]	0.27 [-0.30, 0.79]
EKEN-DIAZ/MD/MMPBSA	6bwq3	17.94 [13.90, 21.50]	16.73 [12.98, 20.62]	16.73 [12.98, 20.62]	0.02 [0.00, 0.84]	-0.47 [-7.66, 1.06]	-0.42 [-0.88, 0.12]
BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	tb3ck	36.61 [28.74, 44.16]	33.90 [25.72, 42.03]	33.90 [25.72, 42.03]	0.02 [0.00, 0.81]	-1.13 [-14.61, 1.41]	-0.27 [-0.73, 0.21]