

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 + jgbg0 + ttmwo	1.74 [1.29, 2.14]	1.36 [0.96, 1.78]	0.08 [-0.57, 0.74]	0.50 [0.29, 0.72]	0.86 [0.59, 1.48]	0.55 [0.31, 0.75]
US/PMF/MT/MD_19	2kb3u + finzb + xdmpa	1.98 [1.18, 2.64]	1.38 [0.89, 1.95]	0.38 [-0.31, 1.14]	0.54 [0.40, 0.77]	1.07 [0.83, 1.76]	0.58 [0.41, 0.74]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	8jxan + e5rqf + j37ec	2.13 [1.48, 2.71]	1.61 [1.12, 2.16]	-0.13 [-0.94, 0.65]	0.18 [0.02, 0.46]	0.43 [0.15, 0.94]	0.39 [0.11, 0.64]
US/PMF/MT/MD_2	2mgw5 + e7w4x + mknyd	2.36 [1.09, 3.51]	1.45 [0.84, 2.22]	0.38 [-0.40, 1.32]	0.52 [0.30, 0.84]	1.20 [0.92, 1.92]	0.64 [0.42, 0.81]
AMOEBA/BAR/Tinker	8fcb6 + jgdj6 + tqhg4	3.00 [1.95, 3.97]	2.19 [1.51, 2.98]	0.10 [-0.92, 1.23]	0.30 [0.04, 0.64]	1.01 [0.42, 1.33]	0.29 [0.05, 0.52]
US/PMF/MT/MD_12	emfe8 + tydzi + j8yon	3.13 [2.37, 3.84]	2.58 [1.94, 3.27]	2.55 [1.89, 3.25]	0.57 [0.36, 0.75]	1.04 [0.84, 1.59]	0.58 [0.39, 0.76]
US/PMF/MT/MD_7	4ndha + y7u8q + dv8mj	3.14 [2.45, 3.77]	2.66 [2.04, 3.32]	2.64 [2.01, 3.31]	0.63 [0.44, 0.79]	1.10 [0.89, 1.68]	0.61 [0.44, 0.77]
US/PMF/MT/MD_5	nb8jk + tj4jx + ubz3m	3.23 [2.66, 3.74]	2.89 [2.36, 3.42]	0.68 [-0.52, 1.85]	0.00 [0.00, 0.22]	-0.06 [-0.69, 0.26]	-0.08 [-0.36, 0.18]
US/PMF/MT/MD_20	j6oi0 + uui3y + zxx8g	3.33 [2.38, 4.18]	2.51 [1.71, 3.36]	-1.01 [-2.23, 0.18]	0.00 [0.00, 0.10]	0.02 [-0.45, 0.36]	-0.02 [-0.29, 0.23]
US/PMF/MT/MD_10	8wns3 + hs2xm + s78rs	3.34 [2.74, 3.90]	2.93 [2.33, 3.55]	0.51 [-0.77, 1.71]	0.02 [0.00, 0.28]	-0.17 [-0.84, 0.14]	-0.08 [-0.39, 0.21]
US/PMF/MT/MD_13	cco6p + gkdce + ikwy8	3.39 [2.73, 4.04]	2.97 [2.36, 3.61]	0.94 [-0.34, 2.13]	0.00 [0.00, 0.10]	-0.02 [-0.47, 0.32]	-0.11 [-0.38, 0.14]
US/PMF/MT/MD_22	4mas4 + iyo2o + qfqyx	3.53 [2.48, 4.44]	2.61 [1.74, 3.54]	2.50 [1.58, 3.47]	0.60 [0.46, 0.76]	1.43 [1.11, 2.27]	0.61 [0.43, 0.76]
US/PMF/MT/MD_4	2vfcf + gt5n0 + m8t0b	3.57 [2.65, 4.40]	2.85 [2.07, 3.69]	2.83 [2.03, 3.68]	0.63 [0.51, 0.79]	1.35 [1.00, 2.18]	0.61 [0.46, 0.75]
US/PMF/MT/MD_15	ib70e + m0qdw + wtm6p	3.62 [3.03, 4.18]	3.23 [2.60, 3.85]	2.39 [1.35, 3.40]	0.01 [0.00, 0.12]	0.10 [-0.32, 0.30]	0.07 [-0.19, 0.30]
US/PMF/MT/MD_9	7ihag + rkitq + pz24v	3.63 [2.64, 4.54]	2.74 [1.88, 3.69]	1.84 [0.71, 3.06]	0.54 [0.30, 0.74]	1.58 [1.27, 2.34]	0.48 [0.26, 0.68]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	f7duk + ibhca + wfs4v	3.73 [3.05, 4.36]	3.33 [2.71, 3.99]	3.08 [2.27, 3.86]	0.47 [0.16, 0.76]	0.99 [0.61, 1.66]	0.54 [0.29, 0.76]
US/PMF/MT/MD_18	70hpk + xcuey + vrsfp	3.77 [3.15, 4.36]	3.42 [2.82, 4.03]	3.42 [2.82, 4.03]	0.57 [0.43, 0.75]	0.91 [0.67, 1.51]	0.54 [0.38, 0.69]
US/PMF/MT/MD_21	45sgk + ftout + tcy06	4.12 [3.09, 5.09]	3.33 [2.47, 4.29]	3.30 [2.41, 4.26]	0.61 [0.48, 0.77]	1.45 [1.11, 2.34]	0.61 [0.43, 0.77]
US/PMF/MT/MD_17	iaz7f + n7b3v + k6f5g	4.15 [3.29, 4.92]	3.60 [2.85, 4.40]	3.60 [2.85, 4.40]	0.60 [0.42, 0.77]	1.23 [0.97, 1.91]	0.62 [0.45, 0.78]
US/PMF/MT/MD_16	50jkg + d6js7 + ogd0g	4.30 [3.51, 5.06]	3.91 [3.27, 4.61]	-0.16 [-1.82, 1.44]	0.09 [0.01, 0.35]	-0.49 [-1.29, -0.15]	-0.20 [-0.43, 0.04]
US/PMF/MT/MD_3	3cxbd + widya + jb047	4.30 [3.43, 5.10]	3.77 [3.01, 4.57]	-0.41 [-2.04, 1.13]	0.06 [0.00, 0.25]	-0.42 [-1.07, -0.08]	-0.20 [-0.44, 0.05]
US/PMF/MT/MD_8	cekua + e032m + mhwfc	4.46 [3.43, 5.48]	3.73 [2.83, 4.70]	0.44 [-1.21, 2.18]	0.02 [0.00, 0.25]	-0.26 [-1.16, 0.19]	-0.15 [-0.41, 0.11]
US/PMF/MT/MD_14	fy660 + oby4 + rc4qr	4.77 [3.72, 5.77]	4.10 [3.21, 5.06]	-0.86 [-2.66, 0.86]	0.10 [0.01, 0.38]	-0.58 [-1.33, -0.21]	-0.27 [-0.52, -0.02]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	3g2hu + 8pqor + iv75a	4.82 [3.68, 5.93]	3.91 [2.89, 5.00]	3.82 [2.75, 4.95]	0.63 [0.40, 0.84]	1.71 [1.36, 2.55]	0.64 [0.44, 0.79]
DDM/GAFF/AM1-BCC/TIP3P	ct5x2 + yedi3 + juz8u	5.29 [4.06, 6.41]	4.29 [3.18, 5.51]	3.23 [1.61, 4.81]	0.51 [0.18, 0.80]	1.92 [1.44, 2.72]	0.56 [0.31, 0.77]
US/PMF/MT/MD_6	bhhbs + egmst + u6tnc	5.35 [4.15, 6.43]	4.46 [3.40, 5.58]	-1.76 [-3.67, 0.09]	0.16 [0.03, 0.49]	-0.78 [-1.83, -0.29]	-0.21 [-0.43, 0.04]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/A	46vw8 + mdqkg + s3kiu	5.44 [4.70, 6.12]	5.03 [4.21, 5.80]	5.00 [4.16, 5.79]	0.41 [0.10, 0.73]	0.90 [0.48, 1.54]	0.52 [0.27, 0.75]
US/PMF/MT/MD_11	6ux0a + 7fk2x + wfrgr	5.57 [4.17, 6.81]	4.50 [3.30, 5.77]	-1.91 [-3.93, 0.01]	0.18 [0.04, 0.52]	-0.88 [-2.01, -0.37]	-0.24 [-0.48, 0.01]
US/PMF/MT/MD_1	4ysuf + t5gev + cbfnz	5.59 [3.58, 7.59]	4.21 [2.97, 5.73]	4.21 [2.97, 5.73]	0.50 [0.28, 0.84]	1.72 [1.31, 2.79]	0.64 [0.42, 0.80]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	bhns3 + qa7zq + xv5oo	6.29 [5.22, 7.33]	5.67 [4.66, 6.71]	5.67 [4.66, 6.71]	0.62 [0.37, 0.83]	1.58 [1.24, 2.36]	0.63 [0.41, 0.80]
NULL1	null1 + null2 + null3	7.29 [6.53, 8.12]	7.02 [6.34, 7.78]	-7.02 [-7.78, -6.34]	0.00 [0.00, 0.00]	0.00 [0.00, 0.00]	nan [nan, nan]
EKEN-DIAZ/MD/MMPBSA	6bwq3 + 8brzp + caknz	13.20 [10.37, 15.81]	11.18 [8.79, 13.75]	11.18 [8.79, 13.75]	0.44 [0.21, 0.72]	2.76 [1.96, 4.27]	0.54 [0.29, 0.74]
BSSE-corrected RI-B3PW91 (SMD)/CBS	5r5n7 + btcyu + sguyt	16.95 [11.75, 22.45]	13.37 [10.03, 17.51]	-3.83 [-10.06, 1.76]	0.31 [0.14, 0.61]	-4.32 [-8.07, -2.46]	-0.48 [-0.66, -0.29]
BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	e85s6 + kuovg + tb3ck	37.39 [33.83, 40.80]	35.81 [31.85, 39.55]	34.82 [29.43, 39.28]	0.00 [0.00, 0.24]	-0.48 [-4.45, 1.65]	0.04 [-0.29, 0.38]