

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 [1.31, 2.21]	1.36 [0.98, 1.84]	0.08 [-0.60, 0.77]	0.50 [0.27, 0.71]	0.86 [0.57, 1.48]	0.55 [0.31, 0.75]
US/PMF/MT/MD_19	2kb3u + finzb + xdmpa	1.98 [1.20, 2.65]	1.38 [0.89, 1.95]	0.38 [-0.31, 1.15]	0.54 [0.39, 0.76]	1.07 [0.83, 1.75]	0.58 [0.41, 0.74]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	8jxan + e5rqf + j37ec	2.13 [1.50, 2.86]	1.61 [1.12, 2.24]	-0.13 [-0.99, 0.68]	0.18 [0.01, 0.48]	0.43 [0.10, 0.95]	0.39 [0.09, 0.63]
US/PMF/MT/MD_2	2mgw5 + e7w4x + mknyd	2.36 [1.09, 3.52]	1.45 [0.85, 2.23]	0.38 [-0.40, 1.34]	0.52 [0.30, 0.84]	1.20 [0.92, 1.93]	0.64 [0.42, 0.80]
AMOEBA/BAR/Tinker	8fcb6 + jgdj6 + tqhg4	3.00 [1.95, 3.97]	2.19 [1.51, 2.97]	0.10 [-0.92, 1.22]	0.30 [0.04, 0.64]	1.01 [0.41, 1.33]	0.29 [0.05, 0.51]
US/PMF/MT/MD_12	emfe8 + tydzi + j8yon	3.13 [2.36, 3.84]	2.58 [1.93, 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, 3.31]	2.64 [2.02, 3.30]	0.63 [0.44, 0.79]	1.10 [0.89, 1.68]	0.61 [0.45, 0.77]
US/PMF/MT/MD_5	nb8jk + tj4jx + ubz3m	3.23 [2.67, 3.76]	2.89 [2.36, 3.44]	0.68 [-0.53, 1.85]	0.00 [0.00, 0.21]	-0.06 [-0.68, 0.27]	-0.08 [-0.35, 0.19]
US/PMF/MT/MD_20	j6oi0 + uui3y + zxx8g	3.33 [2.40, 4.18]	2.51 [1.73, 3.36]	-1.01 [-2.23, 0.16]	0.00 [0.00, 0.10]	0.02 [-0.44, 0.35]	-0.02 [-0.29, 0.23]
US/PMF/MT/MD_10	8wns3 + hs2xm + s78rs	3.34 [2.75, 3.89]	2.93 [2.34, 3.54]	0.51 [-0.77, 1.71]	0.02 [0.00, 0.28]	-0.17 [-0.84, 0.14]	-0.08 [-0.39, 0.22]
US/PMF/MT/MD_13	cco6p + gkdce + ikwy8	3.39 [2.73, 4.03]	2.97 [2.36, 3.60]	0.94 [-0.32, 2.14]	0.00 [0.00, 0.10]	-0.02 [-0.46, 0.32]	-0.11 [-0.38, 0.14]
US/PMF/MT/MD_22	4mas4 + iyo2o + qfqyx	3.53 [2.50, 4.45]	2.61 [1.75, 3.54]	2.50 [1.59, 3.47]	0.60 [0.45, 0.76]	1.43 [1.11, 2.27]	0.61 [0.43, 0.76]
US/PMF/MT/MD_4	2vfcf + gt5n0 + m8t0b	3.57 [2.66, 4.39]	2.85 [2.06, 3.68]	2.83 [2.03, 3.67]	0.63 [0.52, 0.79]	1.35 [1.01, 2.17]	0.61 [0.46, 0.75]
US/PMF/MT/MD_15	ib70e + m0qdw + wtm6p	3.62 [3.04, 4.17]	3.23 [2.61, 3.84]	2.39 [1.33, 3.39]	0.01 [0.00, 0.12]	0.10 [-0.32, 0.31]	0.07 [-0.18, 0.30]
US/PMF/MT/MD_9	7ihag + rkitq + pz24v	3.63 [2.61, 4.53]	2.74 [1.86, 3.68]	1.84 [0.68, 3.05]	0.54 [0.30, 0.74]	1.58 [1.26, 2.34]	0.48 [0.26, 0.68]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	f7duk + ibhca + wfs4v	3.73 [3.04, 4.62]	3.33 [2.64, 4.12]	3.08 [2.15, 3.96]	0.47 [0.09, 0.78]	0.99 [0.49, 1.69]	0.54 [0.25, 0.75]
US/PMF/MT/MD_18	70hpk + xcuey + vrsfp	3.77 [3.16, 4.35]	3.42 [2.83, 4.02]	3.42 [2.83, 4.02]	0.57 [0.44, 0.75]	0.91 [0.68, 1.51]	0.54 [0.38, 0.69]
US/PMF/MT/MD_21	45sgk + ftout + tcy06	4.12 [3.10, 5.09]	3.33 [2.46, 4.28]	3.30 [2.41, 4.26]	0.61 [0.49, 0.77]	1.45 [1.11, 2.32]	0.61 [0.42, 0.77]
US/PMF/MT/MD_17	iaz7f + n7b3v + k6f5g	4.15 [3.31, 4.91]	3.60 [2.86, 4.40]	3.60 [2.86, 4.40]	0.60 [0.43, 0.77]	1.23 [0.97, 1.91]	0.62 [0.45, 0.78]
US/PMF/MT/MD_16	50jkg + d6js7 + ogd0g	4.30 [3.52, 5.07]	3.91 [3.27, 4.61]	-0.16 [-1.82, 1.40]	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 [3.02, 4.57]	-0.41 [-2.07, 1.15]	0.06 [0.00, 0.25]	-0.42 [-1.06, -0.08]	-0.20 [-0.44, 0.05]
US/PMF/MT/MD_8	cekua + e032m + mhwfc	4.46 [3.44, 5.46]	3.73 [2.84, 4.69]	0.44 [-1.19, 2.15]	0.02 [0.00, 0.25]	-0.26 [-1.17, 0.18]	-0.15 [-0.41, 0.10]
US/PMF/MT/MD_14	fy660 + oby4 + rc4qr	4.77 [3.72, 5.77]	4.10 [3.21, 5.05]	-0.86 [-2.66, 0.86]	0.10 [0.01, 0.37]	-0.58 [-1.33, -0.21]	-0.27 [-0.51, -0.01]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	3g2hu + 8pqor + iv75a	4.82 [3.65, 6.09]	3.91 [2.89, 5.08]	3.82 [2.70, 5.02]	0.63 [0.37, 0.84]	1.71 [1.32, 2.58]	0.64 [0.42, 0.80]
DDM/GAFF/AM1-BCC/TIP3P	ct5x2 + yedi3 + juz8u	5.29 [4.06, 6.40]	4.29 [3.16, 5.48]	3.23 [1.63, 4.77]	0.51 [0.19, 0.79]	1.92 [1.44, 2.73]	0.56 [0.31, 0.77]
US/PMF/MT/MD_6	bhhbs + egmst + u6tnc	5.35 [4.13, 6.44]	4.46 [3.39, 5.60]	-1.76 [-3.70, 0.10]	0.16 [0.03, 0.50]	-0.78 [-1.83, -0.29]	-0.21 [-0.43, 0.04]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/A	46vw8 + mdqkg + s3kiu	5.44 [4.69, 6.32]	5.03 [4.27, 5.93]	5.00 [4.06, 5.90]	0.41 [0.06, 0.74]	0.90 [0.39, 1.56]	0.52 [0.22, 0.74]
US/PMF/MT/MD_11	6ux0a + 7fk2x + wfrgr	5.57 [4.16, 6.80]	4.50 [3.30, 5.77]	-1.91 [-3.93, 0.02]	0.18 [0.05, 0.52]	-0.88 [-2.00, -0.38]	-0.24 [-0.48, 0.01]
US/PMF/MT/MD_1	4ysuf + t5gev + cbfnz	5.59 [3.59, 7.60]	4.21 [2.96, 5.72]	4.21 [2.96, 5.72]	0.50 [0.28, 0.85]	1.72 [1.31, 2.77]	0.64 [0.42, 0.80]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	bhns3 + qa7zq + xv5oo	6.29 [5.20, 7.50]	5.67 [4.63, 6.78]	5.67 [4.63, 6.78]	0.62 [0.35, 0.83]	1.58 [1.21, 2.39]	0.63 [0.39, 0.79]
NULL1	null1 + null2 + null3	7.29 [6.53, 8.11]	7.02 [6.34, 7.75]	-7.02 [-7.75, -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 [10.36, 15.84]	11.18 [8.76, 13.78]	11.18 [8.76, 13.78]	0.44 [0.20, 0.72]	2.76 [1.95, 4.27]	0.54 [0.27, 0.72]
BSSE-corrected RI-B3PW91 (SMD)/CBS	5r5n7 + btcyu + sguyt	16.95 [11.70, 22.46]	13.37 [10.00, 17.39]	-3.83 [-9.99, 1.81]	0.31 [0.14, 0.61]	-4.32 [-8.08, -2.50]	-0.48 [-0.66, -0.30]
BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	e85s6 + kuovg + tb3ck	37.39 [33.87, 40.84]	35.81 [31.83, 39.58]	34.82 [29.59, 39.34]	0.00 [0.00, 0.24]	-0.48 [-4.38, 1.64]	0.04 [-0.28, 0.38]