ID	receipt_id	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)	R^2	m	τ
US/PMF/MT/MD_2	e7w4x + mknyd	0.95 [0.64, 1.22]	0.77 [0.51, 1.05]	-0.46 [-0.88, -0.07]	0.85 [0.61, 0.95]	1.39 [1.12, 1.62]	0.74 [0.44, 0.95]
US/PMF/MT/MD_19	2kb3u + finzb	0.96 [0.66, 1.21]	0.77 [0.49, 1.05]	-0.46 [-0.87, -0.05]	0.60 [0.16, 0.85]	0.83 [0.34, 1.22]	0.37 [-0.13, 0.72]
US/PMF/MT/MD_22	4mas4 + iyo2o	1.30 [0.76, 1.82]	0.99 [0.62, 1.44]	0.81 [0.33, 1.33]	0.33 [0.01, 0.76]	0.46 [-0.04, 0.81]	0.33 [-0.14, 0.73]
US/PMF/MT/MD_9	7ihag + rkitq	1.36 [0.87, 1.78]	1.07 [0.68, 1.50]	-0.45 [-1.10, 0.15]	0.01 [0.00, 0.30]	0.06 [-0.23, 0.31]	0.07 [-0.35, 0.44]
US/PMF/MT/MD_23	7uted + zks3c	1.46 [1.15, 1.73]	1.31 [0.99, 1.62]	-0.67 [-1.26, 0.01]	0.34 [0.02, 0.74]	0.75 [0.10, 1.37]	0.31 [-0.17, 0.70]
FEP-MM	n6f0q + w2q3q	1.50 [1.19, 1.79]	1.34 [1.02, 1.68]	-1.18 [-1.62, -0.68]	0.66 [0.31, 0.90]	1.07 [0.60, 1.65]	0.62 [0.22, 0.89]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/D	jgbg0 + ttmwo	1.59 [1.02, 2.15]	1.26 [0.78, 1.81]	0.29 [-0.50, 1.11]	0.79 [0.55, 0.92]	1.87 [1.29, 2.51]	0.70 [0.43, 0.91]
FEP-QM/MM	ahtcq + sdm0h	1.62 [1.29, 1.99]	1.45 [1.12, 1.86]	-1.02 [-1.60, -0.32]	0.76 [0.58, 0.95]	1.55 [0.97, 2.33]	0.77 [0.50, 0.93]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	8jxan + e5rqf	1.76 [1.07, 2.39]	1.33 [0.83, 1.97]	1.04 [0.35, 1.78]	0.78 [0.55, 0.94]	1.74 [1.21, 2.34]	0.70 [0.41, 0.91]
US/PMF/MT/MD_7	4ndha + y7u8q	1.81 [1.36, 2.31]	1.62 [1.24, 2.05]	1.59 [1.18, 2.04]	0.48 [0.07, 0.87]	0.48 [0.17, 0.82]	0.45 [0.07, 0.75]
US/PMF/MT/MD_12	emfe8 + tydzi	1.82 [1.33, 2.29]	1.57 [1.14, 2.03]	1.52 [1.03, 2.01]	0.32 [0.01, 0.76]	0.29 [0.01, 0.57]	0.37 [-0.07, 0.74]
US/PMF/MT/MD_20	uui3y + zxx8g	1.85 [1.04, 2.55]	1.38 [0.83, 2.02]	1.15 [0.48, 1.89]	0.33 [0.01, 0.76]	0.83 [-0.08, 1.46]	0.33 [-0.15, 0.72]
US/PMF/MT/MD_4	gt5n0 + m8t0b	1.99 [1.33, 2.56]	1.59 [1.03, 2.20]	1.56 [0.98, 2.18]	0.42 [0.05, 0.77]	0.86 [0.26, 1.38]	0.35 [-0.08, 0.68]
US/PMF/MT/MD_26	jomge + o3aiv	2.00 [1.29, 2.67]	1.59 [1.02, 2.22]	1.50 [0.87, 2.18]	0.33 [0.01, 0.74]	0.77 [-0.03, 1.34]	0.22 [-0.24, 0.58]
AMOEBA/BAR/Tinker	8fcb6 + jgdj6	2.17 [1.33, 2.89]	1.72 [1.12, 2.41]	-0.85 [-1.85, 0.10]	0.13 [0.00, 0.48]	-0.37 [-0.83, 0.10]	-0.23 [-0.59, 0.15]
US/PMF/MT/MD_25	ei3s2 + vgqcz	2.17 [1.55, 2.76]	1.89 [1.40, 2.44]	1.89 [1.40, 2.44]	0.34 [0.02, 0.74]	0.55 [0.07, 1.00]	0.31 [-0.17, 0.70]
US/PMF/MT/MD_21	45sgk + ftout	2.34 [1.54, 3.07]	1.92 [1.32, 2.61]	1.86 [1.21, 2.59]	0.33 [0.01, 0.76]	0.80 [-0.08, 1.42]	0.33 [-0.15, 0.73]
US/PMF/MT/MD_17	iaz7f + n7b3v	2.40 [1.94, 2.86]	2.22 [1.78, 2.68]	2.22 [1.78, 2.68]	0.46 [0.06, 0.83]	0.35 [0.10, 0.61]	0.39 [-0.07, 0.75]
US/PMF/MT/MD_11	7fk2x + wfrgr	2.41 [1.87, 2.93]	2.18 [1.70, 2.70]	2.18 [1.70, 2.70]	0.32 [0.01, 0.76]	0.41 [0.02, 0.80]	0.37 [-0.07, 0.74]
US/PMF/MT/MD_6	bhhbs + egmst	2.46 [1.96, 3.02]	2.28 [1.86, 2.77]	2.28 [1.86, 2.77]	0.48 [0.08, 0.87]	0.66 [0.23, 1.15]	0.46 [0.08, 0.75]
US/PMF/MT/MD_24	5rmun + aai8i	2.46 [1.80, 3.09]	2.18 [1.66, 2.77]	2.18 [1.66, 2.77]	0.34 [0.02, 0.74]	0.63 [0.08, 1.15]	0.31 [-0.17, 0.70]
FS-DAM/GAFF2/TIP3P	gemch + pbo45	2.50 [1.54, 3.30]	1.90 [1.14, 2.73]	0.76 [-0.46, 1.87]	0.47 [0.02, 0.89]	1.73 [0.17, 2.53]	0.48 [0.02, 0.85]
US/PMF/MT/MD_27	8pxph + kv2ub	2.62 [2.02, 3.22]	2.38 [1.88, 2.95]	2.38 [1.88, 2.95]	0.33 [0.01, 0.74]	0.57 [-0.01, 1.00]	0.22 [-0.23, 0.58]
SQM-opt	c8jfq + vwkb0	2.66 [1.83, 3.42]	2.18 [1.48, 2.96]	1.13 [-0.04, 2.32]	0.09 [0.00, 0.70]	0.64 [-0.50, 2.25]	0.31 [-0.19, 0.76]
US/PMF/MT/MD_18	70hpk + xcuey	2.86 [2.41, 3.32]	2.72 [2.29, 3.17]	2.72 [2.29, 3.17]	0.49 [0.09, 0.81]	0.65 [0.27, 1.00]	0.33 [-0.12, 0.66]
US/PMF/MT/MD_1	4ysuf + t5gev	2.89 [2.21, 3.46]	2.50 [1.79, 3.20]	2.50 [1.79, 3.20]	0.85 [0.61, 0.95]	1.91 [1.54, 2.23]	0.74 [0.44, 0.95]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	8pqor + iv75a	3.03 [2.14, 3.87]	2.49 [1.69, 3.40]	2.35 [1.38, 3.33]	0.82 [0.55, 0.93]	2.21 [1.61, 2.82]	0.70 [0.41, 0.91]
DFT-opt	NB001 + bjyua	3.06 [2.30, 3.74]	2.70 [2.01, 3.42]	-1.57 [-2.80, -0.24]	0.54 [0.08, 0.80]	2.08 [0.61, 2.98]	0.35 [-0.08, 0.68]
US/PMF/MT/MD_14	obyj4 + rc4qr	3.07 [2.37, 3.76]	2.76 [2.12, 3.44]	2.72 [2.03, 3.43]	0.31 [0.01, 0.74]	0.78 [-0.05, 1.32]	0.25 [-0.23, 0.63]
US/PMF/MT/MD_3	3cxbd + widya	3.09 [2.44, 3.70]	2.83 [2.26, 3.46]	2.83 [2.26, 3.46]	0.42 [0.05, 0.77]	0.85 [0.27, 1.36]	0.35 [-0.08, 0.68]
US/PMF/MT/MD_10	hs2xm + s78rs	3.10 [2.46, 3.73]	2.87 [2.34, 3.47]	2.87 [2.34, 3.47]	0.32 [0.01, 0.76]	0.60 [0.01, 1.16]	0.37 [-0.08, 0.74]
US/PMF/MT/MD_5	nb8jk + tj4jx	3.25 [2.58, 3.95]	3.01 [2.46, 3.65]	3.01 [2.46, 3.65]	0.48 [0.08, 0.87]	0.97 [0.34, 1.67]	0.46 [0.08, 0.75]
US/PMF/MT/MD_16	d6js7 + ogd0g	3.28 [2.83, 3.76]	3.16 [2.75, 3.61]	3.16 [2.75, 3.61]	0.46 [0.06, 0.83]	0.49 [0.14, 0.85]	0.40 [-0.06, 0.75]
DDM/GAFF/AM1-BCC/TIP3P	ct5x2 + yedi3	3.38 [2.13, 4.56]	2.66 [1.72, 3.75]	1.02 [-0.68, 2.47]	0.11 [0.00, 0.82]	0.96 [-1.32, 2.67]	0.37 [-0.13, 0.81]
US/PMF/MT/MD_13	gkdce + ikwy8	3.50 [2.74, 4.23]	3.16 [2.44, 3.91]	3.14 [2.39, 3.90]	0.31 [0.01, 0.74]	0.85 [-0.06, 1.44]	0.25 [-0.23, 0.63]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	ibhca + wfs4v	3.69 [2.75, 4.55]	3.24 [2.37, 4.14]	3.24 [2.37, 4.14]	0.81 [0.57, 0.94]	2.08 [1.53, 2.69]	0.73 [0.40, 0.93]
US/PMF/MT/MD_15	ib70e + m0qdw	4.41 [3.90, 4.95]	4.29 [3.84, 4.80]	4.29 [3.84, 4.80]	0.46 [0.06, 0.83]	0.71 [0.21, 1.24]	0.40 [-0.07, 0.75]
US/PMF/MT/MD_8	e032m + mhwfc	4.90 [3.39, 6.26]	4.07 [2.80, 5.46]	2.97 [1.04, 4.85]	0.01 [0.00, 0.30]	0.38 [-1.43, 1.97]	0.07 [-0.35, 0.44]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	bhns3 + qa7zq	4.93 [3.94, 5.86]	4.54 [3.57, 5.52]	4.54 [3.57, 5.52]	0.82 [0.57, 0.93]	2.22 [1.63, 2.85]	0.73 [0.43, 0.91]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/A	mdqkg + s3kiu	5.69 [4.74, 6.59]	5.40 [4.53, 6.32]	5.40 [4.53, 6.32]	0.82 [0.59, 0.94]	2.10 [1.57, 2.70]	0.75 [0.45, 0.93]
NULL1	null2 + null3	5.92 [5.31, 6.53]	5.79 [5.23, 6.40]	-5.79 [-6.40, -5.23]	0.00 [0.00, 0.00]	0.00 [0.00, 0.00]	nan [nan, nan]
EKEN-DIAZ/MD/MMPBSA	8brzp + caknz	7.04 [5.44, 8.53]	6.36 [4.94, 7.88]	6.36 [4.94, 7.88]	0.79 [0.57, 0.93]	2.98 [2.25, 3.85]	0.65 [0.36, 0.84]
BSSE-corrected RI-B3PW91 (SMD)/CBS	5r5n7 + btcyu	16.67 [8.67, 25.21]	12.04 [7.56, 18.50]	5.43 [-3.38, 11.09]	0.33 [0.00, 0.71]	-7.14 [-15.00, 0.96]	-0.23 [-0.66, 0.25]
BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	e85s6 + kuovg	37.74 [34.75, 40.12]	37.14 [33.47, 39.95]	35.28 [27.81, 39.95]	0.11 [0.03, 0.84]	-3.56 [-11.29, 4.12]	0.40 [-0.09, 0.86]

* NB001 was not submitted before the deadline because of a technical issue, and it was received after the experimental results were published.