ID	receipt_id	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)	R^2	m	τ
US/PMF/MT/MD_2	e7w4x	1.20 [0.75, 1.54]	1.03 [0.59, 1.46]	-0.69 [-1.36, -0.00]	0.90 [0.62, 0.99]	1.65 [1.26, 2.00]	0.79 [0.25, 1.00]
US/PMF/MT/MD_19	2kb3u	1.26 [0.91, 1.53]	1.13 [0.71, 1.50]	-0.69 [-1.37, 0.10]	0.27 [0.01, 0.90]	0.43 [-0.43, 1.41]	0.29 [-0.50, 0.90]
Umbrella Sampling/TIP3P	vq30p	1.33 [0.73, 2.08]	1.02 [0.54, 1.86]	-0.07 [-1.14, 0.99]	0.50 [0.00, 0.95]	1.12 [-0.47, 2.59]	0.36 [-0.42, 1.00]
US/PMF/MT/MD_23	zks3c	1.38 [0.95, 1.79]	1.24 [0.83, 1.67]	-0.01 [-0.91, 0.98]	0.19 [0.00, 0.82]	0.53 [-0.59, 1.83]	0.33 [-0.44, 0.96]
FEP-QM/MM	sdm0h	1.49 [0.97, 2.13]	1.32 [0.83, 1.93]	-0.45 [-1.39, 0.68]	0.93 [0.74, 0.99]	2.08 [1.27, 2.84]	0.86 [0.43, 1.00]
FEP-MM	n6f0q	1.52 [1.02, 1.95]	1.31 [0.82, 1.85]	-1.12 [-1.80, -0.35]	0.59 [0.02, 0.97]	1.05 [-0.17, 2.07]	0.50 [-0.30, 1.00]
US/PMF/MT/MD_9	7ihag	1.54 [0.88, 2.06]	1.27 [0.69, 1.89]	-0.82 [-1.72, 0.08]	0.05 [0.00, 0.59]	-0.08 [-0.44, 0.09]	-0.14 [-0.58, 0.42]
US/PMF/MT/MD_22	4mas4	1.66 [0.84, 2.37]	1.31 [0.66, 2.06]	1.04 [0.18, 1.96]	0.08 [0.00, 0.87]	0.24 [-0.82, 1.04]	0.00 [-0.83, 0.67]
US/PMF/MT/MD_4	m8t0b	1.99 [0.61, 2.95]	1.41 [0.53, 2.47]	1.34 [0.42, 2.44]	0.34 [0.00, 0.97]	0.91 [-0.60, 2.27]	0.50 [-0.17, 1.00]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/D	jgbg0	2.05 [1.20, 2.77]	1.72 [0.92, 2.55]	0.48 [-0.93, 1.89]	0.95 [0.73, 0.99]	2.60 [2.12, 3.16]	0.86 [0.48, 1.00]
US/PMF/MT/MD_12	tydzi	2.08 [1.27, 2.79]	1.83 [1.21, 2.57]	1.83 [1.21, 2.57]	0.26 [0.01, 0.97]	0.29 [-0.32, 0.91]	0.36 [-0.39, 1.00]
US/PMF/MT/MD_7	y7u8q	2.11 [1.45, 2.84]	1.92 [1.40, 2.60]	1.92 [1.40, 2.60]	0.43 [0.01, 0.97]	0.48 [-0.18, 1.04]	0.25 [-0.57, 0.83]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	e5rqf	2.11 [0.99, 2.99]	1.58 [0.73, 2.64]	1.40 [0.31, 2.56]	0.94 [0.73, 0.99]	2.24 [1.69, 2.85]	0.86 [0.48, 1.00]
AMOEBA/BAR/Tinker	jgdj6	2.12 [1.07, 3.01]	1.68 [0.86, 2.63]	-0.93 [-2.28, 0.36]	0.07 [0.00, 0.64]	-0.28 [-1.37, 0.48]	-0.07 [-0.67, 0.57]
US/PMF/MT/MD_20	zxx8g	2.39 [1.19, 3.33]	1.96 [1.10, 2.97]	1.54 [0.29, 2.83]	0.08 [0.00, 0.87]	0.43 [-1.48, 1.90]	0.00 [-0.83, 0.67]
US/PMF/MT/MD_26	jomge	2.55 [1.49, 3.45]	2.12 [1.16, 3.12]	2.12 [1.16, 3.12]	0.21 [0.00, 0.90]	0.59 [-1.03, 1.82]	0.07 [-0.83, 0.67]
US/PMF/MT/MD_17	n7b3v	2.59 [1.81, 3.31]	2.40 [1.79, 3.12]	2.40 [1.79, 3.12]	0.29 [0.01, 0.91]	0.33 [-0.38, 1.00]	0.36 [-0.50, 1.00]
US/PMF/MT/MD_25	ei3s2	2.66 [1.75, 3.44]	2.38 [1.62, 3.23]	2.38 [1.62, 3.23]	0.19 [0.00, 0.83]	0.38 [-0.43, 1.34]	0.33 [-0.44, 0.96]
US/PMF/MT/MD_1	t5gev	2.76 [1.51, 3.68]	2.17 [1.01, 3.36]	2.17 [1.01, 3.36]	0.90 [0.62, 0.99]	2.26 [1.74, 2.77]	0.79 [0.25, 1.00]
US/PMF/MT/MD_11	wfrgr	2.79 [2.00, 3.55]	2.59 [1.94, 3.36]	2.59 [1.94, 3.36]	0.27 [0.01, 0.97]	0.41 [-0.44, 1.26]	0.36 [-0.39, 1.00]
US/PMF/MT/MD_21	45sgk	2.87 [1.58, 3.90]	2.35 [1.27, 3.53]	2.24 [1.01, 3.50]	0.08 [0.00, 0.87]	0.41 [-1.44, 1.85]	0.00 [-0.83, 0.67]
US/PMF/MT/MD_6	bhhbs	2.88 [2.16, 3.67]	2.71 [2.14, 3.47]	2.71 [2.14, 3.47]	0.43 [0.01, 0.97]	0.68 [-0.26, 1.46]	0.29 [-0.48, 0.83]
FS-DAM/GAFF2/TIP3P	pbo45	2.91 [1.36, 4.06]	2.24 [1.03, 3.58]	-0.03 [-2.06, 1.95]	0.34 [0.00, 0.96]	1.72 [-1.55, 3.06]	0.29 [-0.57, 1.00]
US/PMF/MT/MD_18	70hpk	2.91 [2.00, 3.70]	2.66 [1.87, 3.51]	2.66 [1.87, 3.51]	0.27 [0.01, 0.90]	0.56 [-0.55, 1.78]	0.29 [-0.50, 0.89]
US/PMF/MT/MD_8	mhwfc	2.97 [2.04, 3.75]	2.58 [1.53, 3.57]	0.38 [-1.78, 2.29]	0.05 [0.00, 0.59]	-0.49 [-2.75, 0.55]	-0.14 [-0.58, 0.42]
US/PMF/MT/MD_3	3cxbd	3.00 [1.77, 4.06]	2.62 [1.71, 3.72]	2.62 [1.71, 3.72]	0.34 [0.00, 0.97]	0.90 [-0.62, 2.28]	0.50 [-0.17, 1.00]
US/PMF/MT/MD_24	5rmun	3.01 [2.04, 3.84]	2.74 [1.92, 3.63]	2.74 [1.92, 3.63]	0.19 [0.00, 0.82]	0.44 [-0.50, 1.54]	0.33 [-0.44, 0.96]
US/PMF/MT/MD_27	kv2ub	3.09 [2.21, 3.91]	2.86 [2.08, 3.71]	2.86 [2.08, 3.71]	0.21 [0.00, 0.90]	0.43 [-0.74, 1.34]	0.07 [-0.83, 0.67]
SQM-opt	vwkb0	3.23 [2.03, 4.26]	2.80 [1.71, 3.94]	2.55 [1.16, 3.89]	0.14 [0.00, 0.90]	0.68 [-1.51, 2.99]	0.36 [-0.50, 1.00]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	8pqor	3.33 [1.72, 4.57]	2.63 [1.32, 4.11]	2.40 [0.79, 4.03]	0.95 [0.73, 0.99]	2.86 [2.31, 3.48]	0.86 [0.48, 1.00]
US/PMF/MT/MD_16	d6js7	3.54 [2.77, 4.29]	3.39 [2.73, 4.14]	3.39 [2.73, 4.14]	0.30 [0.01, 0.91]	0.46 [-0.53, 1.40]	0.36 [-0.50, 1.00]
US/PMF/MT/MD_10	hs2xm	3.67 [2.71, 4.54]	3.45 [2.64, 4.36]	3.45 [2.64, 4.36]	0.27 [0.01, 0.96]	0.60 [-0.65, 1.84]	0.36 [-0.39, 1.00]
US/PMF/MT/MD_14	obyj4	3.69 [2.60, 4.63]	3.29 [2.10, 4.41]	3.21 [1.90, 4.41]	0.10 [0.00, 0.80]	0.50 [-1.47, 1.78]	0.00 [-1.00, 0.57]
DFT-opt	NB001	3.71 [2.77, 4.52]	3.49 [2.62, 4.37]	-2.85 [-4.30, -1.05]	0.57 [0.02, 0.91]	2.03 [-0.11, 4.11]	0.29 [-0.50, 0.90]
US/PMF/MT/MD_5	tj4jx	3.85 [2.84, 4.81]	3.62 [2.78, 4.59]	3.62 [2.78, 4.59]	0.43 [0.01, 0.97]	0.99 [-0.31, 2.12]	0.29 [-0.48, 0.84]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	wfs4v	3.88 [2.46, 5.08]	3.42 [2.14, 4.75]	3.42 [2.14, 4.75]	0.94 [0.73, 0.99]	2.46 [1.87, 3.13]	0.86 [0.48, 1.00]
DDM/GAFF/AM1-BCC/TIP3P	ct5x2	3.89 [1.93, 5.64]	3.12 [1.70, 4.88]	0.25 [-2.67, 2.66]	0.02 [0.00, 0.98]	0.42 [-3.53, 3.70]	0.36 [-0.44, 1.00]
US/PMF/MT/MD_13	ikwy8	4.16 [2.98, 5.16]	3.71 [2.37, 4.95]	3.67 [2.28, 4.94]	0.10 [0.00, 0.81]	0.54 [-1.61, 1.93]	0.00 [-1.00, 0.58]
US/PMF/MT/MD_15	ib70e	4.78 [3.86, 5.63]	4.61 [3.76, 5.50]	4.61 [3.76, 5.50]	0.30 [0.01, 0.91]	0.67 [-0.78, 2.03]	0.36 [-0.50, 1.00]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	qa7zq	5.20 [3.50, 6.64]	4.66 [3.06, 6.30]	4.66 [3.06, 6.30]	0.94 [0.75, 0.99]	2.87 [2.33, 3.53]	0.86 [0.48, 1.00]
NULL1	null2	5.86 [5.03, 6.64]	5.74 [4.95, 6.55]	-5.74 [-6.55, -4.95]	0.00 [0.00, 0.00]	0.00 [0.00, 0.00]	nan [nan, nan]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/A	s3kiu	5.96 [4.57, 7.22]	5.66 [4.40, 7.00]	5.66 [4.40, 7.00]	0.94 [0.72, 1.00]	2.46 [1.88, 3.13]	0.86 [0.48, 1.00]
BSSE-corrected RI-B3PW91 (SMD)/CBS	btcyu	7.00 [4.83, 8.91]	6.23 [4.01, 8.42]	6.23 [4.01, 8.42]	0.00 [0.00, 0.82]	-0.16 [-3.42, 1.71]	-0.14 [-0.83, 0.58]
EKEN-DIAZ/MD/MMPBSA	caknz	7.00 [3.85, 9.54]	5.92 [3.53, 8.68]	5.92 [3.53, 8.68]	0.86 [0.69, 0.99]	3.83 [2.38, 5.64]	0.79 [0.48, 1.00]
BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	e85s6	39.03 [36.23, 41.73]	38.83 [36.14, 41.59]	38.83 [36.14, 41.59]	0.55 [0.02, 0.97]	3.02 [-0.47, 5.67]	0.57 [-0.17, 1.00]

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