

ID	receipt_id	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)	R ²	m	τ
US/PMF/MT/MD_2	e7w4x	1.20 [0.76, 1.54]	1.03 [0.60, 1.46]	-0.69 [-1.36, -0.00]	0.90 [0.62, 0.99]	1.65 [1.28, 2.01]	0.79 [0.25, 1.00]
US/PMF/MT/MD_19	2kb3u	1.26 [0.91, 1.53]	1.13 [0.72, 1.50]	-0.69 [-1.37, 0.08]	0.27 [0.01, 0.90]	0.43 [-0.44, 1.36]	0.29 [-0.50, 0.84]
Umbrella Sampling/TIP3P	vq30p	1.33 [0.70, 1.78]	1.02 [0.44, 1.60]	-0.07 [-0.94, 0.84]	0.50 [0.00, 0.94]	1.12 [-0.39, 2.48]	0.36 [-0.45, 1.00]
US/PMF/MT/MD_23	zks3c	1.38 [0.95, 1.78]	1.24 [0.82, 1.67]	-0.01 [-0.91, 0.98]	0.19 [0.00, 0.83]	0.53 [-0.58, 1.88]	0.33 [-0.45, 0.96]
FEP-QM/MM	sdm0h	1.49 [1.00, 1.92]	1.32 [0.85, 1.80]	-0.45 [-1.35, 0.59]	0.93 [0.80, 1.00]	2.08 [1.34, 2.71]	0.86 [0.50, 1.00]
FEP-MM	n6f0q	1.52 [0.99, 1.94]	1.31 [0.79, 1.83]	-1.12 [-1.79, -0.40]	0.59 [0.02, 0.97]	1.05 [-0.20, 2.01]	0.50 [-0.30, 1.00]
US/PMF/MT/MD_9	7ihag	1.54 [0.89, 2.07]	1.27 [0.70, 1.89]	-0.82 [-1.72, 0.07]	0.05 [0.00, 0.60]	-0.08 [-0.43, 0.08]	-0.14 [-0.58, 0.42]
US/PMF/MT/MD_22	4mas4	1.66 [0.85, 2.37]	1.31 [0.68, 2.05]	1.04 [0.19, 1.97]	0.08 [0.00, 0.87]	0.24 [-0.81, 1.05]	0.00 [-0.83, 0.67]
US/PMF/MT/MD_4	m8t0b	1.99 [0.61, 2.95]	1.41 [0.54, 2.48]	1.34 [0.43, 2.46]	0.34 [0.00, 0.97]	0.91 [-0.57, 2.31]	0.50 [-0.14, 1.00]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/D	jgbg0	2.05 [1.21, 2.74]	1.72 [0.97, 2.52]	0.48 [-0.84, 1.87]	0.95 [0.79, 0.99]	2.60 [2.17, 3.07]	0.86 [0.50, 1.00]
US/PMF/MT/MD_12	tydzi	2.08 [1.27, 2.78]	1.83 [1.21, 2.56]	1.83 [1.21, 2.56]	0.26 [0.01, 0.97]	0.29 [-0.34, 0.93]	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 [-0.14, 1.05]	0.25 [-0.54, 0.83]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	e5rqf	2.11 [0.95, 2.97]	1.58 [0.67, 2.60]	1.40 [0.36, 2.53]	0.94 [0.77, 0.99]	2.24 [1.76, 2.82]	0.86 [0.48, 1.00]
AMOEBA/BAR/Tinker	jgdj6	2.12 [1.08, 3.01]	1.68 [0.86, 2.63]	-0.93 [-2.25, 0.34]	0.07 [0.00, 0.65]	-0.28 [-1.39, 0.49]	-0.07 [-0.67, 0.57]
US/PMF/MT/MD_20	zxx8g	2.39 [1.19, 3.34]	1.96 [1.11, 2.97]	1.54 [0.31, 2.80]	0.08 [0.00, 0.88]	0.43 [-1.50, 1.88]	0.00 [-0.83, 0.67]
US/PMF/MT/MD_26	jomge	2.55 [1.48, 3.45]	2.12 [1.15, 3.13]	2.12 [1.15, 3.13]	0.21 [0.00, 0.92]	0.59 [-1.15, 1.82]	0.07 [-0.84, 0.67]
US/PMF/MT/MD_17	n7b3v	2.59 [1.80, 3.30]	2.40 [1.78, 3.11]	2.40 [1.78, 3.11]	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, 3.43]	2.38 [1.63, 3.22]	2.38 [1.63, 3.22]	0.19 [0.00, 0.82]	0.38 [-0.42, 1.34]	0.33 [-0.43, 0.96]
US/PMF/MT/MD_1	t5gev	2.76 [1.52, 3.68]	2.17 [1.01, 3.35]	2.17 [1.01, 3.35]	0.90 [0.62, 0.99]	2.26 [1.76, 2.79]	0.79 [0.25, 1.00]
US/PMF/MT/MD_11	wfrgr	2.79 [2.01, 3.55]	2.59 [1.94, 3.36]	2.59 [1.94, 3.36]	0.27 [0.01, 0.96]	0.41 [-0.46, 1.27]	0.36 [-0.42, 1.00]
US/PMF/MT/MD_21	45sgk	2.87 [1.59, 3.90]	2.35 [1.28, 3.53]	2.24 [1.06, 3.51]	0.08 [0.00, 0.87]	0.41 [-1.43, 1.82]	0.00 [-0.83, 0.67]
US/PMF/MT/MD_6	bhhbs	2.88 [2.16, 3.69]	2.71 [2.14, 3.49]	2.71 [2.14, 3.49]	0.43 [0.01, 0.97]	0.68 [-0.26, 1.44]	0.29 [-0.50, 0.84]
FS-DAM/GAFF2/TIP3P	pbo45	2.91 [1.36, 4.11]	2.24 [1.04, 3.59]	-0.03 [-2.10, 2.01]	0.34 [0.00, 0.96]	1.72 [-1.54, 3.08]	0.29 [-0.57, 1.00]
US/PMF/MT/MD_18	70hpk	2.91 [2.02, 3.71]	2.66 [1.88, 3.53]	2.66 [1.88, 3.53]	0.27 [0.01, 0.90]	0.56 [-0.54, 1.78]	0.29 [-0.50, 0.91]
US/PMF/MT/MD_8	mhwfc	2.97 [2.05, 3.74]	2.58 [1.55, 3.56]	0.38 [-1.73, 2.28]	0.05 [0.00, 0.59]	-0.49 [-2.85, 0.57]	-0.14 [-0.58, 0.42]
US/PMF/MT/MD_3	3cxbd	3.00 [1.77, 4.07]	2.62 [1.72, 3.73]	2.62 [1.72, 3.73]	0.34 [0.00, 0.97]	0.90 [-0.60, 2.26]	0.50 [-0.13, 1.00]
US/PMF/MT/MD_24	5rmun	3.01 [2.04, 3.85]	2.74 [1.92, 3.64]	2.74 [1.92, 3.64]	0.19 [0.00, 0.81]	0.44 [-0.48, 1.53]	0.33 [-0.43, 0.96]
US/PMF/MT/MD_27	kv2ub	3.09 [2.22, 3.92]	2.86 [2.08, 3.73]	2.86 [2.08, 3.73]	0.21 [0.00, 0.89]	0.43 [-0.76, 1.33]	0.07 [-0.83, 0.65]
SQM-opt	vwkb0	3.23 [2.02, 4.28]	2.80 [1.70, 3.96]	2.55 [1.14, 3.89]	0.14 [0.00, 0.90]	0.68 [-1.56, 3.00]	0.36 [-0.50, 1.00]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	8pqor	3.33 [1.67, 4.54]	2.63 [1.29, 4.06]	2.40 [0.84, 4.00]	0.95 [0.79, 0.99]	2.86 [2.40, 3.41]	0.86 [0.48, 1.00]
US/PMF/MT/MD_16	d6js7	3.54 [2.77, 4.32]	3.39 [2.73, 4.15]	3.39 [2.73, 4.15]	0.30 [0.01, 0.92]	0.46 [-0.53, 1.45]	0.36 [-0.50, 1.00]
US/PMF/MT/MD_10	hs2xm	3.67 [2.72, 4.55]	3.45 [2.65, 4.38]	3.45 [2.65, 4.38]	0.27 [0.01, 0.97]	0.60 [-0.66, 1.84]	0.36 [-0.41, 1.00]
US/PMF/MT/MD_14	obyj4	3.69 [2.62, 4.64]	3.29 [2.13, 4.43]	3.21 [1.92, 4.42]	0.10 [0.00, 0.79]	0.50 [-1.43, 1.74]	0.00 [-1.00, 0.58]
DFT-opt	NB001	3.71 [2.78, 4.53]	3.49 [2.64, 4.38]	-2.85 [-4.30, -1.07]	0.57 [0.02, 0.91]	2.03 [-0.07, 4.11]	0.29 [-0.50, 0.89]
US/PMF/MT/MD_5	tj4jx	3.85 [2.82, 4.82]	3.62 [2.77, 4.60]	3.62 [2.77, 4.60]	0.43 [0.01, 0.97]	0.99 [-0.38, 2.11]	0.29 [-0.48, 0.83]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	wfs4v	3.88 [2.43, 5.06]	3.42 [2.18, 4.74]	3.42 [2.18, 4.74]	0.94 [0.77, 0.99]	2.46 [1.93, 3.12]	0.86 [0.48, 1.00]
DDM/GAFF/AM1-BCC/TIP3P	ct5x2	3.89 [1.92, 5.65]	3.12 [1.70, 4.90]	0.25 [-2.67, 2.66]	0.02 [0.00, 0.98]	0.42 [-3.57, 3.70]	0.36 [-0.44, 1.00]
US/PMF/MT/MD_13	ikwy8	4.16 [2.98, 5.15]	3.71 [2.37, 4.95]	3.67 [2.26, 4.94]	0.10 [0.00, 0.80]	0.54 [-1.56, 1.90]	0.00 [-0.92, 0.57]
US/PMF/MT/MD_15	ib70e	4.78 [3.87, 5.63]	4.61 [3.77, 5.50]	4.61 [3.77, 5.50]	0.30 [0.01, 0.91]	0.67 [-0.78, 2.06]	0.36 [-0.50, 1.00]
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	qa7zq	5.20 [3.48, 6.63]	4.66 [3.07, 6.28]	4.66 [3.07, 6.28]	0.94 [0.79, 0.99]	2.87 [2.39, 3.46]	0.86 [0.48, 1.00]
NULL1	null2	5.86 [5.03, 6.64]	5.74 [4.95, 6.54]	-5.74 [-6.54, -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 [4.58, 7.17]	5.66 [4.44, 6.96]	5.66 [4.44, 6.96]	0.94 [0.76, 0.99]	2.46 [1.93, 3.09]	0.86 [0.50, 1.00]
BSSE-corrected RI-B3PW91 (SMD)/CBS	btcyu	7.00 [4.83, 8.92]	6.23 [4.00, 8.42]	6.23 [4.00, 8.42]	0.00 [0.00, 0.82]	-0.16 [-3.22, 1.85]	-0.14 [-0.83, 0.60]
EKEN-DIAZ/MD/MMPBSA	caknz	7.00 [3.88, 9.50]	5.92 [3.56, 8.67]	5.92 [3.56, 8.67]	0.86 [0.70, 0.99]	3.83 [2.41, 5.65]	0.79 [0.43, 1.00]
BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	e85s6	39.03 [36.27, 41.74]	38.83 [36.18, 41.58]	38.83 [36.18, 41.58]	0.55 [0.01, 0.98]	3.02 [-0.38, 5.67]	0.57 [-0.14, 1.00]

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