ID	name	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)	R^2	m
finzb	US/PMF/MT/MD_19	0.498 [0.285, 0.667]	0.404 [0.209, 0.614]	0.239 [-0.099, 0.529]	0.929 [0.599, 0.988]	0.808 [0.544, 0.994]
mknyd	US/PMF/MT/MD_2	0.604 [0.349, 0.809]	0.509 [0.279, 0.742]	0.239 [-0.146, 0.627]	0.882 [0.248, 0.987]	0.768 [0.494, 0.931]
iyo2o	US/PMF/MT/MD_22	0.803 [0.445, 1.167]	0.674 [0.396, 1.041]	-0.574 [-0.979, -0.180]	0.831 [0.232, 0.994]	1.257 [0.681, 2.307]
ttmwo	SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/D	0.942 [0.611, 1.219]	0.795 [0.442, 1.134]	-0.107 [-0.764, 0.640]	0.754 [0.019, 0.982]	0.606 [0.005, 0.855]
uui3y	US/PMF/MT/MD_20	1.055 [0.455, 1.531]	0.800 [0.361, 1.324]	-0.770 [-1.314, -0.312]	0.829 [0.222, 0.992]	0.692 [0.344, 1.257]
rkitq	US/PMF/MT/MD_9	1.154 [0.490, 1.802]	0.861 [0.443, 1.503]	0.086 [-0.576, 1.034]	0.147 [0.000, 0.858]	0.962 [-0.937, 2.051]
e7w4x	US/PMF/MT/MD_2	1.203 [0.743, 1.543]	1.026 [0.581, 1.465]	0.689 [0.000, 1.375]	0.898 [0.612, 0.992]	0.546 [0.356, 0.639]
o3aiv	US/PMF/MT/MD_26	1.241 [0.742, 1.695]	1.055 [0.617, 1.564]	-0.875 [-1.495, -0.244]	0.653 [0.100, 0.961]	0.675 [-0.614, 0.942]
2kb3u	US/PMF/MT/MD_19	1.263 [0.921, 1.532]	1.127 [0.725, 1.482]	0.687 [-0.084, 1.380]	0.267 [0.007, 0.929]	0.615 [-0.797, 1.505]
8jxan	SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	1.307 [0.716, 1.879]	1.086 [0.659, 1.622]	-0.679 [-1.429, 0.090]	0.719 [0.027, 0.942]	0.540 [0.082, 0.813]
vq30p	Umbrella Sampling/TIP3P	1.325 [0.629, 1.847]	1.015 [0.405, 1.681]	0.071 [-0.845, 1.022]	0.495 [0.003, 0.976]	0.440 [-0.256, 0.821]
zks3c	US/PMF/MT/MD_23	1.384 [0.911, 1.810]	1.241 [0.779, 1.704]	0.009 [-1.024, 0.905]	0.187 [0.002, 0.786]	0.355 [-0.525, 0.938]
4ndha	US/PMF/MT/MD_7	1.460 [1.054, 1.854]	1.319 [0.890, 1.766]	-1.266 [-1.740, -0.751]	0.750 [0.101, 0.950]	1.536 [0.429, 2.430]
w2q3q	FEP-MM	1.479 [1.075, 1.835]	1.359 [0.987, 1.759]	1.231 [0.648, 1.753]	0.737 [0.488, 0.989]	0.676 [0.436, 1.261]
sdm0h	FEP-QM/MM	1.492 [1.021, 1.923]	1.318 [0.840, 1.829]	0.455 [-0.524, 1.336]	0.929 [0.798, 0.994]	0.446 [0.345, 0.605]
emfe8	US/PMF/MT/MD_12	1.504 [1.001, 1.886]	1.309 [0.746, 1.805]	-1.209 [-1.790, -0.539]	0.698 [0.074, 0.946]	2.250 [0.667, 2.960]
n6f0q	FEP-MM	1.515 [1.022, 1.976]	1.314 [0.806, 1.866]	1.124 [0.363, 1.845]	0.588 [0.016, 0.968]	0.562 [-0.139, 0.798]
7uted	US/PMF/MT/MD_23	1.535 [1.128, 1.894]	1.377 [0.923, 1.829]	1.323 [0.765, 1.829]	0.716 [0.013, 0.990]	0.721 [-0.217, 0.966]
7ihag	US/PMF/MT/MD_9	1.543 [0.868, 2.089]	1.274 [0.676, 1.925]	0.824 [-0.081, 1.742]	0.052 [0.000, 0.637]	-0.672 [-2.678, 2.669]
vgqcz	US/PMF/MT/MD_25	1.545 [1.003, 2.128]	1.395 [0.990, 1.925]	-1.395 [-1.923, -0.990]	0.716 [0.009, 0.994]	0.988 [-0.274, 1.379]
ftout	US/PMF/MT/MD_21	1.643 [1.075, 2.148]	1.491 [1.024, 2.026]	-1.491 [-2.016, -1.020]	0.828 [0.248, 0.995]	0.713 [0.420, 1.345]
4mas4	US/PMF/MT/MD_22	1.659 [0.849, 2.375]	1.310 [0.665, 2.061]	-1.040 [-1.936, -0.121]	0.077 [0.000, 0.894]	0.329 [-0.939, 1.449]
ahtcq	FEP-QM/MM	1.737 [1.352, 2.062]	1.590 [1.107, 2.029]	1.590 [1.107, 2.029]	0.814 [0.472, 0.995]	0.715 [0.480, 1.054]
aai8i	US/PMF/MT/MD_24	1.761 [1.224, 2.325]	1.622 [1.207, 2.187]	-1.622 [-2.186, -1.196]	0.715 [0.005, 0.994]	0.864 [-0.254, 1.187]
c8jfq	SQM-opt	1.918 [0.996, 2.664]	1.571 [0.857, 2.388]	0.286 [-1.069, 1.567]	0.179 [0.001, 0.953]	0.257 [-0.279, 2.195]
7fk2x	US/PMF/MT/MD_11	1.939 [1.423, 2.393]	1.770 [1.216, 2.319]	-1.770 [-2.316, -1.208]	0.697 [0.058, 0.948]	1.619 [0.400, 2.104]
egmst	US/PMF/MT/MD_6	1.956 [1.497, 2.389]	1.851 [1.406, 2.329]	-1.851 [-2.321, -1.399]	0.751 [0.132, 0.957]	1.106 [0.348, 1.749]
gt5n0	US/PMF/MT/MD_4	1.980 [1.380, 2.492]	1.770 [1.096, 2.384]	-1.770 [-2.383, -1.096]	0.580 [0.009, 0.923]	0.719 [-0.341, 1.144]
m8t0b	US/PMF/MT/MD_4	1.990 [0.610, 2.932]	1.406 [0.534, 2.421]	-1.341 [-2.406, -0.390]	0.340 [0.002, 0.967]	0.374 [-0.370, 0.786]
gemch	FS-DAM/GAFF2/TIP3P	1.997 [0.920, 2.870]	1.549 [0.785, 2.526]	-1.549 [-2.507, -0.776]	0.837 [0.290, 0.974]	0.496 [0.332, 0.933]
jgbg0	SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/D	2.047 [1.234, 2.743]	1.722 [1.012, 2.549]	-0.480 [-1.925, 0.927]	0.946 [0.791, 0.993]	0.364 [0.287, 0.411]
8pxph	US/PMF/MT/MD_27	2.048 [1.484, 2.566]	1.910 [1.397, 2.445]	-1.910 [-2.429, -1.385]	0.653 [0.096, 0.950]	0.918 [-0.855, 1.306]
tydzi	US/PMF/MT/MD_12	2.085 [1.224, 2.849]	1.831 [1.154, 2.647]	-1.831 [-2.636, -1.140]	0.263 [0.009, 0.979]	0.896 [-1.361, 2.063]
y7u8q	US/PMF/MT/MD_7	2.108 [1.452, 2.840]	1.915 [1.402, 2.611]	-1.915 [-2.606, -1.400]	0.428 [0.012, 0.973]	0.885 [-0.211, 1.414]
e5rqf	SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	2.115 [0.787, 3.004]	1.581 [0.575, 2.660]	-1.404 [-2.543, -0.244]	0.939 [0.785, 0.994]	0.419 [0.302, 0.536]
jgdj6	AMOEBA/BAR/Tinker	2.118 [1.078, 3.026]	1.676 [0.862, 2.635]	0.926 [-0.253, 2.391]	0.069 [0.000, 0.616]	-0.245 [-0.815, 0.627]
iaz7f	US/PMF/MT/MD_17	2.186 [1.696, 2.569]	2.037 [1.415, 2.521]	-2.037 [-2.516, -1.406]	0.913 [0.830, 0.997]	2.443 [1.784, 3.153]
8fcb6	AMOEBA/BAR/Tinker	2.227 [1.014, 3.357]	1.769 [0.970, 2.869]	0.771 [-0.674, 2.319]	0.233 [0.001, 0.976]	-0.509 [-1.523, 0.277]
bjyua	DFT-opt	2.232 [1.231, 3.141]	1.907 [1.163, 2.789]	0.285 [-1.386, 1.692]	0.663 [0.018, 0.941]	0.326 [-0.079, 0.547]
rc4qr	US/PMF/MT/MD_14	2.288 [1.901, 2.624]	2.225 [1.830, 2.572]	-2.225 [-2.572, -1.808]	0.862 [0.067, 0.992]	0.812 [0.143, 1.085]
zxx8g	US/PMF/MT/MD_20	2.391 [1.213, 3.403]	1.961 [1.112, 3.040]	-1.536 [-2.857, -0.266]	0.077 [0.000, 0.868]	0.181 [-0.515, 0.728]
s78rs	US/PMF/MT/MD_10	2.398 [1.925, 2.828]	2.296 [1.835, 2.775]	-2.296 [-2.774, -1.826]	0.699 [0.091, 0.954]	1.109 [0.305, 1.464]
nb8jk	US/PMF/MT/MD_5	2.514 [2.015, 2.971]	2.411 [1.932, 2.908]	-2.411 [-2.897, -1.925]	0.751 [0.128, 0.960]	0.757 [0.304, 1.215]

Continued on next page

ID	name	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)	R^2	m
jomge	US/PMF/MT/MD_26	2.549 [1.501, 3.420]	2.116 [1.209, 3.163]	-2.116 [-3.115, -1.198]	0.207 [0.002, 0.869]	0.350 [-0.689, 0.845]
n7b3v	US/PMF/MT/MD_17	2.591 [1.827, 3.346]	2.400 [1.801, 3.134]	-2.400 [-3.121, -1.783]	0.294 [0.007, 0.921]	0.890 [-1.460, 1.734]
ei3s2	US/PMF/MT/MD_25	2.657 [1.757, 3.503]	2.385 [1.645, 3.284]	-2.385 [-3.270, -1.635]	0.186 [0.003, 0.827]	0.486 [-0.736, 1.387]
gkdce	US/PMF/MT/MD_13	2.683 [2.274, 3.073]	2.612 [2.190, 3.021]	-2.612 [-3.004, -2.188]	0.861 [0.153, 0.994]	0.745 [0.170, 1.023]
iv75a	SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	2.704 [1.701, 3.475]	2.343 [1.361, 3.312]	-2.300 [-3.307, -1.234]	0.754 [0.030, 0.977]	0.458 [0.059, 0.642]
t5gev	US/PMF/MT/MD_1	2.762 [1.392, 3.646]	2.167 [0.949, 3.386]	-2.167 [-3.371, -0.938]	0.898 [0.618, 0.992]	0.396 [0.276, 0.464]
yedi3	DDM/GAFF/AM1-BCC/TIP3P	2.775 [1.519, 3.922]	2.210 [1.165, 3.486]	-1.790 [-3.321, -0.341]	0.406 [0.001, 0.906]	0.296 [-0.830, 0.474]
wfrgr	US/PMF/MT/MD_11	2.795 [2.002, 3.536]	2.593 [1.936, 3.340]	-2.593 [-3.321, -1.922]	0.266 [0.006, 0.973]	0.648 [-1.042, 1.421]
xcuey	US/PMF/MT/MD_18	2.816 [2.507, 3.111]	2.784 [2.477, 3.097]	-2.784 [-3.081, -2.473]	0.929 [0.615, 0.991]	1.284 [0.948, 1.674]
45sgk	US/PMF/MT/MD_21	2.867 [1.548, 4.013]	2.353 [1.265, 3.659]	-2.237 [-3.579, -0.970]	0.077 [0.001, 0.931]	0.186 [-0.535, 0.752]
bhhbs	US/PMF/MT/MD_6	2.881 [2.154, 3.671]	2.710 [2.139, 3.476]	-2.710 [-3.474, -2.139]	0.430 [0.011, 0.974]	0.636 [-1.374, 1.009]
pbo45	FS-DAM/GAFF2/TIP3P	2.910 [1.384, 4.168]	2.241 [1.007, 3.683]	0.034 [-2.025, 2.056]	0.339 [0.002, 0.971]	0.197 [-0.220, 0.389]
70hpk	US/PMF/MT/MD_18	2.912 [2.014, 3.712]	2.656 [1.894, 3.515]	-2.656 [-3.502, -1.883]	0.267 [0.005, 0.917]	0.474 [-0.626, 1.066]
mhwfc	US/PMF/MT/MD_8	2.970 [2.037, 3.775]	2.576 [1.510, 3.536]	-0.376 [-2.323, 1.865]	0.054 [0.000, 0.619]	-0.109 [-0.460, 0.309]
ogd0g	US/PMF/MT/MD_16	2.992 [2.540, 3.338]	2.925 [2.426, 3.324]	-2.925 [-3.315, -2.421]	0.914 [0.818, 0.997]	1.756 [1.259, 2.285]
5r5n7	BSSE-corrected RI-B3PW91 (SMD)/CBS	22.511 [11.410, 34.382]	17.855 [11.072, 28.749]	-4.628 [-14.953, 13.281]	0.605 [0.002, 0.964]	-0.046 [-0.233, 0.132]
3cxbd	US/PMF/MT/MD_3	3.002 [1.797, 4.094]	2.623 [1.730, 3.756]	-2.623 [-3.749, -1.711]	0.339 [0.000, 0.966]	0.376 [-0.172, 0.775]
5rmun	US/PMF/MT/MD_24	3.006 [2.003, 3.893]	2.736 [1.907, 3.686]	-2.736 [-3.653, -1.875]	0.186 [0.004, 0.905]	0.425 [-0.630, 1.197]
4ysuf	US/PMF/MT/MD_1	3.007 [2.253, 3.717]	2.829 [2.140, 3.620]	-2.829 [-3.585, -2.140]	0.882 [0.226, 0.990]	0.558 [0.338, 0.670]
kv2ub	US/PMF/MT/MD_27	3.090 [2.199, 3.962]	2.855 [2.060, 3.779]	-2.855 [-3.738, -2.021]	0.207 [0.001, 0.848]	0.477 [-0.896, 1.174]
widya	US/PMF/MT/MD_3	3.171 [2.562, 3.728]	3.046 [2.439, 3.649]	-3.046 [-3.640, -2.435]	0.581 [0.017, 0.903]	0.726 [-0.082, 1.213]
vwkb0	SQM-opt	3.232 [1.938, 4.278]	2.798 [1.645, 3.922]	-2.550 [-3.870, -1.018]	0.140 [0.001, 0.897]	0.206 [-0.382, 0.702]
8pqor	SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	3.325 [1.656, 4.519]	2.629 [1.250, 4.085]	-2.401 [-4.029, -0.787]	0.946 [0.805, 0.994]	0.330 [0.255, 0.376]
ibhca	SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	3.479 [2.152, 4.671]	3.054 [1.894, 4.329]	-3.054 [-4.306, -1.848]	0.720 [0.030, 0.951]	0.408 [0.006, 0.615]
d6js7	US/PMF/MT/MD_16	3.544 [2.785, 4.325]	3.390 [2.741, 4.145]	-3.390 [-4.134, -2.734]	0.296 [0.006, 0.905]	0.641 [-0.981, 1.346]
hs2xm	US/PMF/MT/MD_10	3.666 [2.783, 4.547]	3.449 [2.695, 4.374]	-3.449 [-4.365, -2.667]	0.266 [0.007, 0.941]	0.443 [-0.675, 0.998]
obyj4	US/PMF/MT/MD_14	3.689 [2.518, 4.607]	3.290 [2.065, 4.412]	-3.207 [-4.406, -1.789]	0.099 [0.000, 0.776]	0.201 [-0.399, 0.872]
tj4jx	US/PMF/MT/MD_5	3.850 [2.782, 4.804]	3.618 [2.738, 4.554]	-3.618 [-4.546, -2.714]	0.429 [0.008, 0.977]	0.435 [-0.089, 0.695]
wfs4v	SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	3.885 [2.494, 5.014]	3.419 [2.191, 4.741]	-3.419 [-4.700, -2.171]	0.939 [0.772, 0.993]	0.381 [0.284, 0.439]
ct5x2	DDM/GAFF/AM1-BCC/TIP3P	3.891 [1.911, 5.592]	3.117 [1.673, 4.785]	-0.248 [-2.769, 2.688]	0.016 [0.000, 0.984]	0.038 [-0.221, 0.325]
kuovg	BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	36.413 [31.161, 40.117]	35.456 [29.071, 40.014]	-31.727 [-39.978, -17.799]	0.435 [0.184, 0.945]	-0.048 [-0.069, 0.259]
e85s6	BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	39.031 [36.511, 41.672]	38.831 [36.410, 41.518]	-38.831 [-41.501, -36.355]	0.548 [0.030, 0.972]	0.181 [-0.059, 0.249]
m0qdw	US/PMF/MT/MD_15	4.000 [3.709, 4.265]	3.979 [3.681, 4.255]	-3.979 [-4.252, -3.670]	0.914 [0.816, 0.996]	1.201 [0.884, 1.520]
ikwy8	US/PMF/MT/MD_13	4.161 [3.048, 5.172]	3.713 [2.429, 4.921]	-3.673 [-4.909, -2.314]	0.099 [0.000, 0.759]	0.184 [-0.367, 0.767]
bhns3	SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	4.637 [3.565, 5.522]	4.414 [3.335, 5.430]	-4.414 [-5.406, -3.331]	0.768 [0.017, 0.978]	0.459 [0.001, 0.620]
ib70e	US/PMF/MT/MD_15	4.777 [3.893, 5.690]	4.607 [3.770, 5.572]	-4.607 [-5.555, -3.760]	0.296 [0.009, 0.914]	0.439 [-0.719, 0.893]
qa7zq	SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	5.202 [3.251, 6.628]	4.659 [2.894, 6.295]	-4.659 [-6.263, -2.875]	0.945 [0.796, 0.992]	0.329 [0.257, 0.387]
mdqkg	SOMD/AM1BCC-GAFF-TIP3P/MBAR/A	5.406 [4.214, 6.547]	5.145 [4.105, 6.338]	-5.145 [-6.321, -4.088]	0.744 [0.058, 0.954]	0.412 [0.145, 0.606]
s3kiu	Alchemical Free Energy Calculations	5.957 [4.423, 7.261]	5.664 [4.340, 7.065]	-5.664 [-7.034, -4.309]	0.938 [0.772, 0.995]	0.381 [0.284, 0.480]
e032m	US/PMF/MT/MD_8	6.262 [4.143, 8.085]	5.569 [3.484, 7.679]	-5.569 [-7.629, -3.435]	0.148 [0.001, 0.893]	0.154 [-0.146, 0.363]
caknz	EKEN-DIAZ/MD/MMPBSA	6.999 [3.938, 9.614]	5.922 [3.618, 8.723]	-5.922 [-8.691, -3.602]	0.862 [0.700, 0.988]	0.225 [0.147, 0.347]
btcyu	BSSE-corrected RI-B3PW91 (SMD)/CBS	6.999 [4.789, 8.970]	6.233 [3.916, 8.428]	-6.233 [-8.386, -3.895]	0.004 [0.000, 0.802]	-0.026 [-0.208, 0.515]
8brzp	EKEN-DIAZ/MD/MMPBSA	7.073 [5.599, 8.570]	6.802 [5.522, 8.361]	-6.802 [-8.308, -5.518]	0.843 [0.126, 0.976]	0.379 [0.181, 0.466]