

		ID	name	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)	R ²	m			
d4twv	SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/D	1.923	[1.154, 2.494]	1.506	[0.793, 2.170]	0.237	[-0.808, 1.445]	0.128	[0.001, 0.715]	0.436	[-0.802, 1.634]
wtm6p	US/PMF/MT/MD_15	1.990	[1.332, 2.527]	1.686	[1.093, 2.302]	0.379	[-0.691, 1.523]	0.358	[0.072, 0.698]	0.459	[0.091, 1.065]
sguyt	BSSE-corrected RI-B3PW91 (SMD)/CBS	17.262	[12.005, 22.095]	14.879	[10.555, 19.854]	14.406	[9.522, 19.695]	0.000	[0.000, 0.470]	0.002	[-0.091, 0.077]
6bwq3	EKEN-DIAZ/MD/MMPBSA	17.801	[14.414, 20.852]	16.694	[13.519, 19.889]	-16.694	[-19.849, -13.501]	0.001	[0.000, 0.659]	-0.007	[-0.138, 0.171]
j37ec	SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	2.584	[1.392, 3.467]	2.021	[1.159, 3.026]	1.834	[0.866, 2.972]	0.125	[0.001, 0.741]	0.512	[-0.835, 2.253]
xdmpa	US/PMF/MT/MD_19	2.881	[1.662, 3.842]	2.278	[1.215, 3.344]	-1.611	[-3.023, -0.136]	0.075	[0.000, 0.530]	0.237	[-0.257, 0.871]
ubz3m	US/PMF/MT/MD_5	3.187	[2.282, 4.021]	2.720	[1.749, 3.681]	2.720	[1.749, 3.681]	0.385	[0.001, 0.777]	0.577	[-0.146, 0.988]
cco6p	US/PMF/MT/MD_13	3.231	[2.015, 4.344]	2.683	[1.672, 3.852]	2.268	[0.890, 3.666]	0.243	[0.020, 0.741]	0.352	[0.081, 1.143]
2mgw5	US/PMF/MT/MD_2	3.507	[1.328, 5.392]	2.442	[1.123, 4.283]	-1.609	[-3.681, 0.139]	0.045	[0.000, 0.661]	0.132	[-0.433, 0.843]
8wns3	US/PMF/MT/MD_10	3.665	[2.571, 4.594]	3.021	[1.745, 4.322]	2.932	[1.569, 4.304]	0.227	[0.000, 0.679]	0.368	[-0.123, 0.859]
cekua	US/PMF/MT/MD_8	3.729	[2.704, 4.640]	3.238	[2.181, 4.372]	3.238	[2.181, 4.372]	0.338	[0.002, 0.777]	0.492	[-0.151, 0.981]
tqhg4	AMOEBA/BAR/Tinker	3.732	[1.880, 5.156]	2.721	[1.473, 4.084]	-1.184	[-3.074, 0.541]	0.140	[0.001, 0.747]	0.169	[-0.145, 0.493]
f7duk	SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	3.789	[2.729, 4.732]	3.477	[2.569, 4.424]	-2.841	[-4.275, -1.111]	0.125	[0.001, 0.662]	0.261	[-0.438, 1.098]
tb3ck	BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	36.987	[29.994, 43.540]	34.285	[27.162, 41.438]	-34.285	[-41.287, -27.052]	0.000	[0.000, 0.545]	-0.002	[-0.058, 0.086]
3z83m	HREM/BAR/RESP/Force-Matching/TIP3P	4.321	[3.191, 5.399]	3.816	[2.734, 4.991]	-2.198	[-4.005, -0.046]	0.487	[0.129, 0.811]	0.254	[0.069, 0.472]
j8yon	US/PMF/MT/MD_12	4.387	[3.291, 5.240]	4.037	[3.013, 5.020]	-4.037	[-5.012, -2.990]	0.227	[0.001, 0.684]	0.594	[-0.193, 1.360]
dv8mj	US/PMF/MT/MD_7	4.409	[3.622, 5.111]	4.168	[3.284, 4.985]	-4.168	[-4.985, -3.280]	0.386	[0.001, 0.791]	0.933	[-0.234, 1.644]
j6oi0	US/PMF/MT/MD_20	4.716	[3.455, 5.909]	4.162	[2.804, 5.486]	4.162	[2.804, 5.486]	0.300	[0.076, 0.789]	0.385	[0.116, 1.089]
vrsfp	US/PMF/MT/MD_18	4.786	[3.776, 5.568]	4.432	[3.172, 5.445]	-4.432	[-5.433, -3.161]	0.075	[0.000, 0.522]	0.554	[-0.592, 2.089]
2vfcf	US/PMF/MT/MD_4	5.053	[3.882, 6.111]	4.683	[3.561, 5.909]	-4.683	[-5.881, -3.552]	0.286	[0.040, 0.739]	0.471	[0.101, 1.005]
46vw8	SOMD/AM1BCC-GAFF-TIP3P/MBAR/A	5.068	[3.851, 6.083]	4.475	[2.971, 5.777]	-4.409	[-5.751, -2.779]	0.128	[0.001, 0.718]	0.264	[-0.490, 1.128]
qfqyx	US/PMF/MT/MD_22	5.306	[4.116, 6.396]	4.962	[3.825, 6.104]	-4.962	[-6.095, -3.815]	0.300	[0.067, 0.777]	0.479	[0.152, 1.368]
6jsye	DDM/Force-Matching/FEP/HREM/MBAR	5.429	[3.979, 6.764]	4.769	[3.479, 6.084]	-1.126	[-3.881, 1.909]	0.256	[0.001, 0.699]	0.145	[-0.057, 0.386]
50jkg	US/PMF/MT/MD_16	5.445	[4.174, 6.674]	4.997	[3.695, 6.347]	4.997	[3.695, 6.347]	0.358	[0.049, 0.721]	0.408	[0.068, 0.903]
pz24v	US/PMF/MT/MD_9	5.452	[4.279, 6.400]	5.166	[4.080, 6.175]	-5.166	[-6.165, -4.070]	0.338	[0.001, 0.804]	0.542	[-0.146, 1.120]
jb047	US/PMF/MT/MD_3	5.608	[4.229, 6.729]	5.138	[3.703, 6.468]	5.138	[3.703, 6.468]	0.287	[0.047, 0.758]	0.376	[0.092, 0.808]
tcy06	US/PMF/MT/MD_21	5.814	[4.498, 7.048]	5.390	[4.178, 6.729]	-5.390	[-6.708, -4.166]	0.299	[0.058, 0.788]	0.392	[0.094, 1.151]
k6f5g	US/PMF/MT/MD_17	5.818	[4.915, 6.606]	5.617	[4.727, 6.507]	-5.617	[-6.501, -4.717]	0.358	[0.097, 0.729]	0.742	[0.165, 1.760]
fy660	US/PMF/MT/MD_14	6.486	[5.158, 7.864]	6.050	[4.785, 7.506]	6.050	[4.785, 7.506]	0.243	[0.018, 0.794]	0.345	[0.060, 1.200]
3g2hu	SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	6.613	[4.967, 8.089]	5.988	[4.233, 7.601]	-5.963	[-7.555, -4.142]	0.128	[0.001, 0.704]	0.222	[-0.326, 0.842]
juz8u	DDM/GAFF/AM1-BCC/TIP3P	7.212	[5.588, 8.541]	6.648	[4.986, 8.253]	-6.439	[-8.188, -4.359]	0.292	[0.002, 0.718]	0.257	[-0.042, 0.655]
u6tnc	US/PMF/MT/MD_6	7.834	[6.760, 8.802]	7.625	[6.582, 8.640]	7.625	[6.582, 8.640]	0.386	[0.002, 0.811]	0.514	[-0.159, 0.889]
xv5oo	SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	7.868	[6.243, 9.417]	7.331	[5.424, 8.982]	-7.331	[-8.936, -5.383]	0.127	[0.001, 0.719]	0.222	[-0.382, 0.831]
cbfnz	US/PMF/MT/MD_1	8.044	[4.700, 11.166]	6.704	[4.117, 9.696]	-6.704	[-9.640, -4.066]	0.045	[0.000, 0.627]	0.087	[-0.164, 0.562]
6ux0a	US/PMF/MT/MD_11	8.225	[6.810, 9.425]	7.865	[6.381, 9.205]	7.865	[6.381, 9.205]	0.227	[0.001, 0.664]	0.327	[-0.110, 0.763]