ID	name	MAE	RMSE	Pearson's r	τ	Spearman's Rho
1	55_NaCl_0Mg_TP3_GAF_40_1ns_unres	1.42 [0.45, 2.52]	1.98 [0.85, 2.78]	0.76 [0.29, 1.00]	0.47 [-0.17, 1.00]	0.66 [-0.23, 1.00]
2	55_NaCl_2Mg_TP3_GAF_40_1ns_unres	2.20 [1.46, 2.86]	2.37 [1.76, 2.92]	0.90 [0.71, 1.00]	0.73 [-0.09, 1.00]	0.83 [0.00, 1.00]
3	55_NaCl_3Mg_TP3_GAF_40_1ns_unres	2.97 [2.34, 3.82]	3.11 [2.39, 3.93]	0.56 [0.10, 1.00]	0.73 [0.23, 1.00]	0.89 [0.45, 1.00]
4	55_NaCl_0Mg_TP3_GAF_40_1ns_BBres	2.24 [1.31, 3.09]	2.48 [1.67, 3.16]	0.65 [0.12, 1.00]	0.73 [-0.09, 1.00]	0.89 [0.00, 1.00]
5	55_NaCl_2Mg_TP3_GAF_40_1ns_BBres	2.62 [1.59, 3.63]	2.91 [1.86, 3.69]	0.66 [0.05, 1.00]	0.73 [-0.09, 1.00]	0.89 [0.00, 1.00]
6	55_NaCl_3Mg_TP3_GAF_40_1ns_BBres	2.70 [1.40, 4.11]	3.21 [1.45, 4.38]	0.38 [-0.32, 1.00]	0.33 [-0.50, 1.00]	0.43 [-0.74, 1.00]
7	55_NaCl_2Mg_OPC_GAF_40_1ns_unres	2.25 [1.03, 3.48]	2.78 [1.11, 3.77]	0.27 [-0.66, 1.00]	0.33 [-0.54, 1.00]	0.54 [-0.64, 1.00]
8	55_NaCl_2Mg_TP3_OFF_40_1ns_unres	2.45 [1.47, 3.65]	2.80 [1.60, 3.91]	0.50 [-0.35, 0.99]	0.47 [-0.23, 1.00]	0.71 [-0.09, 1.00]
9	55_NaCl_3Mg_TP3_OFF_40_1ns_unres	2.36 [1.28, 3.53]	2.73 [1.59, 3.81]	0.70 [-0.22, 1.00]	0.47 [-0.64, 1.00]	0.60 [-0.80, 1.00]
10	55_KCl_2Mg_TP3_GAF_40_1ns_unres	1.91 [0.72, 3.26]	2.47 [0.92, 3.64]	0.35 [-0.99, 1.00]	0.07 [-1.00, 1.00]	0.14 [-1.00, 1.00]
11	55_KCl_3Mg_TP3_GAF_40_1ns_unres	2.39 [1.37, 3.71]	2.79 [1.44, 3.96]	0.46 [-0.10, 1.00]	0.47 [-0.45, 1.00]	0.60 [-0.60, 1.00]
12	150_KCl_2Mg_TP3_GAF_40_1ns_unres	1.73 [0.68, 3.29]	2.46 [0.71, 3.99]	0.23 [-0.76, 1.00]	0.47 [-0.33, 1.00]	0.60 [-0.50, 1.00]
13	0_NaCl_3Mg_TP3_GAF_40_1ns_unres	2.53 [1.79, 3.41]	2.74 [1.86, 3.57]	0.82 [-0.28, 1.00]	0.47 [-0.54, 1.00]	0.60 [-0.64, 1.00]
14	55_NaCl_2Mg_TP3_GAF_80_1ns_unres	2.80 [2.21, 3.55]	2.91 [2.27, 3.63]	0.89 [0.68, 1.00]	0.73 [-0.09, 1.00]	0.89 [0.00, 1.00]
15	55_NaCl_2Mg_TP3_GAF_40_2ns_unres	2.81 [1.98, 3.51]	2.96 [2.13, 3.53]	0.85 [0.25, 0.99]	0.60 [-0.23, 1.00]	0.77 [-0.09, 1.00]
16	55_NaCl_2Mg_TP3_GAF_80_1ns_BBres	2.16 [1.39, 3.01]	2.40 [1.50, 3.13]	0.73 [0.17, 1.00]	0.87 [0.33, 1.00]	0.94 [0.50, 1.00]
17	55_NaCl_2Mg_TP3_GAF_40_2ns_BBres	2.41 [1.50, 3.29]	2.63 [1.76, 3.41]	0.56 [0.05, 1.00]	0.60 [-0.23, 1.00]	0.71 [-0.33, 1.00]
18	55_NaCl_0Mg_TP3_GAF_80_1ns_BBres	1.81 [1.03, 2.44]	2.00 [1.38, 2.53]	0.84 [0.60, 1.00]	0.73 [0.11, 1.00]	0.89 [0.20, 1.00]
19	55_NaCl_0Mg_TP3_GAF_40_2ns_BBres	2.26 [1.35, 3.37]	2.60 [1.44, 3.72]	0.54 [-0.04, 1.00]	0.73 [-0.09, 1.00]	0.89 [0.00, 1.00]
20	MMGBSA_for_RNA_salt_Mg	8.27 [6.42, 10.08]	8.54 [6.76, 10.25]	0.32 [-0.68, 1.00]	0.47 [-0.64, 1.00]	0.60 [-0.80, 1.00]
21	MMGBSA_for_RNA_salt	7.81 [5.18, 10.44]	8.61 [5.52, 11.20]	0.08 [-0.91, 1.00]	0.47 [-0.64, 1.00]	0.43 [-0.80, 1.00]

Notes

- Mean and 95% confidence intervals of performance statistics were calculated by bootstrapping with 1000 samples.