MSE_o 0.030 0 34 36 28 47 22 44 41 11 6 24 30 3 16 14 Force prediction error $(kcal/mol A)^2$ 0.025 2 26 49 12 43 39 25 7 37 48 17 Mean 10 35 15 1 8 32 5 0.020 0.015 23 31 13 38 9 4 45 0.010 0.005

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Cluster index

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0.000

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