

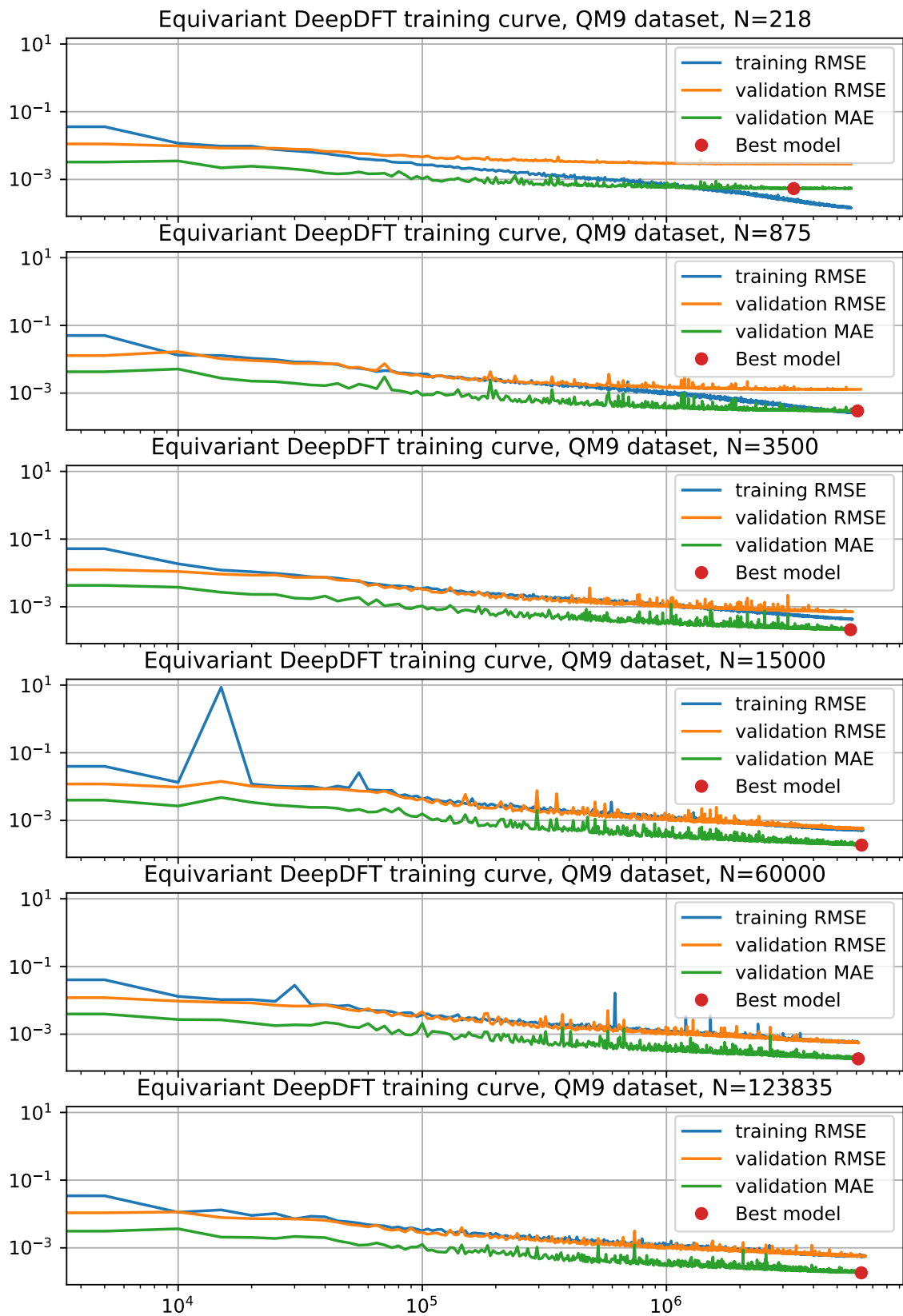
Supplementary information to: Equivariant graph neural networks for fast electron density estimation of molecules, liquids, and solids

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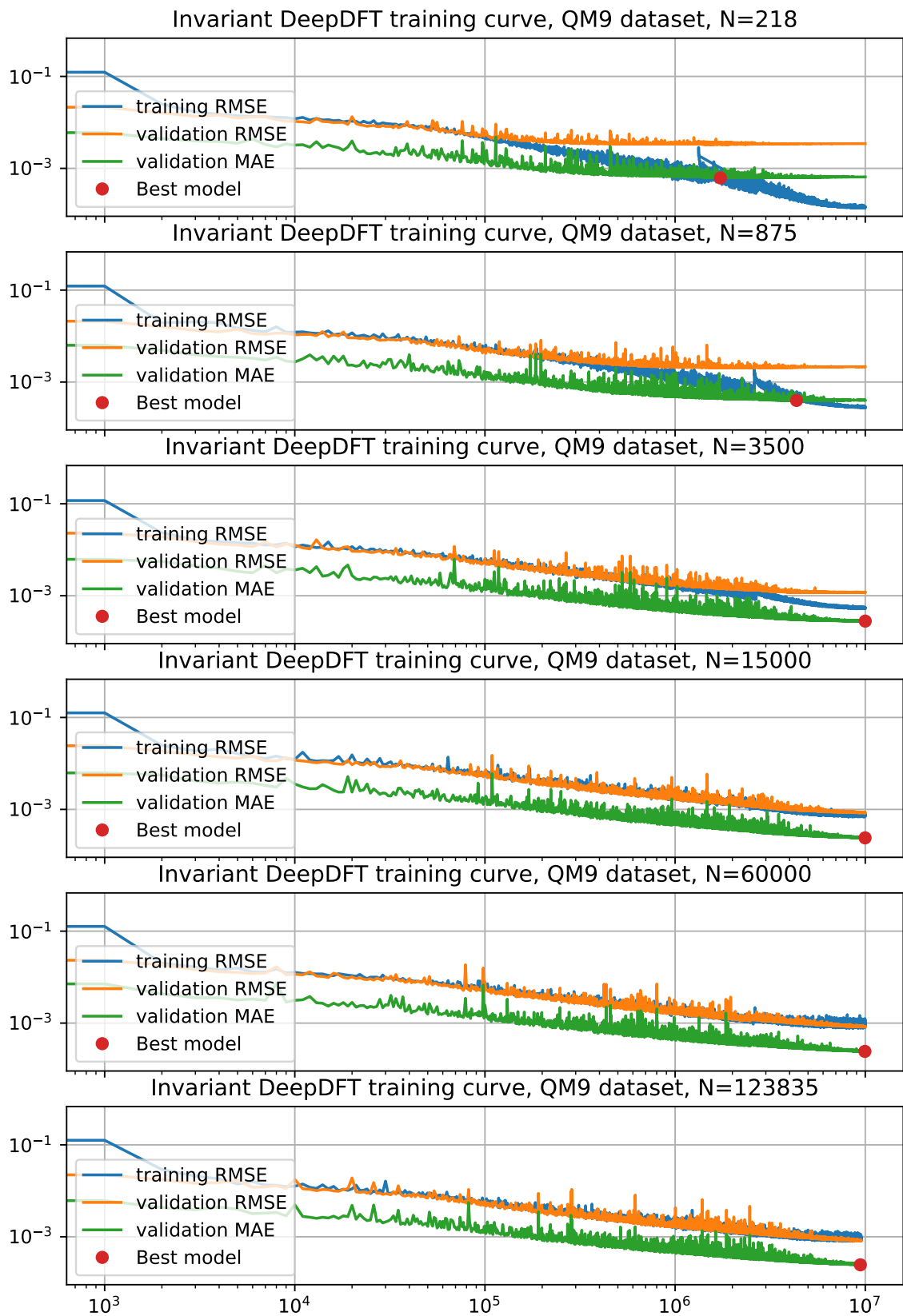
July 27, 2022

1 Training curves for equivariant and invariant DeepDFT models with different training set sizes

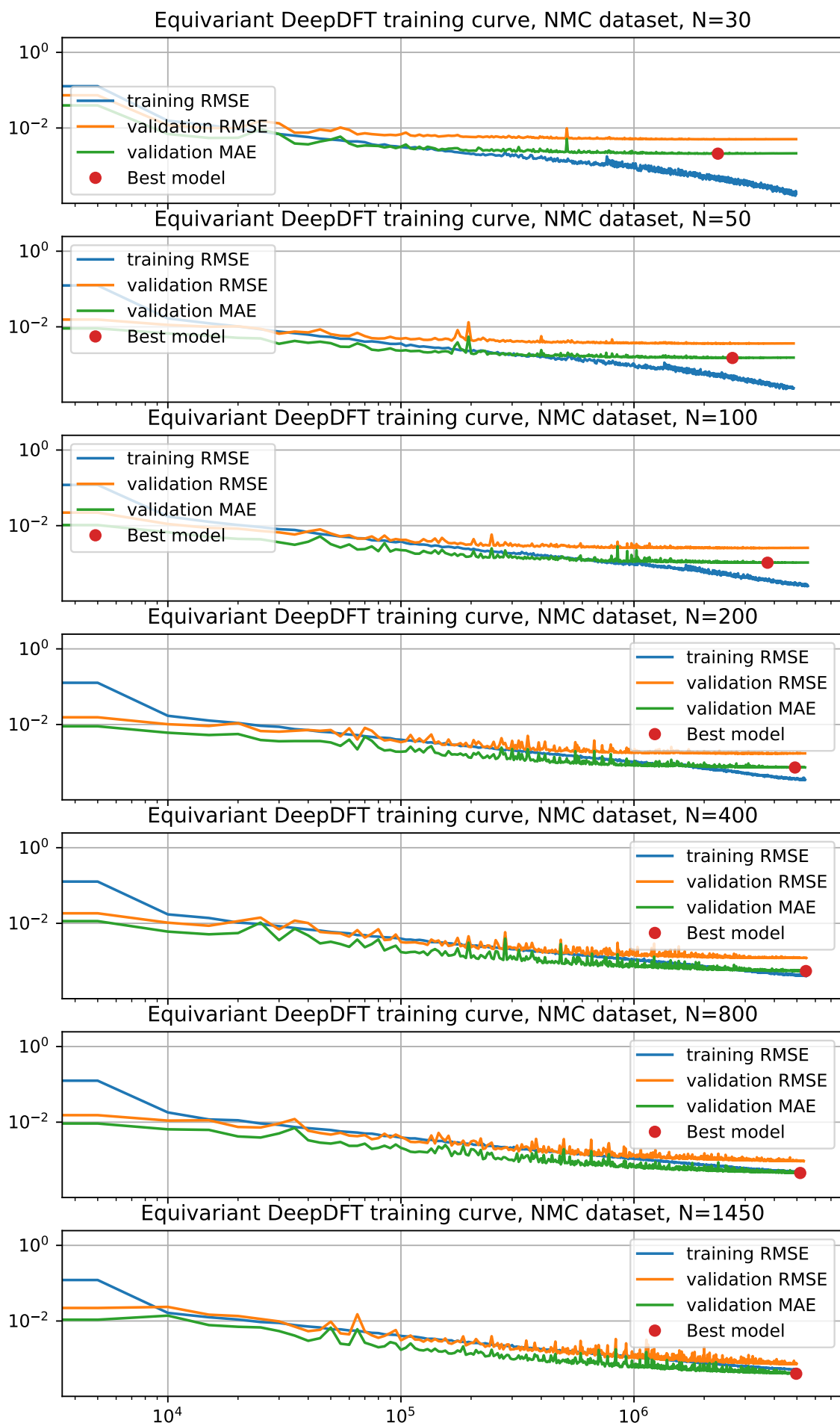
During training of the equivariant and invariant DeepDFT models the cost function is tracked for a sample of the validation set and a running cost is tracked for the training set. The validation mean absolute error (MAE) is used as the selection criteria for the best model.



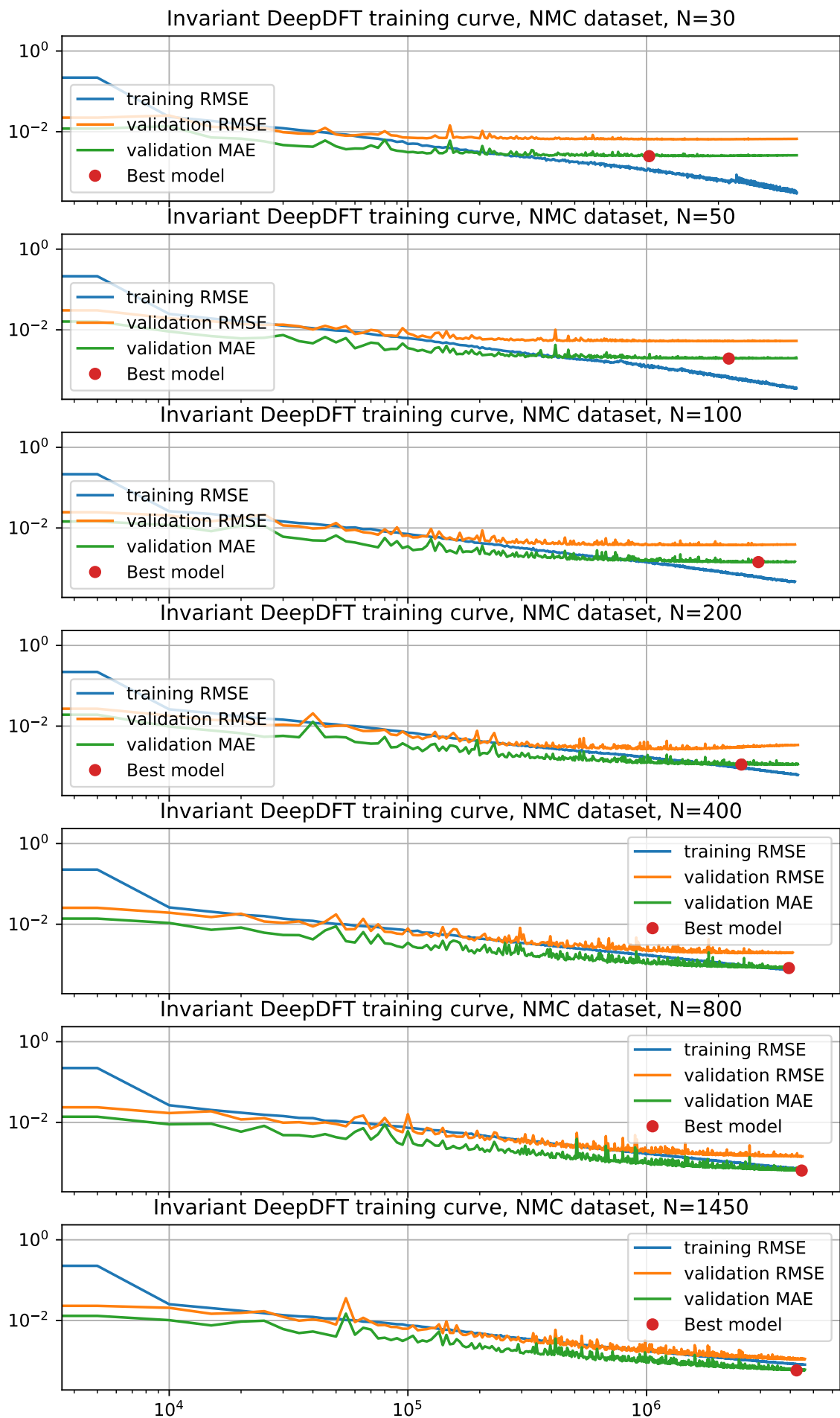
Supplementary Figure 1: Equivariant model QM9 dataset training curves.



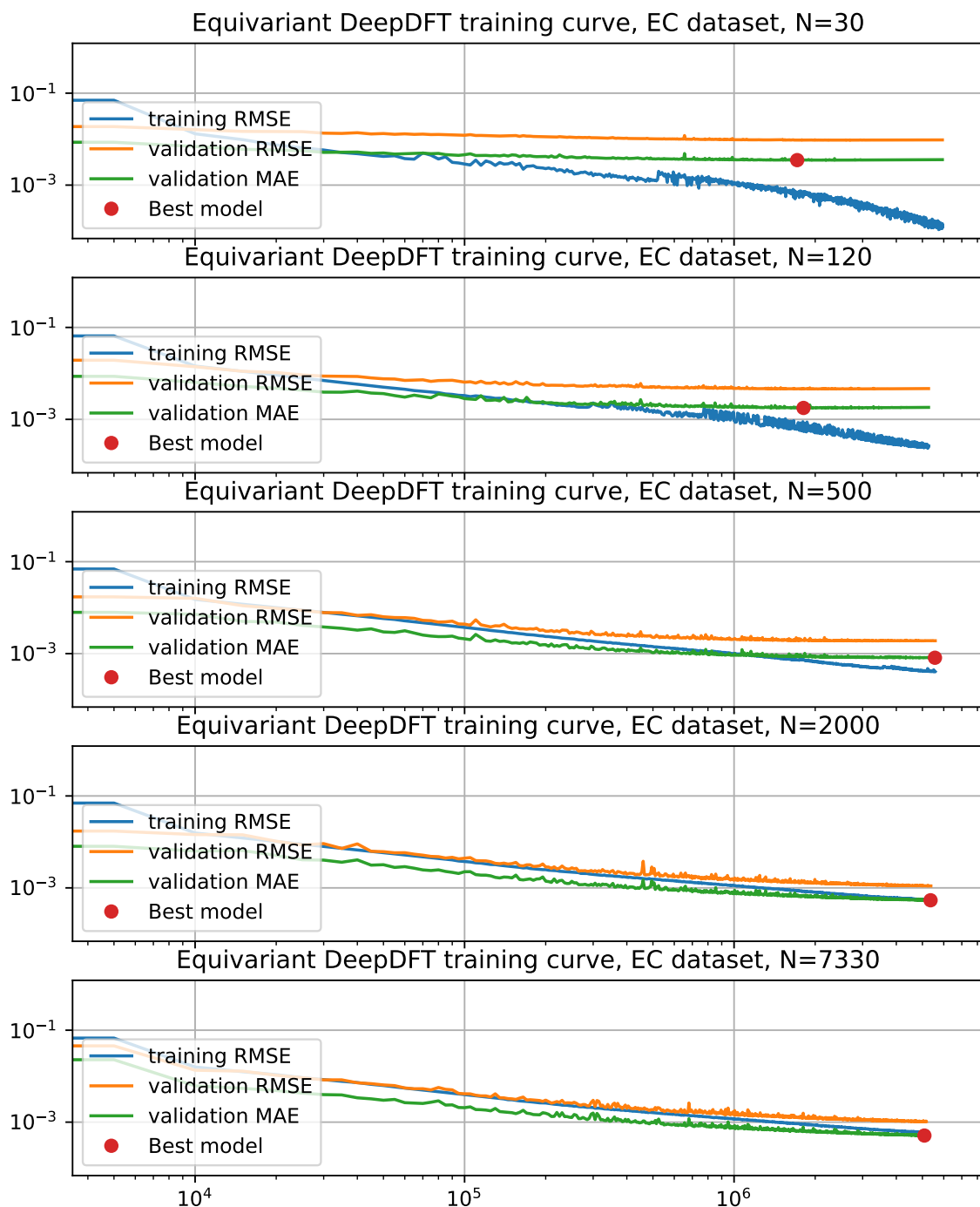
Supplementary Figure 2: Equivariant model QM9 dataset training curves.



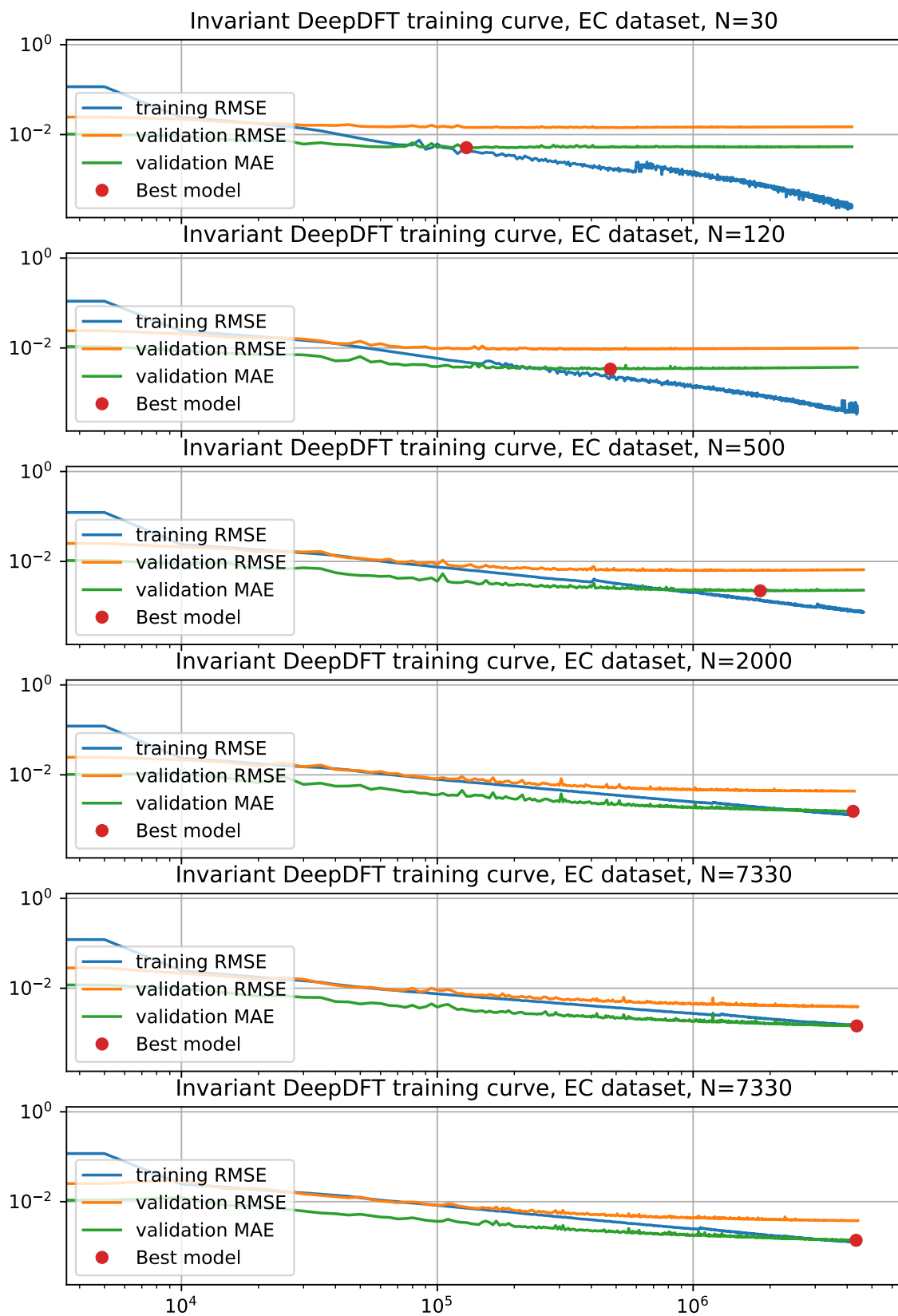
Supplementary Figure 3: Equivariant model LIB cathode dataset training curves.



Supplementary Figure 4: Invariant model LIB cathode dataset training curves.



Supplementary Figure 5: Equivariant model ethylene carbonate dataset training curves.



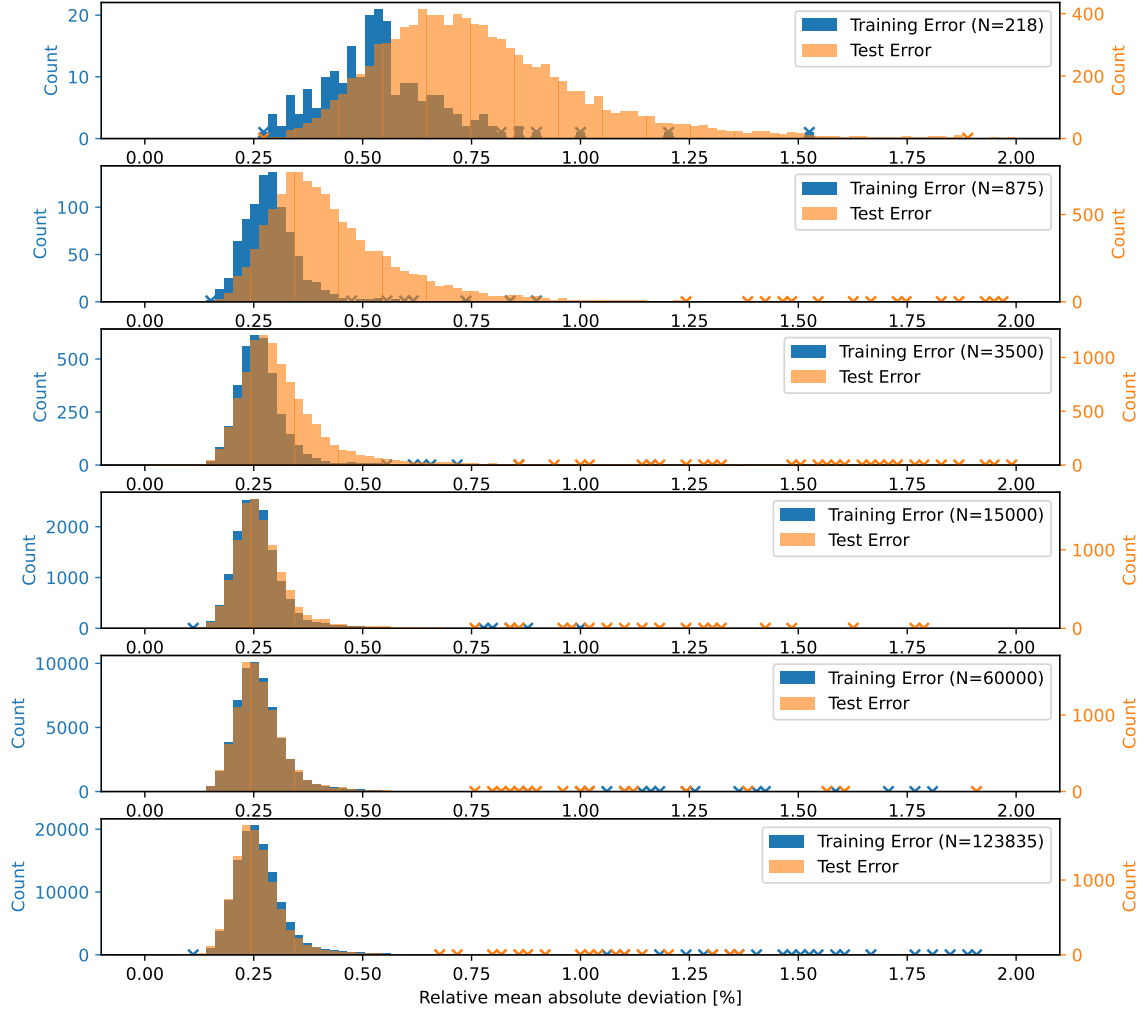
Supplementary Figure 6: Invariant model ethylene carbonate dataset training curves.

2 Distribution of prediction errors for test and training data

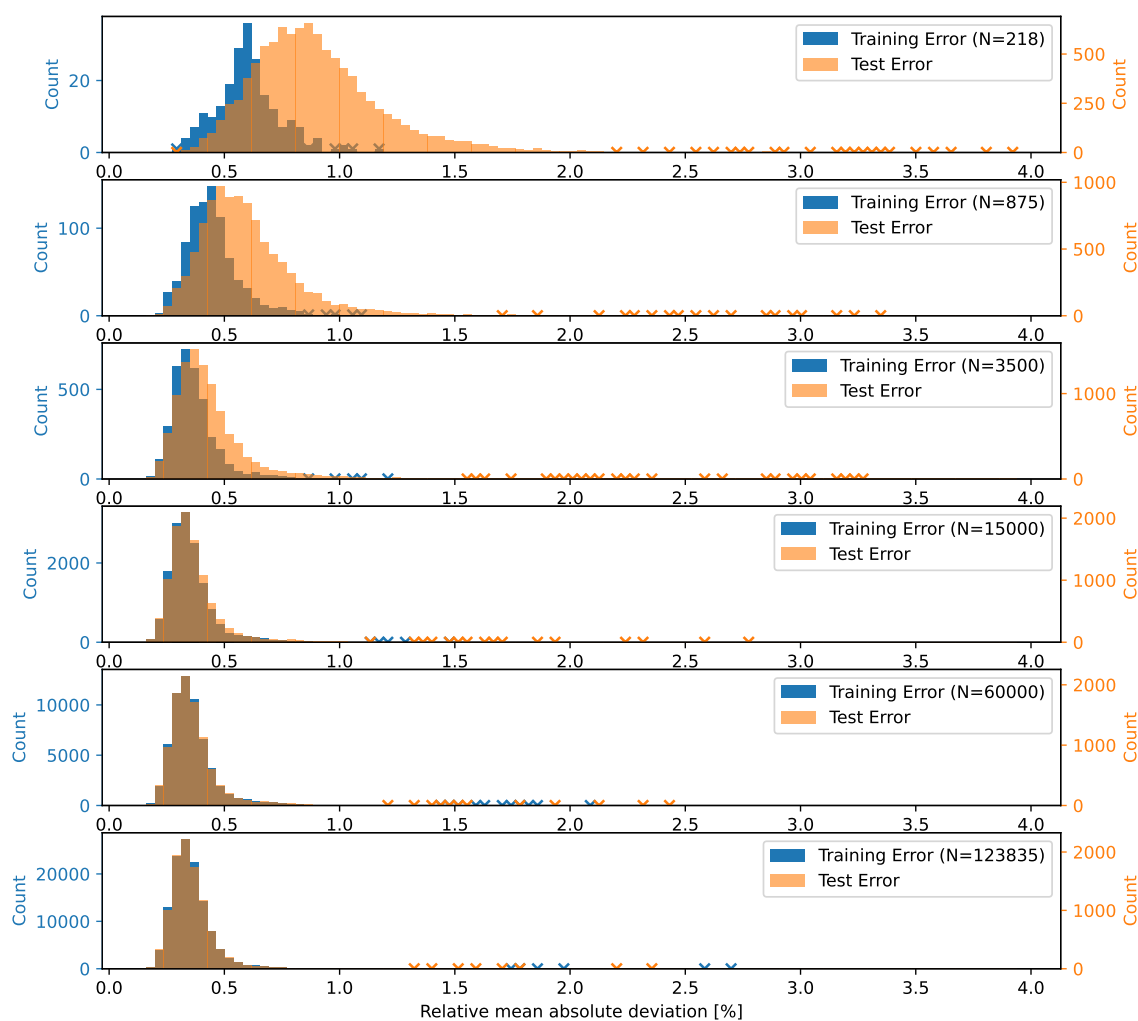
The figures in this section shows the distribution of prediction errors on training and test set using the normalised error metric:

$$\varepsilon_{|\text{mae}|} = \frac{\int_{x \in V} |\rho(x) - \hat{\rho}(x)|}{\int_{x \in V} |\rho(x)|} \quad (1)$$

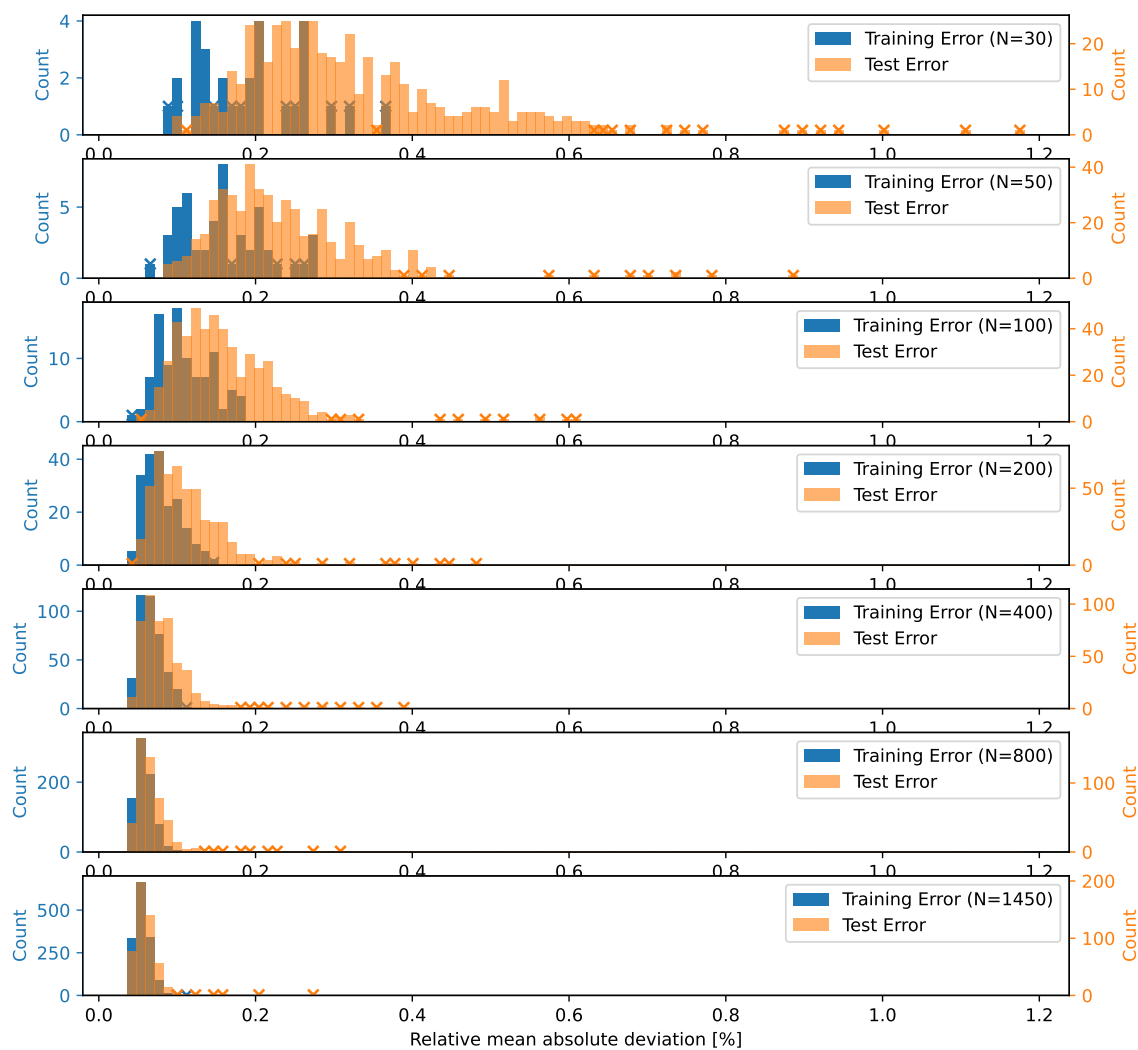
For each case the model was selected during training as the model with the lowest mean absolute error on the validation set. The markers show histogram bin with only a single occurrence, to show the extent of the tail of the distributions.



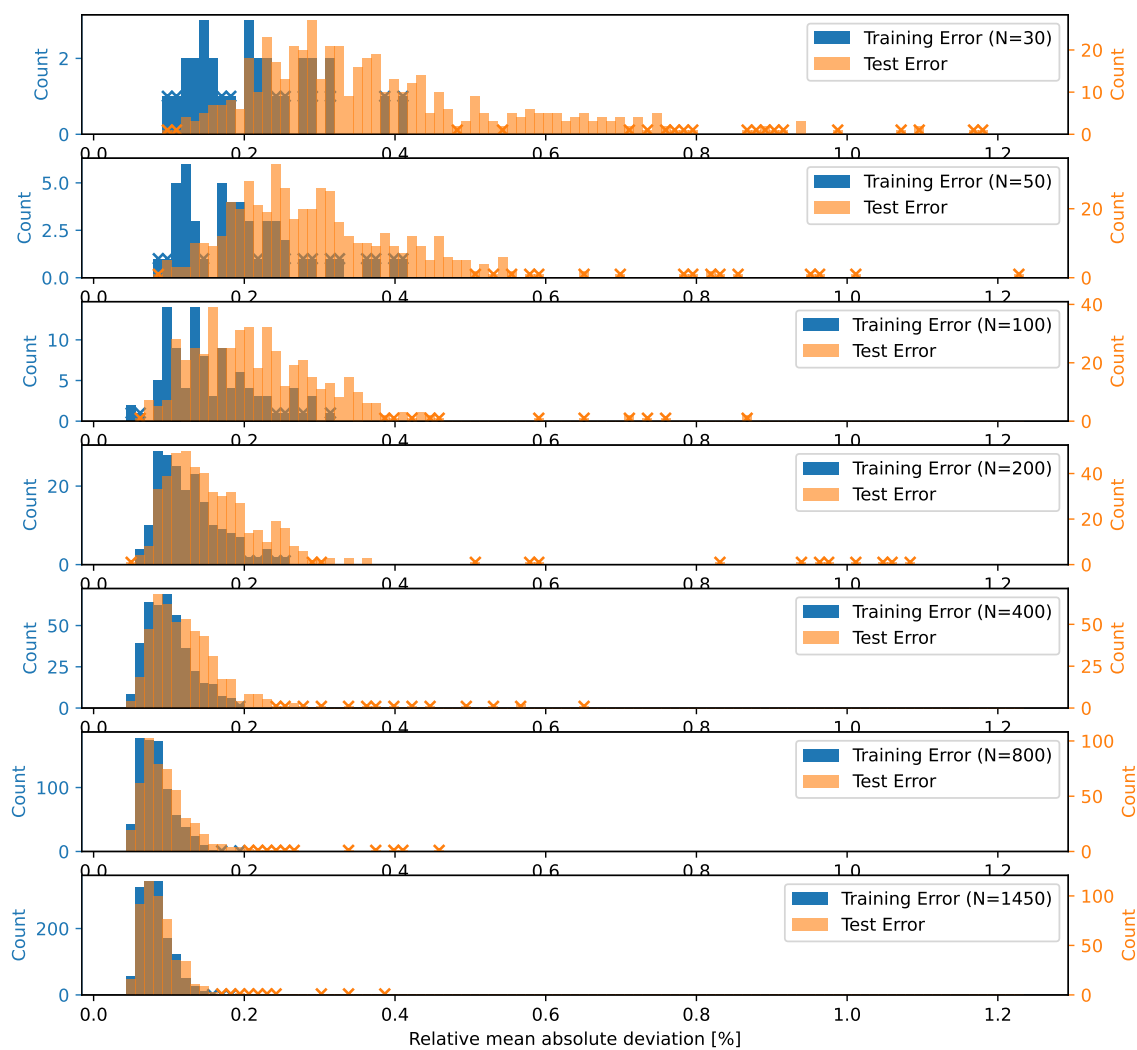
Supplementary Figure 7: Equivariant model QM9 dataset train and test set predictions



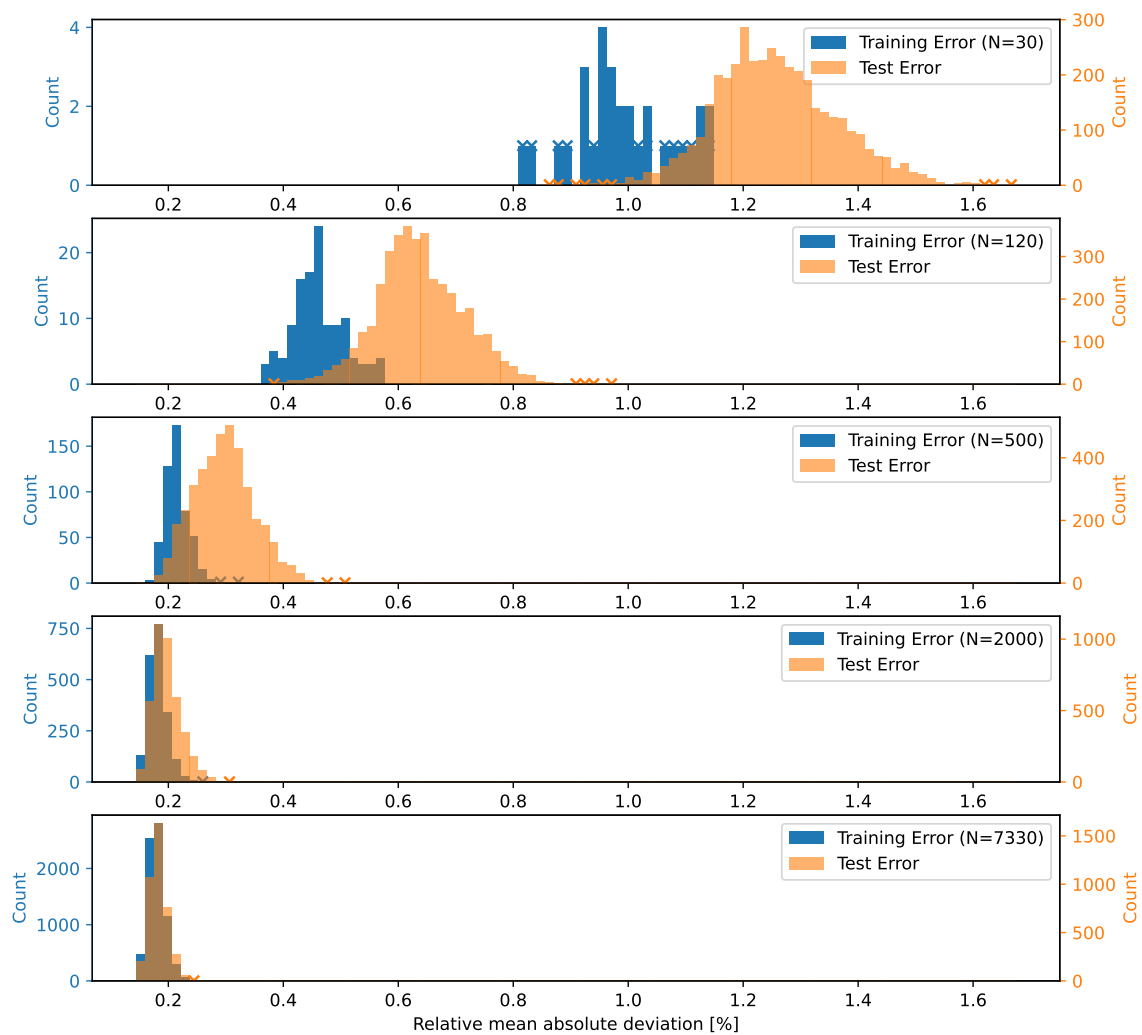
Supplementary Figure 8: Invariant model QM9 dataset train and test set predictions



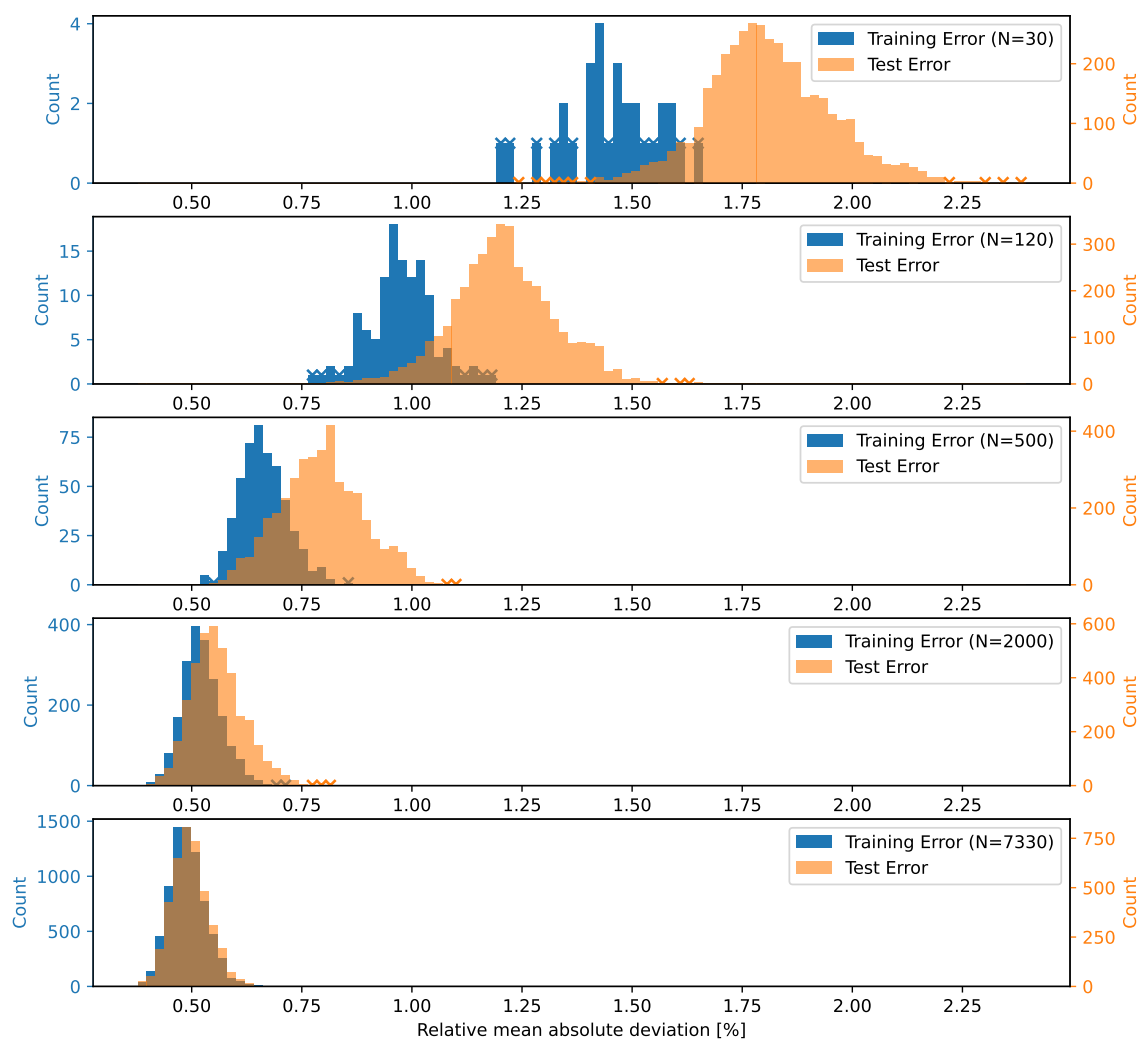
Supplementary Figure 9: Equivariant model LIB cathode dataset train and test set predictions



Supplementary Figure 10: Invariant model LIB cathode dataset train and test set predictions



Supplementary Figure 11: Equivariant model ethylene carbonate dataset train and test set predictions



Supplementary Figure 12: Invariant model ethylene carbonate dataset train and test set predictions