

# Evaluating Dropout and L2 Regularization for Generalizability of ANI-1 Neural Network

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## Introduction

Recent advances in machine learning, such as deep learning, have been shown to drastically improve the development of molecular potential energy models with a significantly smaller computational cost. One of the most prominent contributions in this area is the ANI-1 model, which demonstrated that neural network potentials (NNPs) trained on density functional theory (DFT) data can generalize well to diverse organic molecules (Smith et al., 2017). ANI-1 achieved this by combining a molecular representation based on atomic environment vectors (AEVs) with a high-capacity feedforward neural network architecture, allowing for accurate energy predictions for molecules larger than those seen during training.

While ANI-1 shows an advanced ability for generalization as mentioned in the paper mentioned above, its training strategy did not include key regularization techniques commonly used in modern deep learning. Specifically, the model omitted dropout and L2 regularization, two widely adopted methods for controlling overfitting and improving model performance. Instead, ANI-1 relied on architectural tuning, learning rate decay, and max-norm constraints to regularize training. However, with neural network potentials often trained on limited and highly correlated data, especially in smaller chemical domains, not including dropout and L2 leaves open questions about their potential to further stabilize learning and improve generalization. These regularization techniques can affect not only predictive performance but also convergence behavior and transferability. While these methods have been studied extensively in general deep learning contexts, their combined effects have not been systematically studied in the setting of molecular energy prediction, especially within architectures like ANI. In this project, we aim to systematically investigate the individual and combined effects of dropout and L2 regularization on the training and performance of ANI-style neural network potentials.

## Methods

We used the publicly available ANI-1 dataset (Smith et al., 2017), which consists of approximately 20 million DFT-calculated energies for small organic molecules composed of H, C, N, and O atoms. For this study, we subset the data to include only molecules with at least four heavy atoms to ensure more challenging learning dynamics.

Each molecule is represented using the Atomic Environment Vector (AEV) formalism. We utilize the AEV implementation from the TorchANI package (Gao et al., 2020), which efficiently computes AEVs and supports batched training, using the same feature configuration and symmetry function parameters as the original ANI-1 paper. Our only architectural changes to the original model are the inclusion of dropout and L2 regularization, applied to investigate their individual and combined impact on model generalization.

Models are trained with the Adam optimizer and a learning rate of 0.001 over a total of 100 epochs. We include 4 hidden layers as we determined that this was the most optimal. Unlike the original ANI-1 model, which used a larger batch size of 1024, we opted for a larger batch size of 512. We decided to do

this in order to reduce gradient noise, allowing for more stable updates and potentially faster convergence. We used two datasets:

Small set: First 5,000 molecules from the training and validation splits

Large set: Full dataset (all available training and validation molecules)

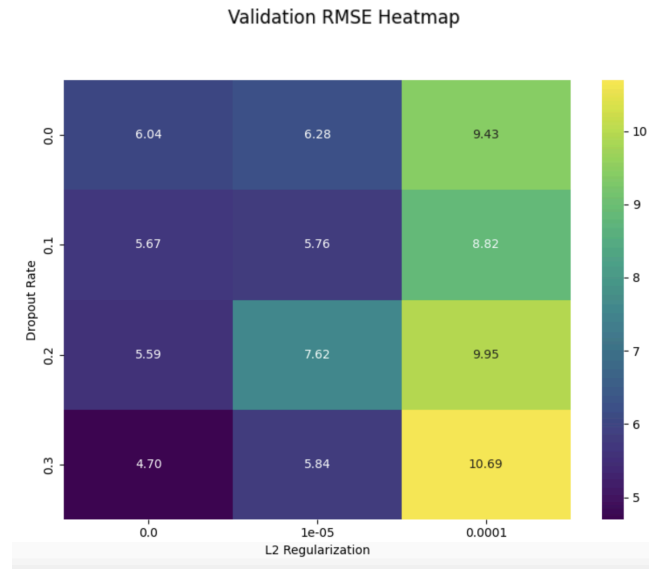
We performed a grid search over dropout and L2 weight decay values to explore their effects and interactions:

Dropout Rate	L2 Weight Decay
None	0
0.1	1e-5
0.2	1e-4
0.3	

**Table 1.** Values of dropout rate and L2 weight decay to be tested using a grid search.

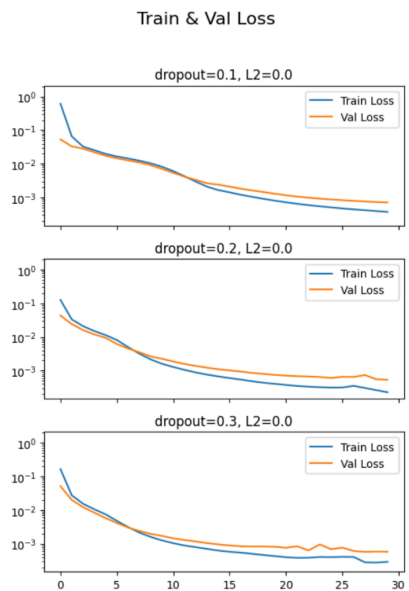
## Results and Discussion

To evaluate the impact of combining L2 regularization and dropout on the ANI-1 model, we conducted a grid search over four dropout rates and three L2 weight decay values. The model architecture consisted of four hidden layers with ReLU activation, a batch size of 512, and a fixed learning rate of 0.001. Each configuration was trained for 100 epochs, and root mean square error (RMSE) was used to assess model performance (Figure 1). Three configurations, dropout = 0.3, L2 = 0.0, dropout = 0.1, L2 = 0.0, and dropout = 0.2, L2 = 0.0 achieved RMSE values around 5 kcal/mol, with the first achieving an RMSE below 5 kcal/mol.



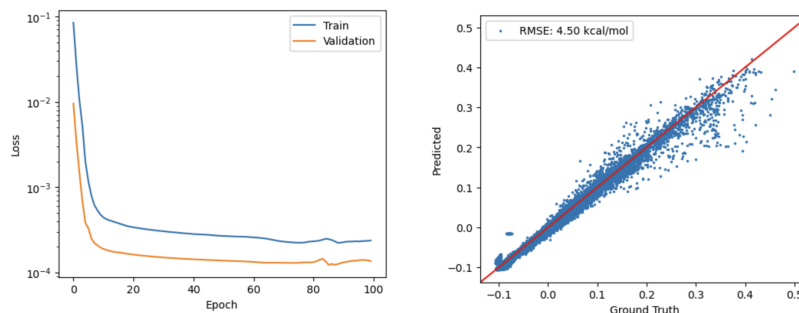
**Figure 1.** Heatmap of RMSE values of models trained with grid search for dropout rate and L2 regularization. All models had identical architecture of batch size 512, learning rate of 0.001, and 4 hidden layers.

To identify the most promising configuration among the three, we analyzed training and validation loss curves over 30 epochs (Figure 2). Across all configurations, the validation and training curves exhibited signs of overfitting, indicated by the cross between the two curves. While dropout and L2 regularization typically improve generalization, the persistent overfitting observed here is likely due to the use of a constant learning rate. Future iterations of the models may benefit from implementing a learning rate schedule following Simulated Annealing (as discussed in the course) to mitigate this issue.



**Figure 2.** Training and validation loss curves for models with no L2 regularization, batch size 512, 4 hidden layers, and learning rate 0.001. Each had a dropout rate of either 0.1, 0.2, or 0.3.

Among the tested configurations, the model with dropout = 0.3 and L2 = 0.0 showed the most stable training and validation curves. To further evaluate this configuration and assess whether increased training time could reduce overfitting, we retrained the model for 100 epochs (Figure 3) and conducted a 5-fold cross-validation with three runs per fold. This retraining yielded an RMSE of approximately 4.50, and cross-validation produced an average RMSE of  $3.4312 \pm 0.4773$  kcal/mol. These results suggest that adding dropout at a rate of 0.3 without L2 regularization enhances the model’s generalizability while maintaining low prediction error.



**Figure 3.** (Left) Training and Validation loss curves for model with no L2 regularization, batch size 512, 4 hidden layers, and learning rate 0.001, and dropout rate 0.3. Model trained at 100 epochs. (Right) Accuracy of prediction with RMSE.

While our findings demonstrate the potential of dropout to improve performance, several differences exist between our experimental setup and the original ANI-1 training regime. In relation to the learning rate, although both models employed an initial learning rate of 0.001, the ANI-1 model reduced this value by an order of magnitude at six intervals during training. This gradual decay strategy facilitates weight fine-tuning and helps prevent overshooting during optimization, thereby improving convergence. In contrast, our use of a fixed learning rate may have constrained model performance.

Additionally, the ANI-1 model utilized a batch size of 1024, while our model utilized a batch size of 512. Larger batch sizes typically yield more stable gradient estimates and improve training robustness, especially on large datasets. This smaller batch size, while enabling more frequent updates, introduced greater variance in the training and validation curves during hyperparameter tuning.

While we additionally employed mean squared error as the loss function, ANI-1 used an exponential loss function designed to reduce sensitivity to outliers and a max-norm regularization function instead of L2 regularization. Furthermore, while ANI-1 implemented early stopping based on validation error, our training proceeded for a fixed number of epochs. Although this approach helps ensure consistency across each model trained, it may have allowed some overfitting that could be accounted for with early stopping in future iterations.

## Conclusion

In this study, we investigated the effects of incorporating dropout and L2 regularization into the ANI-1 neural network potential architecture. Through a comprehensive grid search and cross-validation analysis, we found that introducing a dropout rate of 0.3 without L2 regularization led to improved model generalization. While both dropout and L2 are widely used in deep learning to combat overfitting, our results indicate that dropout alone provides the most benefit within the ANI-1 framework under a constant learning rate of 0.001 and a batch size of 512.

While these results are promising, our training procedure diverged from the original ANI-1 model in several key ways, including the use of a fixed learning rate, smaller batch size, and mean squared error loss. These differences likely contributed to overfitting observed in training and validation curves. Future work exploring the integration of learning rate schedules, such as exponential decay or simulated annealing, and early stopping mechanisms may provide further insight into the generalizability of Smith et. al.'s ANI-1 model.

# ani\_model\_final\_proj

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```
[4]: import torch
import torch.nn as nn
import numpy as np
import matplotlib
import matplotlib.pyplot as plt
from tqdm import tqdm
import torchani
from torchani.data import TransformableIterable
import pandas as pd
import seaborn as sns

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
```

```
[5]: def init_aev_computer():
    Rcr = 5.2
    Rca = 3.5
    EtaR = torch.tensor([16], dtype=torch.float, device=device)
    ShfR = torch.tensor([
        0.900000, 1.168750, 1.437500, 1.706250,
        1.975000, 2.243750, 2.512500, 2.781250,
        3.050000, 3.318750, 3.587500, 3.856250,
        4.125000, 4.393750, 4.662500, 4.931250
    ], dtype=torch.float, device=device)
    EtaA = torch.tensor([8], dtype=torch.float, device=device)
    Zeta = torch.tensor([32], dtype=torch.float, device=device)
    ShfA = torch.tensor([0.90, 1.55, 2.20, 2.85], dtype=torch.float,
↪device=device)
    ShfZ = torch.tensor([
        0.19634954, 0.58904862, 0.9817477, 1.37444680,
        1.76714590, 2.15984490, 2.5525440, 2.94524300
    ], dtype=torch.float, device=device)
    return torchani.AEVComputer(Rcr, Rca, EtaR, ShfR, EtaA, Zeta, ShfA, ShfZ,
↪num_species=4)

aev_computer = init_aev_computer()
```

```
[6]: class AtomicNet(nn.Module):
    def __init__(self, dropout_rate=None):
        super().__init__()
        layers = [
            nn.Linear(384, 256), nn.ReLU(),
            nn.Dropout(dropout_rate) if dropout_rate else nn.Identity(),
            nn.Linear(256, 192), nn.ReLU(),
            nn.Dropout(dropout_rate) if dropout_rate else nn.Identity(),
            nn.Linear(192, 128), nn.ReLU(),
            nn.Dropout(dropout_rate) if dropout_rate else nn.Identity(),
            nn.Linear(128, 64), nn.ReLU(),
            nn.Dropout(dropout_rate) if dropout_rate else nn.Identity(),
            nn.Linear(64, 1)
        ]
        self.layers = nn.Sequential(*layers)

    def forward(self, x):
        return self.layers(x)

[7]: def load_ani_dataset(dspath):
    energy_shifter = torchani.utils.EnergyShifter(None)
    species_order = ['H', 'C', 'N', 'O']
    dataset = torchani.data.load(dspath)
    dataset = dataset.subtract_self_energies(energy_shifter, species_order)
    dataset = dataset.species_to_indices(species_order)
    dataset = dataset.shuffle()
    return dataset

dataset = load_ani_dataset("./ani_gdb_s01_to_s04.h5")
train_data, val_data, test_data = dataset.split(0.8, 0.1, 0.1)

[8]: def get_data_subset(dataset, size):
    dataset = list(dataset)
    if size == 'small':
        return TransformableIterable(dataset[:5000])
    elif size == 'large':
        return TransformableIterable(dataset[:20000])
    else:
        return TransformableIterable(dataset)

train_subset = get_data_subset(train_data, '')
val_subset = get_data_subset(val_data, '')

[9]: def build_model(dropout, l2, device):
    nets = [AtomicNet(dropout).to(device) for _ in range(4)]
    ani_model = torchani.ANIModel(nets)
    return nn.Sequential(aev_computer, ani_model).to(device)
```

```

[10]: class ANITrainer:
    def __init__(self, model, batch_size=512, learning_rate=1e-3, epoch=100,
↳ l2=0.0):
        self.model = model
        self.batch_size = batch_size
        self.optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate,
↳ weight_decay=l2)
        self.epoch = epoch

    def train(self, train_data, val_data, early_stop=True, draw_curve=True):
        self.model.train()
        train_loader = train_data.collate(self.batch_size).cache()
        loss_func = nn.MSELoss()
        train_loss_list = []
        val_loss_list = []
        val_rmse_list = []
        best_model = None
        lowest_val_loss = float('inf')

        for ep in tqdm(range(self.epoch), desc="Epochs"):
            total_train_loss = 0.0
            for batch in train_loader:
                species = batch['species'].to(device)
                coords = batch['coordinates'].to(device)
                energies = batch['energies'].to(device).float()

                _, pred = self.model((species, coords))
                loss = loss_func(energies, pred)

                self.optimizer.zero_grad()
                loss.backward()
                self.optimizer.step()
                total_train_loss += loss.item()

            val_loss, val_rmse = self.evaluate(val_data)
            train_loss_list.append(total_train_loss)
            val_loss_list.append(val_loss)
            val_rmse_list.append(val_rmse)

            print(f"Epoch {ep+1} - Train Loss: {total_train_loss:.4f}, Val Loss:
↳ {val_loss:.4f}, RMSE: {val_rmse:.2f} kcal/mol")

            if early_stop and val_loss < lowest_val_loss:
                lowest_val_loss = val_loss
                best_model = self.model.state_dict()

        if draw_curve:

```



```

fig, ax1 = plt.subplots()
ax1.plot(train_loss_list, label="Train Loss")
ax1.plot(val_loss_list, label="Val Loss")
ax1.set_yscale("log")
ax1.set_xlabel("Epoch")
ax1.set_ylabel("MSE Loss")

ax2 = ax1.twinx()
ax2.plot(val_rmse_list, 'r--', label="Val RMSE")
ax2.set_ylabel("RMSE (kcal/mol)", color='red')

fig.legend(loc='upper right')
plt.title("Training Curve")
plt.show()

if early_stop and best_model:
    self.model.load_state_dict(best_model)

return train_loss_list, val_loss_list, val_rmse_list

def evaluate(self, data, draw_plot=False):
    data_loader = data.collate(self.batch_size).cache()
    loss_func = nn.MSELoss()
    total_loss = 0.0
    true_all, pred_all = [], []

    self.model.eval()
    with torch.no_grad():
        for batch in data_loader:
            species = batch['species'].to(device)
            coords = batch['coordinates'].to(device)
            true = batch['energies'].to(device).float()
            _, pred = self.model((species, coords))

            total_loss += loss_func(true, pred).item()
            true_all.append(true.cpu().numpy())
            pred_all.append(pred.cpu().numpy())

    true_all = np.concatenate(true_all).flatten()
    pred_all = np.concatenate(pred_all).flatten()
    rmse = np.sqrt(np.mean((true_all - pred_all) ** 2)) * 627.509

    if draw_plot:
        plt.scatter(true_all, pred_all, s=2)
        plt.plot([true_all.min(), true_all.max()], [true_all.min(),
→true_all.max()], 'r--')
        plt.xlabel("True Energy")

```

```

plt.ylabel("Predicted Energy")
plt.title(f"Validation RMSE: {rmse:.2f} kcal/mol")
plt.show()

return total_loss, rmse

```

```

[15]: results = []
dropout_list = [None, 0.1, 0.2, 0.3]
l2_list = [0.0, 1e-5, 1e-4]

num_rows = len(dropout_list)
num_cols = len(l2_list)
fig_loss, axes_loss = plt.subplots(num_rows, num_cols, figsize=(15, 10),
    ↪sharex=True, sharey=True)
fig_rmse, axes_rmse = plt.subplots(num_rows, num_cols, figsize=(15, 10),
    ↪sharex=True, sharey=True)

for i, dropout in enumerate(dropout_list):
    for j, l2 in enumerate(l2_list):
        print(f"\nTraining model with dropout={dropout}, L2={l2}")
        model = build_model(dropout, l2, device)
        trainer = ANITrainer(model, epoch=30, l2=l2)
        train_losses, val_losses, val_rmse = trainer.train(
            train_subset, val_subset, early_stop=True, draw_curve=False
        )

        final_rmse = val_rmse[-1]
        results.append({'dropout': dropout if dropout else 0.0, 'l2': l2,
    ↪'val_rmse': final_rmse})

        # Plot losses
        ax_loss = axes_loss[i][j]
        ax_loss.plot(train_losses, label='Train Loss')
        ax_loss.plot(val_losses, label='Val Loss')
        ax_loss.set_yscale('log')
        ax_loss.set_title(f"dropout={dropout}, L2={l2}")
        ax_loss.legend()

        # Plot RMSE
        ax_rmse = axes_rmse[i][j]
        ax_rmse.plot(val_rmse, color='red', label='Val RMSE')
        ax_rmse.set_title(f"dropout={dropout}, L2={l2}")
        ax_rmse.set_ylabel("RMSE (kcal/mol)")
        ax_rmse.set_xlabel("Epoch")
        ax_rmse.legend()

fig_loss.suptitle("Train & Validation Loss Curves", fontsize=16)

```

```
fig_rmse.suptitle("Validation RMSE Curves", fontsize=16)
fig_loss.tight_layout(rect=[0, 0, 1, 0.97])
fig_rmse.tight_layout(rect=[0, 0, 1, 0.97])
plt.show()
```

Training model with dropout=None, L2=0.0

```
Epochs:   3%|                                     | 1/30 [00:06<03:02,  6.30s/it]
Epoch 1 - Train Loss: 0.3069, Val Loss: 0.0773, RMSE: 55.24 kcal/mol
Epochs:   7%|                                     | 2/30 [00:10<02:29,  5.34s/it]
Epoch 2 - Train Loss: 0.0530, Val Loss: 0.0386, RMSE: 39.08 kcal/mol
Epochs:  10%|                                     | 3/30 [00:15<02:17,  5.08s/it]
Epoch 3 - Train Loss: 0.0262, Val Loss: 0.0176, RMSE: 26.37 kcal/mol
Epochs:  13%|                                     | 4/30 [00:21<02:14,  5.19s/it]
Epoch 4 - Train Loss: 0.0148, Val Loss: 0.0138, RMSE: 23.45 kcal/mol
Epochs:  17%|                                     | 5/30 [00:26<02:11,  5.27s/it]
Epoch 5 - Train Loss: 0.0112, Val Loss: 0.0109, RMSE: 20.85 kcal/mol
Epochs:  20%|                                     | 6/30 [00:32<02:12,  5.53s/it]
Epoch 6 - Train Loss: 0.0091, Val Loss: 0.0090, RMSE: 18.92 kcal/mol
Epochs:  23%|                                     | 7/30 [00:37<02:06,  5.49s/it]
Epoch 7 - Train Loss: 0.0074, Val Loss: 0.0074, RMSE: 17.19 kcal/mol
Epochs:  27%|                                     | 8/30 [00:47<02:31,  6.91s/it]
Epoch 8 - Train Loss: 0.0056, Val Loss: 0.0059, RMSE: 15.32 kcal/mol
Epochs:  30%|                                     | 9/30 [00:55<02:29,  7.10s/it]
Epoch 9 - Train Loss: 0.0043, Val Loss: 0.0048, RMSE: 13.85 kcal/mol
Epochs:  33%|                                     | 10/30 [01:03<02:29,  7.47s/it]
Epoch 10 - Train Loss: 0.0033, Val Loss: 0.0039, RMSE: 12.43 kcal/mol
Epochs:  37%|                                     | 11/30 [01:10<02:20,  7.41s/it]
Epoch 11 - Train Loss: 0.0026, Val Loss: 0.0032, RMSE: 11.26 kcal/mol
Epochs:  40%|                                     | 12/30 [01:19<02:19,  7.73s/it]
Epoch 12 - Train Loss: 0.0021, Val Loss: 0.0027, RMSE: 10.38 kcal/mol
Epochs:  43%|                                     | 13/30 [01:28<02:17,  8.10s/it]
Epoch 13 - Train Loss: 0.0018, Val Loss: 0.0023, RMSE:  9.67 kcal/mol
Epochs:  47%|                                     | 14/30 [01:35<02:07,  7.95s/it]
```

Epoch 14 - Train Loss: 0.0015, Val Loss: 0.0020, RMSE: 9.01 kcal/mol  
Epochs: 50%| | 15/30 [01:43<01:57, 7.85s/it]

Epoch 15 - Train Loss: 0.0013, Val Loss: 0.0018, RMSE: 8.46 kcal/mol  
Epochs: 53%| | 16/30 [01:50<01:47, 7.65s/it]

Epoch 16 - Train Loss: 0.0012, Val Loss: 0.0016, RMSE: 7.90 kcal/mol  
Epochs: 57%| | 17/30 [01:58<01:38, 7.56s/it]

Epoch 17 - Train Loss: 0.0010, Val Loss: 0.0014, RMSE: 7.56 kcal/mol  
Epochs: 60%| | 18/30 [02:04<01:27, 7.31s/it]

Epoch 18 - Train Loss: 0.0008, Val Loss: 0.0013, RMSE: 7.12 kcal/mol  
Epochs: 63%| | 19/30 [02:12<01:20, 7.34s/it]

Epoch 19 - Train Loss: 0.0007, Val Loss: 0.0011, RMSE: 6.75 kcal/mol  
Epochs: 67%| | 20/30 [02:19<01:14, 7.43s/it]

Epoch 20 - Train Loss: 0.0007, Val Loss: 0.0010, RMSE: 6.44 kcal/mol  
Epochs: 70%| | 21/30 [02:27<01:07, 7.51s/it]

Epoch 21 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.35 kcal/mol  
Epochs: 73%| | 22/30 [02:36<01:02, 7.81s/it]

Epoch 22 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.96 kcal/mol  
Epochs: 77%| | 23/30 [02:43<00:53, 7.70s/it]

Epoch 23 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.83 kcal/mol  
Epochs: 80%| | 24/30 [02:51<00:46, 7.73s/it]

Epoch 24 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.79 kcal/mol  
Epochs: 83%| | 25/30 [02:59<00:39, 7.99s/it]

Epoch 25 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.73 kcal/mol  
Epochs: 87%| | 26/30 [03:07<00:31, 7.97s/it]

Epoch 26 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.65 kcal/mol  
Epochs: 90%| | 27/30 [03:16<00:24, 8.26s/it]

Epoch 27 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.44 kcal/mol  
Epochs: 93%| | 28/30 [03:24<00:15, 7.94s/it]

Epoch 28 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.24 kcal/mol  
Epochs: 97%| | 29/30 [03:33<00:08, 8.30s/it]

Epoch 29 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.51 kcal/mol  
Epochs: 100%| | 30/30 [03:40<00:00, 7.33s/it]

Epoch 30 - Train Loss: 0.0004, Val Loss: 0.0009, RMSE: 6.04 kcal/mol

Training model with dropout=None, L2=1e-05

Epochs: 3%| | 1/30 [00:08<03:55, 8.12s/it]

Epoch 1 - Train Loss: 0.9701, Val Loss: 0.0678, RMSE: 51.75 kcal/mol

Epochs: 7%| | 2/30 [00:18<04:22, 9.37s/it]

Epoch 2 - Train Loss: 0.0988, Val Loss: 0.0449, RMSE: 42.12 kcal/mol

Epochs: 10%| | 3/30 [00:26<03:54, 8.68s/it]

Epoch 3 - Train Loss: 0.0441, Val Loss: 0.0319, RMSE: 35.56 kcal/mol

Epochs: 13%| | 4/30 [00:35<03:52, 8.93s/it]

Epoch 4 - Train Loss: 0.0289, Val Loss: 0.0259, RMSE: 32.02 kcal/mol

Epochs: 17%| | 5/30 [00:43<03:38, 8.75s/it]

Epoch 5 - Train Loss: 0.0209, Val Loss: 0.0197, RMSE: 27.98 kcal/mol

Epochs: 20%| | 6/30 [00:51<03:19, 8.32s/it]

Epoch 6 - Train Loss: 0.0171, Val Loss: 0.0165, RMSE: 25.65 kcal/mol

Epochs: 23%| | 7/30 [00:58<03:02, 7.94s/it]

Epoch 7 - Train Loss: 0.0142, Val Loss: 0.0138, RMSE: 23.45 kcal/mol

Epochs: 27%| | 8/30 [01:05<02:48, 7.68s/it]

Epoch 8 - Train Loss: 0.0115, Val Loss: 0.0107, RMSE: 20.63 kcal/mol

Epochs: 30%| | 9/30 [01:14<02:45, 7.89s/it]

Epoch 9 - Train Loss: 0.0083, Val Loss: 0.0072, RMSE: 16.93 kcal/mol

Epochs: 33%| | 10/30 [01:22<02:40, 8.01s/it]

Epoch 10 - Train Loss: 0.0054, Val Loss: 0.0049, RMSE: 13.89 kcal/mol

Epochs: 37%| | 11/30 [01:30<02:34, 8.11s/it]

Epoch 11 - Train Loss: 0.0038, Val Loss: 0.0037, RMSE: 12.12 kcal/mol

Epochs: 40%| | 12/30 [01:38<02:23, 7.98s/it]

Epoch 12 - Train Loss: 0.0029, Val Loss: 0.0031, RMSE: 11.13 kcal/mol

Epochs: 43%| | 13/30 [01:45<02:11, 7.73s/it]

Epoch 13 - Train Loss: 0.0024, Val Loss: 0.0026, RMSE: 10.20 kcal/mol

Epochs: 47%| | 14/30 [01:54<02:09, 8.08s/it]

Epoch 14 - Train Loss: 0.0019, Val Loss: 0.0022, RMSE: 9.28 kcal/mol

Epochs: 50%| | 15/30 [02:02<01:58, 7.92s/it]

Epoch 15 - Train Loss: 0.0017, Val Loss: 0.0020, RMSE: 8.79 kcal/mol  
Epochs: 53%| | 16/30 [02:11<01:56, 8.33s/it]  
Epoch 16 - Train Loss: 0.0015, Val Loss: 0.0018, RMSE: 8.41 kcal/mol  
Epochs: 57%| | 17/30 [02:19<01:45, 8.15s/it]  
Epoch 17 - Train Loss: 0.0014, Val Loss: 0.0016, RMSE: 7.92 kcal/mol  
Epochs: 60%| | 18/30 [02:27<01:38, 8.18s/it]  
Epoch 18 - Train Loss: 0.0012, Val Loss: 0.0015, RMSE: 7.59 kcal/mol  
Epochs: 63%| | 19/30 [02:35<01:29, 8.17s/it]  
Epoch 19 - Train Loss: 0.0011, Val Loss: 0.0014, RMSE: 7.35 kcal/mol  
Epochs: 67%| | 20/30 [02:42<01:18, 7.86s/it]  
Epoch 20 - Train Loss: 0.0010, Val Loss: 0.0013, RMSE: 7.08 kcal/mol  
Epochs: 70%| | 21/30 [02:50<01:12, 8.01s/it]  
Epoch 21 - Train Loss: 0.0009, Val Loss: 0.0012, RMSE: 6.89 kcal/mol  
Epochs: 73%| | 22/30 [02:58<01:04, 8.02s/it]  
Epoch 22 - Train Loss: 0.0009, Val Loss: 0.0012, RMSE: 6.86 kcal/mol  
Epochs: 77%| | 23/30 [03:08<00:58, 8.37s/it]  
Epoch 23 - Train Loss: 0.0008, Val Loss: 0.0012, RMSE: 6.96 kcal/mol  
Epochs: 80%| | 24/30 [03:19<00:55, 9.31s/it]  
Epoch 24 - Train Loss: 0.0008, Val Loss: 0.0011, RMSE: 6.74 kcal/mol  
Epochs: 83%| | 25/30 [03:26<00:43, 8.63s/it]  
Epoch 25 - Train Loss: 0.0007, Val Loss: 0.0012, RMSE: 6.92 kcal/mol  
Epochs: 87%| | 26/30 [03:33<00:32, 8.20s/it]  
Epoch 26 - Train Loss: 0.0007, Val Loss: 0.0011, RMSE: 6.57 kcal/mol  
Epochs: 90%| | 27/30 [03:40<00:23, 7.87s/it]  
Epoch 27 - Train Loss: 0.0007, Val Loss: 0.0011, RMSE: 6.58 kcal/mol  
Epochs: 93%| | 28/30 [03:47<00:15, 7.61s/it]  
Epoch 28 - Train Loss: 0.0007, Val Loss: 0.0011, RMSE: 6.70 kcal/mol  
Epochs: 97%| | 29/30 [03:55<00:07, 7.64s/it]  
Epoch 29 - Train Loss: 0.0007, Val Loss: 0.0010, RMSE: 6.44 kcal/mol  
Epochs: 100%| | 30/30 [04:03<00:00, 8.11s/it]  
Epoch 30 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.28 kcal/mol

Training model with dropout=None, L2=0.0001

Epochs: 3% | 1/30 [00:06<03:16, 6.79s/it]  
Epoch 1 - Train Loss: 0.2930, Val Loss: 0.1206, RMSE: 69.01 kcal/mol  
Epochs: 7% | 2/30 [00:15<03:38, 7.81s/it]  
Epoch 2 - Train Loss: 0.0604, Val Loss: 0.0372, RMSE: 38.38 kcal/mol  
Epochs: 10% | 3/30 [00:23<03:40, 8.18s/it]  
Epoch 3 - Train Loss: 0.0273, Val Loss: 0.0242, RMSE: 30.94 kcal/mol  
Epochs: 13% | 4/30 [00:33<03:49, 8.82s/it]  
Epoch 4 - Train Loss: 0.0214, Val Loss: 0.0194, RMSE: 27.75 kcal/mol  
Epochs: 17% | 5/30 [00:44<03:54, 9.37s/it]  
Epoch 5 - Train Loss: 0.0169, Val Loss: 0.0165, RMSE: 25.60 kcal/mol  
Epochs: 20% | 6/30 [00:51<03:25, 8.55s/it]  
Epoch 6 - Train Loss: 0.0139, Val Loss: 0.0132, RMSE: 22.93 kcal/mol  
Epochs: 23% | 7/30 [00:59<03:17, 8.60s/it]  
Epoch 7 - Train Loss: 0.0105, Val Loss: 0.0095, RMSE: 19.42 kcal/mol  
Epochs: 27% | 8/30 [01:08<03:09, 8.62s/it]  
Epoch 8 - Train Loss: 0.0076, Val Loss: 0.0071, RMSE: 16.78 kcal/mol  
Epochs: 30% | 9/30 [01:18<03:08, 8.98s/it]  
Epoch 9 - Train Loss: 0.0058, Val Loss: 0.0056, RMSE: 14.94 kcal/mol  
Epochs: 33% | 10/30 [01:26<02:52, 8.64s/it]  
Epoch 10 - Train Loss: 0.0045, Val Loss: 0.0047, RMSE: 13.69 kcal/mol  
Epochs: 37% | 11/30 [01:33<02:35, 8.19s/it]  
Epoch 11 - Train Loss: 0.0040, Val Loss: 0.0046, RMSE: 13.54 kcal/mol  
Epochs: 40% | 12/30 [01:40<02:22, 7.94s/it]  
Epoch 12 - Train Loss: 0.0034, Val Loss: 0.0037, RMSE: 12.14 kcal/mol  
Epochs: 43% | 13/30 [01:52<02:34, 9.09s/it]  
Epoch 13 - Train Loss: 0.0031, Val Loss: 0.0042, RMSE: 12.92 kcal/mol  
Epochs: 47% | 14/30 [02:11<03:15, 12.23s/it]  
Epoch 14 - Train Loss: 0.0030, Val Loss: 0.0033, RMSE: 11.36 kcal/mol  
Epochs: 50% | 15/30 [02:23<03:00, 12.06s/it]  
Epoch 15 - Train Loss: 0.0027, Val Loss: 0.0029, RMSE: 10.80 kcal/mol  
Epochs: 53% | 16/30 [02:34<02:45, 11.84s/it]

Epoch 16 - Train Loss: 0.0025, Val Loss: 0.0032, RMSE: 11.18 kcal/mol  
Epochs: 57%| | 17/30 [02:44<02:25, 11.21s/it]

Epoch 17 - Train Loss: 0.0025, Val Loss: 0.0031, RMSE: 11.09 kcal/mol  
Epochs: 60%| | 18/30 [02:53<02:05, 10.47s/it]

Epoch 18 - Train Loss: 0.0025, Val Loss: 0.0037, RMSE: 12.02 kcal/mol  
Epochs: 63%| | 19/30 [03:02<01:49, 9.96s/it]

Epoch 19 - Train Loss: 0.0026, Val Loss: 0.0027, RMSE: 10.27 kcal/mol  
Epochs: 67%| | 20/30 [03:09<01:33, 9.32s/it]

Epoch 20 - Train Loss: 0.0023, Val Loss: 0.0025, RMSE: 9.88 kcal/mol  
Epochs: 70%| | 21/30 [03:17<01:19, 8.79s/it]

Epoch 21 - Train Loss: 0.0021, Val Loss: 0.0030, RMSE: 10.96 kcal/mol  
Epochs: 73%| | 22/30 [03:26<01:11, 8.95s/it]

Epoch 22 - Train Loss: 0.0023, Val Loss: 0.0027, RMSE: 10.30 kcal/mol  
Epochs: 77%| | 23/30 [03:34<01:00, 8.57s/it]

Epoch 23 - Train Loss: 0.0021, Val Loss: 0.0023, RMSE: 9.56 kcal/mol  
Epochs: 80%| | 24/30 [03:43<00:52, 8.79s/it]

Epoch 24 - Train Loss: 0.0020, Val Loss: 0.0025, RMSE: 9.85 kcal/mol  
Epochs: 83%| | 25/30 [03:52<00:44, 8.87s/it]

Epoch 25 - Train Loss: 0.0020, Val Loss: 0.0036, RMSE: 11.97 kcal/mol  
Epochs: 87%| | 26/30 [04:00<00:33, 8.44s/it]

Epoch 26 - Train Loss: 0.0026, Val Loss: 0.0025, RMSE: 10.01 kcal/mol  
Epochs: 90%| | 27/30 [04:07<00:24, 8.20s/it]

Epoch 27 - Train Loss: 0.0021, Val Loss: 0.0022, RMSE: 9.29 kcal/mol  
Epochs: 93%| | 28/30 [04:19<00:18, 9.14s/it]

Epoch 28 - Train Loss: 0.0019, Val Loss: 0.0027, RMSE: 10.28 kcal/mol  
Epochs: 97%| | 29/30 [04:32<00:10, 10.44s/it]

Epoch 29 - Train Loss: 0.0020, Val Loss: 0.0029, RMSE: 10.76 kcal/mol  
Epochs: 100%| | 30/30 [04:41<00:00, 9.37s/it]

Epoch 30 - Train Loss: 0.0021, Val Loss: 0.0023, RMSE: 9.43 kcal/mol

Training model with dropout=0.1, L2=0.0

Epochs: 3%| | 1/30 [00:10<05:12, 10.76s/it]



Epoch 1 - Train Loss: 1.2534, Val Loss: 0.0263, RMSE: 32.30 kcal/mol  
Epochs: 7%| | 2/30 [00:18<04:14, 9.10s/it]

Epoch 2 - Train Loss: 0.0961, Val Loss: 0.0218, RMSE: 29.40 kcal/mol  
Epochs: 10%| | 3/30 [00:31<04:56, 11.00s/it]

Epoch 3 - Train Loss: 0.0394, Val Loss: 0.0212, RMSE: 29.01 kcal/mol  
Epochs: 13%| | 4/30 [00:39<04:07, 9.51s/it]

Epoch 4 - Train Loss: 0.0251, Val Loss: 0.0205, RMSE: 28.52 kcal/mol  
Epochs: 17%| | 5/30 [00:47<03:43, 8.93s/it]

Epoch 5 - Train Loss: 0.0189, Val Loss: 0.0184, RMSE: 27.05 kcal/mol  
Epochs: 20%| | 6/30 [00:53<03:09, 7.91s/it]

Epoch 6 - Train Loss: 0.0164, Val Loss: 0.0158, RMSE: 25.01 kcal/mol  
Epochs: 23%| | 7/30 [00:59<02:47, 7.30s/it]

Epoch 7 - Train Loss: 0.0138, Val Loss: 0.0139, RMSE: 23.52 kcal/mol  
Epochs: 27%| | 8/30 [01:04<02:30, 6.84s/it]

Epoch 8 - Train Loss: 0.0118, Val Loss: 0.0119, RMSE: 21.75 kcal/mol  
Epochs: 30%| | 9/30 [01:10<02:14, 6.43s/it]

Epoch 9 - Train Loss: 0.0100, Val Loss: 0.0101, RMSE: 19.99 kcal/mol  
Epochs: 33%| | 10/30 [01:15<02:02, 6.13s/it]

Epoch 10 - Train Loss: 0.0083, Val Loss: 0.0083, RMSE: 18.16 kcal/mol  
Epochs: 37%| | 11/30 [01:21<01:53, 5.97s/it]

Epoch 11 - Train Loss: 0.0067, Val Loss: 0.0067, RMSE: 16.31 kcal/mol  
Epochs: 40%| | 12/30 [01:28<01:52, 6.25s/it]

Epoch 12 - Train Loss: 0.0053, Val Loss: 0.0054, RMSE: 14.58 kcal/mol  
Epochs: 43%| | 13/30 [01:35<01:50, 6.51s/it]

Epoch 13 - Train Loss: 0.0041, Val Loss: 0.0043, RMSE: 12.99 kcal/mol  
Epochs: 47%| | 14/30 [01:45<02:01, 7.62s/it]

Epoch 14 - Train Loss: 0.0033, Val Loss: 0.0035, RMSE: 11.82 kcal/mol  
Epochs: 50%| | 15/30 [01:52<01:49, 7.29s/it]

Epoch 15 - Train Loss: 0.0027, Val Loss: 0.0030, RMSE: 10.94 kcal/mol  
Epochs: 53%| | 16/30 [02:01<01:51, 7.99s/it]

Epoch 16 - Train Loss: 0.0022, Val Loss: 0.0026, RMSE: 10.05 kcal/mol  
Epochs: 57%| | 17/30 [02:08<01:36, 7.46s/it]

Epoch 17 - Train Loss: 0.0019, Val Loss: 0.0022, RMSE: 9.31 kcal/mol  
Epochs: 60%| | 18/30 [02:13<01:21, 6.81s/it]  
Epoch 18 - Train Loss: 0.0017, Val Loss: 0.0019, RMSE: 8.75 kcal/mol  
Epochs: 63%| | 19/30 [02:19<01:11, 6.47s/it]  
Epoch 19 - Train Loss: 0.0015, Val Loss: 0.0017, RMSE: 8.26 kcal/mol  
Epochs: 67%| | 20/30 [02:24<01:01, 6.18s/it]  
Epoch 20 - Train Loss: 0.0013, Val Loss: 0.0015, RMSE: 7.81 kcal/mol  
Epochs: 70%| | 21/30 [02:31<00:56, 6.31s/it]  
Epoch 21 - Train Loss: 0.0011, Val Loss: 0.0014, RMSE: 7.44 kcal/mol  
Epochs: 73%| | 22/30 [02:39<00:54, 6.84s/it]  
Epoch 22 - Train Loss: 0.0010, Val Loss: 0.0013, RMSE: 7.13 kcal/mol  
Epochs: 77%| | 23/30 [02:46<00:48, 6.96s/it]  
Epoch 23 - Train Loss: 0.0009, Val Loss: 0.0012, RMSE: 6.86 kcal/mol  
Epochs: 80%| | 24/30 [02:53<00:41, 6.85s/it]  
Epoch 24 - Train Loss: 0.0009, Val Loss: 0.0011, RMSE: 6.61 kcal/mol  
Epochs: 83%| | 25/30 [02:59<00:33, 6.68s/it]  
Epoch 25 - Train Loss: 0.0008, Val Loss: 0.0010, RMSE: 6.38 kcal/mol  
Epochs: 87%| | 26/30 [03:05<00:26, 6.63s/it]  
Epoch 26 - Train Loss: 0.0007, Val Loss: 0.0010, RMSE: 6.19 kcal/mol  
Epochs: 90%| | 27/30 [03:12<00:19, 6.56s/it]  
Epoch 27 - Train Loss: 0.0007, Val Loss: 0.0009, RMSE: 6.03 kcal/mol  
Epochs: 93%| | 28/30 [03:17<00:12, 6.29s/it]  
Epoch 28 - Train Loss: 0.0006, Val Loss: 0.0009, RMSE: 5.89 kcal/mol  
Epochs: 97%| | 29/30 [03:23<00:06, 6.21s/it]  
Epoch 29 - Train Loss: 0.0006, Val Loss: 0.0008, RMSE: 5.76 kcal/mol  
Epochs: 100%| | 30/30 [03:30<00:00, 7.01s/it]  
Epoch 30 - Train Loss: 0.0006, Val Loss: 0.0008, RMSE: 5.67 kcal/mol

Training model with dropout=0.1, L2=1e-05

Epochs: 3%| | 1/30 [00:07<03:32, 7.33s/it]  
Epoch 1 - Train Loss: 0.1118, Val Loss: 0.0267, RMSE: 32.53 kcal/mol  
Epochs: 7%| | 2/30 [00:14<03:21, 7.19s/it]

Epoch 2 - Train Loss: 0.0302, Val Loss: 0.0284, RMSE: 33.56 kcal/mol  
Epochs: 10%| | 3/30 [00:21<03:13, 7.18s/it]

Epoch 3 - Train Loss: 0.0201, Val Loss: 0.0186, RMSE: 27.18 kcal/mol  
Epochs: 13%| | 4/30 [00:28<02:59, 6.92s/it]

Epoch 4 - Train Loss: 0.0150, Val Loss: 0.0137, RMSE: 23.33 kcal/mol  
Epochs: 17%| | 5/30 [00:34<02:48, 6.73s/it]

Epoch 5 - Train Loss: 0.0116, Val Loss: 0.0113, RMSE: 21.19 kcal/mol  
Epochs: 20%| | 6/30 [00:40<02:39, 6.64s/it]

Epoch 6 - Train Loss: 0.0091, Val Loss: 0.0091, RMSE: 18.99 kcal/mol  
Epochs: 23%| | 7/30 [00:47<02:32, 6.61s/it]

Epoch 7 - Train Loss: 0.0067, Val Loss: 0.0064, RMSE: 15.94 kcal/mol  
Epochs: 27%| | 8/30 [00:53<02:24, 6.55s/it]

Epoch 8 - Train Loss: 0.0047, Val Loss: 0.0047, RMSE: 13.64 kcal/mol  
Epochs: 30%| | 9/30 [01:00<02:15, 6.43s/it]

Epoch 9 - Train Loss: 0.0034, Val Loss: 0.0038, RMSE: 12.21 kcal/mol  
Epochs: 33%| | 10/30 [01:07<02:11, 6.59s/it]

Epoch 10 - Train Loss: 0.0026, Val Loss: 0.0032, RMSE: 11.32 kcal/mol  
Epochs: 37%| | 11/30 [01:12<02:00, 6.35s/it]

Epoch 11 - Train Loss: 0.0021, Val Loss: 0.0025, RMSE: 9.97 kcal/mol  
Epochs: 40%| | 12/30 [01:20<02:02, 6.80s/it]

Epoch 12 - Train Loss: 0.0017, Val Loss: 0.0021, RMSE: 9.18 kcal/mol  
Epochs: 43%| | 13/30 [01:27<01:53, 6.67s/it]

Epoch 13 - Train Loss: 0.0014, Val Loss: 0.0019, RMSE: 8.63 kcal/mol  
Epochs: 47%| | 14/30 [01:33<01:46, 6.67s/it]

Epoch 14 - Train Loss: 0.0013, Val Loss: 0.0017, RMSE: 8.20 kcal/mol  
Epochs: 50%| | 15/30 [01:39<01:35, 6.38s/it]

Epoch 15 - Train Loss: 0.0011, Val Loss: 0.0015, RMSE: 7.81 kcal/mol  
Epochs: 53%| | 16/30 [01:44<01:25, 6.12s/it]

Epoch 16 - Train Loss: 0.0010, Val Loss: 0.0014, RMSE: 7.50 kcal/mol  
Epochs: 57%| | 17/30 [01:50<01:17, 5.94s/it]

Epoch 17 - Train Loss: 0.0009, Val Loss: 0.0013, RMSE: 7.25 kcal/mol  
Epochs: 60%| | 18/30 [01:56<01:10, 5.85s/it]

Epoch 18 - Train Loss: 0.0009, Val Loss: 0.0012, RMSE: 6.99 kcal/mol  
 Epochs: 63%| | 19/30 [02:05<01:15, 6.84s/it]  
 Epoch 19 - Train Loss: 0.0008, Val Loss: 0.0012, RMSE: 6.79 kcal/mol  
 Epochs: 67%| | 20/30 [02:10<01:04, 6.49s/it]  
 Epoch 20 - Train Loss: 0.0007, Val Loss: 0.0011, RMSE: 6.53 kcal/mol  
 Epochs: 70%| | 21/30 [02:17<00:57, 6.38s/it]  
 Epoch 21 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.28 kcal/mol  
 Epochs: 73%| | 22/30 [02:22<00:49, 6.14s/it]  
 Epoch 22 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.26 kcal/mol  
 Epochs: 77%| | 23/30 [02:28<00:42, 6.06s/it]  
 Epoch 23 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.33 kcal/mol  
 Epochs: 80%| | 24/30 [02:34<00:36, 6.13s/it]  
 Epoch 24 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.36 kcal/mol  
 Epochs: 83%| | 25/30 [02:40<00:30, 6.04s/it]  
 Epoch 25 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.21 kcal/mol  
 Epochs: 87%| | 26/30 [02:46<00:23, 5.90s/it]  
 Epoch 26 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 6.12 kcal/mol  
 Epochs: 90%| | 27/30 [02:52<00:18, 6.07s/it]  
 Epoch 27 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 6.10 kcal/mol  
 Epochs: 93%| | 28/30 [02:59<00:12, 6.23s/it]  
 Epoch 28 - Train Loss: 0.0005, Val Loss: 0.0010, RMSE: 6.19 kcal/mol  
 Epochs: 97%| | 29/30 [03:07<00:06, 6.96s/it]  
 Epoch 29 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.92 kcal/mol  
 Epochs: 100%| | 30/30 [03:13<00:00, 6.45s/it]  
 Epoch 30 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.76 kcal/mol

Training model with dropout=0.1, L2=0.0001

Epochs: 3%| | 1/30 [00:05<02:42, 5.59s/it]  
 Epoch 1 - Train Loss: 0.8473, Val Loss: 0.1541, RMSE: 78.00 kcal/mol  
 Epochs: 7%| | 2/30 [00:12<03:00, 6.43s/it]  
 Epoch 2 - Train Loss: 0.1380, Val Loss: 0.0756, RMSE: 54.63 kcal/mol  
 Epochs: 10%| | 3/30 [00:18<02:51, 6.36s/it]

Epoch 3 - Train Loss: 0.0604, Val Loss: 0.0494, RMSE: 44.20 kcal/mol  
Epochs: 13%| | 4/30 [00:23<02:31, 5.83s/it]

Epoch 4 - Train Loss: 0.0330, Val Loss: 0.0200, RMSE: 28.14 kcal/mol  
Epochs: 17%| | 5/30 [00:29<02:19, 5.58s/it]

Epoch 5 - Train Loss: 0.0168, Val Loss: 0.0157, RMSE: 24.95 kcal/mol  
Epochs: 20%| | 6/30 [00:34<02:09, 5.39s/it]

Epoch 6 - Train Loss: 0.0132, Val Loss: 0.0128, RMSE: 22.56 kcal/mol  
Epochs: 23%| | 7/30 [00:39<02:02, 5.32s/it]

Epoch 7 - Train Loss: 0.0111, Val Loss: 0.0113, RMSE: 21.16 kcal/mol  
Epochs: 27%| | 8/30 [00:44<01:54, 5.21s/it]

Epoch 8 - Train Loss: 0.0094, Val Loss: 0.0097, RMSE: 19.63 kcal/mol  
Epochs: 30%| | 9/30 [00:49<01:48, 5.17s/it]

Epoch 9 - Train Loss: 0.0079, Val Loss: 0.0081, RMSE: 17.91 kcal/mol  
Epochs: 33%| | 10/30 [00:54<01:43, 5.19s/it]

Epoch 10 - Train Loss: 0.0064, Val Loss: 0.0067, RMSE: 16.29 kcal/mol  
Epochs: 37%| | 11/30 [01:02<01:52, 5.94s/it]

Epoch 11 - Train Loss: 0.0053, Val Loss: 0.0059, RMSE: 15.28 kcal/mol  
Epochs: 40%| | 12/30 [01:09<01:52, 6.25s/it]

Epoch 12 - Train Loss: 0.0046, Val Loss: 0.0055, RMSE: 14.77 kcal/mol  
Epochs: 43%| | 13/30 [01:15<01:47, 6.33s/it]

Epoch 13 - Train Loss: 0.0042, Val Loss: 0.0050, RMSE: 14.15 kcal/mol  
Epochs: 47%| | 14/30 [01:21<01:38, 6.13s/it]

Epoch 14 - Train Loss: 0.0039, Val Loss: 0.0045, RMSE: 13.41 kcal/mol  
Epochs: 50%| | 15/30 [01:27<01:31, 6.10s/it]

Epoch 15 - Train Loss: 0.0037, Val Loss: 0.0041, RMSE: 12.75 kcal/mol  
Epochs: 53%| | 16/30 [01:33<01:26, 6.17s/it]

Epoch 16 - Train Loss: 0.0034, Val Loss: 0.0038, RMSE: 12.24 kcal/mol  
Epochs: 57%| | 17/30 [01:40<01:21, 6.26s/it]

Epoch 17 - Train Loss: 0.0031, Val Loss: 0.0036, RMSE: 11.87 kcal/mol  
Epochs: 60%| | 18/30 [01:46<01:14, 6.21s/it]

Epoch 18 - Train Loss: 0.0029, Val Loss: 0.0034, RMSE: 11.68 kcal/mol  
Epochs: 63%| | 19/30 [01:52<01:08, 6.26s/it]

Epoch 19 - Train Loss: 0.0027, Val Loss: 0.0032, RMSE: 11.27 kcal/mol  
 Epochs: 67%| | 20/30 [01:58<01:01, 6.11s/it]

Epoch 20 - Train Loss: 0.0025, Val Loss: 0.0029, RMSE: 10.63 kcal/mol  
 Epochs: 70%| | 21/30 [02:03<00:52, 5.84s/it]

Epoch 21 - Train Loss: 0.0023, Val Loss: 0.0027, RMSE: 10.25 kcal/mol  
 Epochs: 73%| | 22/30 [02:08<00:45, 5.70s/it]

Epoch 22 - Train Loss: 0.0022, Val Loss: 0.0025, RMSE: 9.96 kcal/mol  
 Epochs: 77%| | 23/30 [02:15<00:42, 6.07s/it]

Epoch 23 - Train Loss: 0.0021, Val Loss: 0.0024, RMSE: 9.72 kcal/mol  
 Epochs: 80%| | 24/30 [02:28<00:48, 8.07s/it]

Epoch 24 - Train Loss: 0.0020, Val Loss: 0.0023, RMSE: 9.52 kcal/mol  
 Epochs: 83%| | 25/30 [02:35<00:38, 7.62s/it]

Epoch 25 - Train Loss: 0.0019, Val Loss: 0.0022, RMSE: 9.39 kcal/mol  
 Epochs: 87%| | 26/30 [02:49<00:38, 9.61s/it]

Epoch 26 - Train Loss: 0.0019, Val Loss: 0.0022, RMSE: 9.27 kcal/mol  
 Epochs: 90%| | 27/30 [02:58<00:28, 9.54s/it]

Epoch 27 - Train Loss: 0.0018, Val Loss: 0.0021, RMSE: 9.16 kcal/mol  
 Epochs: 93%| | 28/30 [03:07<00:18, 9.31s/it]

Epoch 28 - Train Loss: 0.0018, Val Loss: 0.0021, RMSE: 9.05 kcal/mol  
 Epochs: 97%| | 29/30 [03:14<00:08, 8.72s/it]

Epoch 29 - Train Loss: 0.0017, Val Loss: 0.0020, RMSE: 8.94 kcal/mol  
 Epochs: 100%| | 30/30 [03:21<00:00, 6.73s/it]

Epoch 30 - Train Loss: 0.0017, Val Loss: 0.0020, RMSE: 8.82 kcal/mol

Training model with dropout=0.2, L2=0.0

Epochs: 3%| | 1/30 [00:07<03:26, 7.13s/it]

Epoch 1 - Train Loss: 0.9063, Val Loss: 0.0737, RMSE: 53.97 kcal/mol  
 Epochs: 7%| | 2/30 [00:12<02:57, 6.34s/it]

Epoch 2 - Train Loss: 0.0941, Val Loss: 0.0364, RMSE: 37.94 kcal/mol  
 Epochs: 10%| | 3/30 [00:19<02:52, 6.39s/it]

Epoch 3 - Train Loss: 0.0453, Val Loss: 0.0273, RMSE: 32.87 kcal/mol  
 Epochs: 13%| | 4/30 [00:25<02:47, 6.43s/it]

Epoch 4 - Train Loss: 0.0289, Val Loss: 0.0226, RMSE: 29.97 kcal/mol  
Epochs: 17%| | 5/30 [00:31<02:35, 6.22s/it]

Epoch 5 - Train Loss: 0.0213, Val Loss: 0.0195, RMSE: 27.86 kcal/mol  
Epochs: 20%| | 6/30 [00:38<02:30, 6.27s/it]

Epoch 6 - Train Loss: 0.0172, Val Loss: 0.0168, RMSE: 25.82 kcal/mol  
Epochs: 23%| | 7/30 [00:43<02:18, 6.02s/it]

Epoch 7 - Train Loss: 0.0142, Val Loss: 0.0142, RMSE: 23.73 kcal/mol  
Epochs: 27%| | 8/30 [00:48<02:01, 5.54s/it]

Epoch 8 - Train Loss: 0.0122, Val Loss: 0.0122, RMSE: 22.02 kcal/mol  
Epochs: 30%| | 9/30 [00:52<01:45, 5.04s/it]

Epoch 9 - Train Loss: 0.0102, Val Loss: 0.0102, RMSE: 20.09 kcal/mol  
Epochs: 33%| | 10/30 [00:54<01:26, 4.35s/it]

Epoch 10 - Train Loss: 0.0082, Val Loss: 0.0080, RMSE: 17.85 kcal/mol  
Epochs: 37%| | 11/30 [00:57<01:13, 3.86s/it]

Epoch 11 - Train Loss: 0.0063, Val Loss: 0.0062, RMSE: 15.73 kcal/mol  
Epochs: 40%| | 12/30 [01:00<01:03, 3.54s/it]

Epoch 12 - Train Loss: 0.0048, Val Loss: 0.0050, RMSE: 14.04 kcal/mol  
Epochs: 43%| | 13/30 [01:03<00:56, 3.32s/it]

Epoch 13 - Train Loss: 0.0038, Val Loss: 0.0041, RMSE: 12.69 kcal/mol  
Epochs: 47%| | 14/30 [01:06<00:50, 3.16s/it]

Epoch 14 - Train Loss: 0.0031, Val Loss: 0.0036, RMSE: 11.92 kcal/mol  
Epochs: 50%| | 15/30 [01:08<00:45, 3.04s/it]

Epoch 15 - Train Loss: 0.0026, Val Loss: 0.0031, RMSE: 11.04 kcal/mol  
Epochs: 53%| | 16/30 [01:11<00:41, 2.96s/it]

Epoch 16 - Train Loss: 0.0022, Val Loss: 0.0027, RMSE: 10.30 kcal/mol  
Epochs: 57%| | 17/30 [01:14<00:37, 2.92s/it]

Epoch 17 - Train Loss: 0.0019, Val Loss: 0.0024, RMSE: 9.77 kcal/mol  
Epochs: 60%| | 18/30 [01:17<00:35, 2.92s/it]

Epoch 18 - Train Loss: 0.0017, Val Loss: 0.0022, RMSE: 9.33 kcal/mol  
Epochs: 63%| | 19/30 [01:20<00:34, 3.13s/it]

Epoch 19 - Train Loss: 0.0015, Val Loss: 0.0020, RMSE: 8.88 kcal/mol  
Epochs: 67%| | 20/30 [01:23<00:30, 3.09s/it]

Epoch 20 - Train Loss: 0.0013, Val Loss: 0.0018, RMSE: 8.37 kcal/mol  
 Epochs: 70%| | 21/30 [01:26<00:26, 2.98s/it]  
 Epoch 21 - Train Loss: 0.0011, Val Loss: 0.0016, RMSE: 7.94 kcal/mol  
 Epochs: 73%| | 22/30 [01:29<00:23, 2.92s/it]  
 Epoch 22 - Train Loss: 0.0010, Val Loss: 0.0014, RMSE: 7.52 kcal/mol  
 Epochs: 77%| | 23/30 [01:32<00:20, 2.88s/it]  
 Epoch 23 - Train Loss: 0.0009, Val Loss: 0.0013, RMSE: 7.13 kcal/mol  
 Epochs: 80%| | 24/30 [01:34<00:17, 2.85s/it]  
 Epoch 24 - Train Loss: 0.0008, Val Loss: 0.0012, RMSE: 6.80 kcal/mol  
 Epochs: 83%| | 25/30 [01:37<00:14, 2.82s/it]  
 Epoch 25 - Train Loss: 0.0007, Val Loss: 0.0011, RMSE: 6.54 kcal/mol  
 Epochs: 87%| | 26/30 [01:40<00:11, 2.79s/it]  
 Epoch 26 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.29 kcal/mol  
 Epochs: 90%| | 27/30 [01:43<00:08, 2.79s/it]  
 Epoch 27 - Train Loss: 0.0006, Val Loss: 0.0009, RMSE: 6.09 kcal/mol  
 Epochs: 93%| | 28/30 [01:46<00:05, 2.85s/it]  
 Epoch 28 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.92 kcal/mol  
 Epochs: 97%| | 29/30 [01:48<00:02, 2.83s/it]  
 Epoch 29 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.71 kcal/mol  
 Epochs: 100%| | 30/30 [01:51<00:00, 3.73s/it]  
 Epoch 30 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.59 kcal/mol

Training model with dropout=0.2, L2=1e-05

Epochs: 3%| | 1/30 [00:03<01:45, 3.64s/it]  
 Epoch 1 - Train Loss: 0.9525, Val Loss: 0.0392, RMSE: 39.46 kcal/mol  
 Epochs: 7%| | 2/30 [00:06<01:26, 3.09s/it]  
 Epoch 2 - Train Loss: 0.0663, Val Loss: 0.0308, RMSE: 34.97 kcal/mol  
 Epochs: 10%| | 3/30 [00:09<01:22, 3.05s/it]  
 Epoch 3 - Train Loss: 0.0332, Val Loss: 0.0311, RMSE: 35.16 kcal/mol  
 Epochs: 13%| | 4/30 [00:12<01:16, 2.93s/it]  
 Epoch 4 - Train Loss: 0.0269, Val Loss: 0.0262, RMSE: 32.25 kcal/mol  
 Epochs: 17%| | 5/30 [00:14<01:12, 2.88s/it]



Epoch 5 - Train Loss: 0.0222, Val Loss: 0.0219, RMSE: 29.46 kcal/mol  
Epochs: 20%| | 6/30 [00:17<01:08, 2.85s/it]

Epoch 6 - Train Loss: 0.0187, Val Loss: 0.0184, RMSE: 27.02 kcal/mol  
Epochs: 23%| | 7/30 [00:20<01:04, 2.82s/it]

Epoch 7 - Train Loss: 0.0161, Val Loss: 0.0161, RMSE: 25.32 kcal/mol  
Epochs: 27%| | 8/30 [00:23<01:02, 2.83s/it]

Epoch 8 - Train Loss: 0.0141, Val Loss: 0.0142, RMSE: 23.73 kcal/mol  
Epochs: 30%| | 9/30 [00:26<00:58, 2.80s/it]

Epoch 9 - Train Loss: 0.0119, Val Loss: 0.0116, RMSE: 21.50 kcal/mol  
Epochs: 33%| | 10/30 [00:28<00:56, 2.80s/it]

Epoch 10 - Train Loss: 0.0094, Val Loss: 0.0092, RMSE: 19.11 kcal/mol  
Epochs: 37%| | 11/30 [00:31<00:53, 2.80s/it]

Epoch 11 - Train Loss: 0.0073, Val Loss: 0.0071, RMSE: 16.79 kcal/mol  
Epochs: 40%| | 12/30 [00:34<00:50, 2.79s/it]

Epoch 12 - Train Loss: 0.0058, Val Loss: 0.0057, RMSE: 15.05 kcal/mol  
Epochs: 43%| | 13/30 [00:37<00:47, 2.77s/it]

Epoch 13 - Train Loss: 0.0047, Val Loss: 0.0048, RMSE: 13.85 kcal/mol  
Epochs: 47%| | 14/30 [00:39<00:44, 2.78s/it]

Epoch 14 - Train Loss: 0.0040, Val Loss: 0.0042, RMSE: 12.95 kcal/mol  
Epochs: 50%| | 15/30 [00:42<00:41, 2.78s/it]

Epoch 15 - Train Loss: 0.0034, Val Loss: 0.0037, RMSE: 12.13 kcal/mol  
Epochs: 53%| | 16/30 [00:45<00:39, 2.79s/it]

Epoch 16 - Train Loss: 0.0029, Val Loss: 0.0033, RMSE: 11.47 kcal/mol  
Epochs: 57%| | 17/30 [00:48<00:36, 2.81s/it]

Epoch 17 - Train Loss: 0.0026, Val Loss: 0.0031, RMSE: 11.09 kcal/mol  
Epochs: 60%| | 18/30 [00:51<00:33, 2.83s/it]

Epoch 18 - Train Loss: 0.0024, Val Loss: 0.0029, RMSE: 10.76 kcal/mol  
Epochs: 63%| | 19/30 [00:54<00:31, 2.82s/it]

Epoch 19 - Train Loss: 0.0022, Val Loss: 0.0028, RMSE: 10.47 kcal/mol  
Epochs: 67%| | 20/30 [00:56<00:28, 2.86s/it]

Epoch 20 - Train Loss: 0.0020, Val Loss: 0.0026, RMSE: 10.09 kcal/mol  
Epochs: 70%| | 21/30 [00:59<00:25, 2.83s/it]

Epoch 21 - Train Loss: 0.0019, Val Loss: 0.0024, RMSE: 9.70 kcal/mol  
 Epochs: 73%| | 22/30 [01:02<00:22, 2.80s/it]  
 Epoch 22 - Train Loss: 0.0018, Val Loss: 0.0022, RMSE: 9.39 kcal/mol  
 Epochs: 77%| | 23/30 [01:05<00:19, 2.80s/it]  
 Epoch 23 - Train Loss: 0.0017, Val Loss: 0.0021, RMSE: 9.12 kcal/mol  
 Epochs: 80%| | 24/30 [01:09<00:18, 3.13s/it]  
 Epoch 24 - Train Loss: 0.0016, Val Loss: 0.0020, RMSE: 8.81 kcal/mol  
 Epochs: 83%| | 25/30 [01:13<00:17, 3.42s/it]  
 Epoch 25 - Train Loss: 0.0015, Val Loss: 0.0018, RMSE: 8.56 kcal/mol  
 Epochs: 87%| | 26/30 [01:17<00:14, 3.57s/it]  
 Epoch 26 - Train Loss: 0.0014, Val Loss: 0.0018, RMSE: 8.35 kcal/mol  
 Epochs: 90%| | 27/30 [01:19<00:10, 3.34s/it]  
 Epoch 27 - Train Loss: 0.0013, Val Loss: 0.0017, RMSE: 8.13 kcal/mol  
 Epochs: 93%| | 28/30 [01:22<00:06, 3.17s/it]  
 Epoch 28 - Train Loss: 0.0012, Val Loss: 0.0016, RMSE: 7.94 kcal/mol  
 Epochs: 97%| | 29/30 [01:25<00:03, 3.05s/it]  
 Epoch 29 - Train Loss: 0.0012, Val Loss: 0.0015, RMSE: 7.77 kcal/mol  
 Epochs: 100%| | 30/30 [01:28<00:00, 2.94s/it]  
 Epoch 30 - Train Loss: 0.0011, Val Loss: 0.0015, RMSE: 7.62 kcal/mol

Training model with dropout=0.2, L2=0.0001

Epochs: 3%| | 1/30 [00:03<01:45, 3.65s/it]  
 Epoch 1 - Train Loss: 1.1561, Val Loss: 0.0366, RMSE: 38.10 kcal/mol  
 Epochs: 7%| | 2/30 [00:06<01:27, 3.14s/it]  
 Epoch 2 - Train Loss: 0.0896, Val Loss: 0.0356, RMSE: 37.59 kcal/mol  
 Epochs: 10%| | 3/30 [00:09<01:19, 2.95s/it]  
 Epoch 3 - Train Loss: 0.0450, Val Loss: 0.0347, RMSE: 37.09 kcal/mol  
 Epochs: 13%| | 4/30 [00:11<01:15, 2.89s/it]  
 Epoch 4 - Train Loss: 0.0324, Val Loss: 0.0326, RMSE: 35.96 kcal/mol  
 Epochs: 17%| | 5/30 [00:14<01:11, 2.85s/it]  
 Epoch 5 - Train Loss: 0.0282, Val Loss: 0.0288, RMSE: 33.81 kcal/mol  
 Epochs: 20%| | 6/30 [00:17<01:07, 2.81s/it]

Epoch 6 - Train Loss: 0.0251, Val Loss: 0.0254, RMSE: 31.77 kcal/mol  
Epochs: 23%| | 7/30 [00:20<01:04, 2.80s/it]

Epoch 7 - Train Loss: 0.0226, Val Loss: 0.0227, RMSE: 30.01 kcal/mol  
Epochs: 27%| | 8/30 [00:23<01:01, 2.80s/it]

Epoch 8 - Train Loss: 0.0197, Val Loss: 0.0193, RMSE: 27.67 kcal/mol  
Epochs: 30%| | 9/30 [00:25<00:58, 2.79s/it]

Epoch 9 - Train Loss: 0.0166, Val Loss: 0.0162, RMSE: 25.38 kcal/mol  
Epochs: 33%| | 10/30 [00:28<00:55, 2.78s/it]

Epoch 10 - Train Loss: 0.0138, Val Loss: 0.0133, RMSE: 23.02 kcal/mol  
Epochs: 37%| | 11/30 [00:31<00:53, 2.82s/it]

Epoch 11 - Train Loss: 0.0113, Val Loss: 0.0107, RMSE: 20.64 kcal/mol  
Epochs: 40%| | 12/30 [00:34<00:50, 2.81s/it]

Epoch 12 - Train Loss: 0.0089, Val Loss: 0.0084, RMSE: 18.28 kcal/mol  
Epochs: 43%| | 13/30 [00:37<00:47, 2.81s/it]

Epoch 13 - Train Loss: 0.0070, Val Loss: 0.0068, RMSE: 16.41 kcal/mol  
Epochs: 47%| | 14/30 [00:39<00:44, 2.78s/it]

Epoch 14 - Train Loss: 0.0057, Val Loss: 0.0057, RMSE: 15.01 kcal/mol  
Epochs: 50%| | 15/30 [00:42<00:41, 2.78s/it]

Epoch 15 - Train Loss: 0.0048, Val Loss: 0.0049, RMSE: 13.95 kcal/mol  
Epochs: 53%| | 16/30 [00:45<00:38, 2.78s/it]

Epoch 16 - Train Loss: 0.0042, Val Loss: 0.0045, RMSE: 13.29 kcal/mol  
Epochs: 57%| | 17/30 [00:48<00:36, 2.78s/it]

Epoch 17 - Train Loss: 0.0037, Val Loss: 0.0041, RMSE: 12.71 kcal/mol  
Epochs: 60%| | 18/30 [00:50<00:33, 2.79s/it]

Epoch 18 - Train Loss: 0.0034, Val Loss: 0.0038, RMSE: 12.22 kcal/mol  
Epochs: 63%| | 19/30 [00:53<00:30, 2.78s/it]

Epoch 19 - Train Loss: 0.0032, Val Loss: 0.0036, RMSE: 12.00 kcal/mol  
Epochs: 67%| | 20/30 [00:56<00:27, 2.78s/it]

Epoch 20 - Train Loss: 0.0031, Val Loss: 0.0036, RMSE: 11.93 kcal/mol  
Epochs: 70%| | 21/30 [00:59<00:24, 2.76s/it]

Epoch 21 - Train Loss: 0.0029, Val Loss: 0.0035, RMSE: 11.80 kcal/mol  
Epochs: 73%| | 22/30 [01:02<00:22, 2.78s/it]

Epoch 22 - Train Loss: 0.0028, Val Loss: 0.0034, RMSE: 11.57 kcal/mol  
 Epochs: 77%| | 23/30 [01:04<00:19, 2.78s/it]  
 Epoch 23 - Train Loss: 0.0027, Val Loss: 0.0032, RMSE: 11.31 kcal/mol  
 Epochs: 80%| | 24/30 [01:07<00:16, 2.77s/it]  
 Epoch 24 - Train Loss: 0.0026, Val Loss: 0.0030, RMSE: 10.98 kcal/mol  
 Epochs: 83%| | 25/30 [01:10<00:13, 2.77s/it]  
 Epoch 25 - Train Loss: 0.0024, Val Loss: 0.0029, RMSE: 10.69 kcal/mol  
 Epochs: 87%| | 26/30 [01:13<00:11, 2.78s/it]  
 Epoch 26 - Train Loss: 0.0023, Val Loss: 0.0028, RMSE: 10.50 kcal/mol  
 Epochs: 90%| | 27/30 [01:15<00:08, 2.78s/it]  
 Epoch 27 - Train Loss: 0.0023, Val Loss: 0.0027, RMSE: 10.35 kcal/mol  
 Epochs: 93%| | 28/30 [01:18<00:05, 2.78s/it]  
 Epoch 28 - Train Loss: 0.0022, Val Loss: 0.0026, RMSE: 10.20 kcal/mol  
 Epochs: 97%| | 29/30 [01:21<00:02, 2.80s/it]  
 Epoch 29 - Train Loss: 0.0022, Val Loss: 0.0026, RMSE: 10.07 kcal/mol  
 Epochs: 100%| | 30/30 [01:24<00:00, 2.81s/it]  
 Epoch 30 - Train Loss: 0.0021, Val Loss: 0.0025, RMSE: 9.95 kcal/mol

Training model with dropout=0.3, L2=0.0

Epochs: 3%| | 1/30 [00:03<01:47, 3.71s/it]  
 Epoch 1 - Train Loss: 0.1832, Val Loss: 0.0681, RMSE: 51.81 kcal/mol  
 Epochs: 7%| | 2/30 [00:06<01:28, 3.17s/it]  
 Epoch 2 - Train Loss: 0.0373, Val Loss: 0.0308, RMSE: 34.99 kcal/mol  
 Epochs: 10%| | 3/30 [00:09<01:20, 2.98s/it]  
 Epoch 3 - Train Loss: 0.0221, Val Loss: 0.0223, RMSE: 29.76 kcal/mol  
 Epochs: 13%| | 4/30 [00:12<01:15, 2.90s/it]  
 Epoch 4 - Train Loss: 0.0182, Val Loss: 0.0156, RMSE: 24.91 kcal/mol  
 Epochs: 17%| | 5/30 [00:14<01:10, 2.83s/it]  
 Epoch 5 - Train Loss: 0.0141, Val Loss: 0.0134, RMSE: 23.04 kcal/mol  
 Epochs: 20%| | 6/30 [00:17<01:07, 2.81s/it]  
 Epoch 6 - Train Loss: 0.0115, Val Loss: 0.0109, RMSE: 20.80 kcal/mol  
 Epochs: 23%| | 7/30 [00:20<01:04, 2.81s/it]

Epoch 7 - Train Loss: 0.0089, Val Loss: 0.0080, RMSE: 17.87 kcal/mol  
Epochs: 27%| | 8/30 [00:23<01:01, 2.79s/it]

Epoch 8 - Train Loss: 0.0063, Val Loss: 0.0058, RMSE: 15.17 kcal/mol  
Epochs: 30%| | 9/30 [00:25<00:58, 2.81s/it]

Epoch 9 - Train Loss: 0.0045, Val Loss: 0.0043, RMSE: 13.11 kcal/mol  
Epochs: 33%| | 10/30 [00:28<00:56, 2.82s/it]

Epoch 10 - Train Loss: 0.0033, Val Loss: 0.0034, RMSE: 11.54 kcal/mol  
Epochs: 37%| | 11/30 [00:31<00:53, 2.83s/it]

Epoch 11 - Train Loss: 0.0025, Val Loss: 0.0027, RMSE: 10.39 kcal/mol  
Epochs: 40%| | 12/30 [00:34<00:50, 2.82s/it]

Epoch 12 - Train Loss: 0.0020, Val Loss: 0.0023, RMSE: 9.59 kcal/mol  
Epochs: 43%| | 13/30 [00:37<00:48, 2.83s/it]

Epoch 13 - Train Loss: 0.0016, Val Loss: 0.0020, RMSE: 8.87 kcal/mol  
Epochs: 47%| | 14/30 [00:40<00:44, 2.81s/it]

Epoch 14 - Train Loss: 0.0014, Val Loss: 0.0017, RMSE: 8.23 kcal/mol  
Epochs: 50%| | 15/30 [00:42<00:42, 2.81s/it]

Epoch 15 - Train Loss: 0.0011, Val Loss: 0.0015, RMSE: 7.64 kcal/mol  
Epochs: 53%| | 16/30 [00:45<00:39, 2.79s/it]

Epoch 16 - Train Loss: 0.0010, Val Loss: 0.0013, RMSE: 7.13 kcal/mol  
Epochs: 57%| | 17/30 [00:48<00:36, 2.80s/it]

Epoch 17 - Train Loss: 0.0008, Val Loss: 0.0011, RMSE: 6.70 kcal/mol  
Epochs: 60%| | 18/30 [00:51<00:33, 2.80s/it]

Epoch 18 - Train Loss: 0.0007, Val Loss: 0.0010, RMSE: 6.36 kcal/mol  
Epochs: 63%| | 19/30 [00:53<00:30, 2.78s/it]

Epoch 19 - Train Loss: 0.0007, Val Loss: 0.0009, RMSE: 6.07 kcal/mol  
Epochs: 67%| | 20/30 [00:56<00:27, 2.77s/it]

Epoch 20 - Train Loss: 0.0006, Val Loss: 0.0009, RMSE: 5.89 kcal/mol  
Epochs: 70%| | 21/30 [00:59<00:24, 2.77s/it]

Epoch 21 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.90 kcal/mol  
Epochs: 73%| | 22/30 [01:02<00:22, 2.78s/it]

Epoch 22 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.84 kcal/mol  
Epochs: 77%| | 23/30 [01:05<00:19, 2.78s/it]

Epoch 23 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.60 kcal/mol  
 Epochs: 80%| | 24/30 [01:07<00:16, 2.79s/it]  
 Epoch 24 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.36 kcal/mol  
 Epochs: 83%| | 25/30 [01:10<00:13, 2.79s/it]  
 Epoch 25 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.21 kcal/mol  
 Epochs: 87%| | 26/30 [01:13<00:11, 2.79s/it]  
 Epoch 26 - Train Loss: 0.0003, Val Loss: 0.0007, RMSE: 5.11 kcal/mol  
 Epochs: 90%| | 27/30 [01:16<00:08, 2.80s/it]  
 Epoch 27 - Train Loss: 0.0003, Val Loss: 0.0006, RMSE: 5.00 kcal/mol  
 Epochs: 93%| | 28/30 [01:19<00:05, 2.88s/it]  
 Epoch 28 - Train Loss: 0.0003, Val Loss: 0.0006, RMSE: 4.86 kcal/mol  
 Epochs: 97%| | 29/30 [01:22<00:02, 2.84s/it]  
 Epoch 29 - Train Loss: 0.0003, Val Loss: 0.0006, RMSE: 4.75 kcal/mol  
 Epochs: 100%| | 30/30 [01:24<00:00, 2.83s/it]  
 Epoch 30 - Train Loss: 0.0002, Val Loss: 0.0006, RMSE: 4.70 kcal/mol

Training model with dropout=0.3, L2=1e-05

Epochs: 3%| | 1/30 [00:03<01:49, 3.78s/it]  
 Epoch 1 - Train Loss: 0.1418, Val Loss: 0.0421, RMSE: 40.83 kcal/mol  
 Epochs: 7%| | 2/30 [00:06<01:32, 3.29s/it]  
 Epoch 2 - Train Loss: 0.0249, Val Loss: 0.0202, RMSE: 28.33 kcal/mol  
 Epochs: 10%| | 3/30 [00:09<01:25, 3.16s/it]  
 Epoch 3 - Train Loss: 0.0162, Val Loss: 0.0144, RMSE: 23.95 kcal/mol  
 Epochs: 13%| | 4/30 [00:12<01:18, 3.03s/it]  
 Epoch 4 - Train Loss: 0.0119, Val Loss: 0.0112, RMSE: 21.10 kcal/mol  
 Epochs: 17%| | 5/30 [00:15<01:13, 2.95s/it]  
 Epoch 5 - Train Loss: 0.0090, Val Loss: 0.0086, RMSE: 18.47 kcal/mol  
 Epochs: 20%| | 6/30 [00:18<01:09, 2.89s/it]  
 Epoch 6 - Train Loss: 0.0066, Val Loss: 0.0065, RMSE: 16.05 kcal/mol  
 Epochs: 23%| | 7/30 [00:20<01:05, 2.86s/it]  
 Epoch 7 - Train Loss: 0.0048, Val Loss: 0.0046, RMSE: 13.55 kcal/mol  
 Epochs: 27%| | 8/30 [00:23<01:02, 2.85s/it]

Epoch 8 - Train Loss: 0.0036, Val Loss: 0.0037, RMSE: 12.10 kcal/mol  
Epochs: 30%| | 9/30 [00:26<00:59, 2.82s/it]

Epoch 9 - Train Loss: 0.0029, Val Loss: 0.0033, RMSE: 11.39 kcal/mol  
Epochs: 33%| | 10/30 [00:29<00:56, 2.81s/it]

Epoch 10 - Train Loss: 0.0024, Val Loss: 0.0026, RMSE: 10.07 kcal/mol  
Epochs: 37%| | 11/30 [00:32<00:53, 2.79s/it]

Epoch 11 - Train Loss: 0.0019, Val Loss: 0.0022, RMSE: 9.31 kcal/mol  
Epochs: 40%| | 12/30 [00:34<00:50, 2.79s/it]

Epoch 12 - Train Loss: 0.0016, Val Loss: 0.0019, RMSE: 8.69 kcal/mol  
Epochs: 43%| | 13/30 [00:37<00:47, 2.79s/it]

Epoch 13 - Train Loss: 0.0014, Val Loss: 0.0019, RMSE: 8.61 kcal/mol  
Epochs: 47%| | 14/30 [00:40<00:44, 2.77s/it]

Epoch 14 - Train Loss: 0.0012, Val Loss: 0.0017, RMSE: 8.09 kcal/mol  
Epochs: 50%| | 15/30 [00:43<00:41, 2.78s/it]

Epoch 15 - Train Loss: 0.0011, Val Loss: 0.0015, RMSE: 7.68 kcal/mol  
Epochs: 53%| | 16/30 [00:45<00:38, 2.78s/it]

Epoch 16 - Train Loss: 0.0010, Val Loss: 0.0014, RMSE: 7.53 kcal/mol  
Epochs: 57%| | 17/30 [00:48<00:36, 2.78s/it]

Epoch 17 - Train Loss: 0.0010, Val Loss: 0.0013, RMSE: 7.28 kcal/mol  
Epochs: 60%| | 18/30 [00:51<00:34, 2.84s/it]

Epoch 18 - Train Loss: 0.0009, Val Loss: 0.0012, RMSE: 6.93 kcal/mol  
Epochs: 63%| | 19/30 [00:54<00:31, 2.84s/it]

Epoch 19 - Train Loss: 0.0008, Val Loss: 0.0012, RMSE: 6.87 kcal/mol  
Epochs: 67%| | 20/30 [00:57<00:28, 2.85s/it]

Epoch 20 - Train Loss: 0.0008, Val Loss: 0.0013, RMSE: 7.12 kcal/mol  
Epochs: 70%| | 21/30 [01:00<00:25, 2.82s/it]

Epoch 21 - Train Loss: 0.0008, Val Loss: 0.0012, RMSE: 6.79 kcal/mol  
Epochs: 73%| | 22/30 [01:03<00:22, 2.85s/it]

Epoch 22 - Train Loss: 0.0008, Val Loss: 0.0010, RMSE: 6.24 kcal/mol  
Epochs: 77%| | 23/30 [01:06<00:21, 3.13s/it]

Epoch 23 - Train Loss: 0.0006, Val Loss: 0.0009, RMSE: 6.13 kcal/mol  
Epochs: 80%| | 24/30 [01:11<00:21, 3.64s/it]

Epoch 24 - Train Loss: 0.0006, Val Loss: 0.0011, RMSE: 6.59 kcal/mol  
 Epochs: 83%| | 25/30 [01:16<00:19, 3.87s/it]  
 Epoch 25 - Train Loss: 0.0007, Val Loss: 0.0012, RMSE: 6.94 kcal/mol  
 Epochs: 87%| | 26/30 [01:19<00:15, 3.84s/it]  
 Epoch 26 - Train Loss: 0.0008, Val Loss: 0.0014, RMSE: 7.42 kcal/mol  
 Epochs: 90%| | 27/30 [01:22<00:10, 3.53s/it]  
 Epoch 27 - Train Loss: 0.0008, Val Loss: 0.0010, RMSE: 6.13 kcal/mol  
 Epochs: 93%| | 28/30 [01:25<00:06, 3.30s/it]  
 Epoch 28 - Train Loss: 0.0007, Val Loss: 0.0010, RMSE: 6.22 kcal/mol  
 Epochs: 97%| | 29/30 [01:28<00:03, 3.14s/it]  
 Epoch 29 - Train Loss: 0.0006, Val Loss: 0.0008, RMSE: 5.76 kcal/mol  
 Epochs: 100%| | 30/30 [01:31<00:00, 3.03s/it]  
 Epoch 30 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.84 kcal/mol

Training model with dropout=0.3, L2=0.0001

Epochs: 3%| | 1/30 [00:03<01:50, 3.81s/it]  
 Epoch 1 - Train Loss: 4.3262, Val Loss: 0.1521, RMSE: 77.55 kcal/mol  
 Epochs: 7%| | 2/30 [00:06<01:30, 3.21s/it]  
 Epoch 2 - Train Loss: 0.2846, Val Loss: 0.1366, RMSE: 73.46 kcal/mol  
 Epochs: 10%| | 3/30 [00:09<01:23, 3.09s/it]  
 Epoch 3 - Train Loss: 0.1142, Val Loss: 0.0797, RMSE: 56.16 kcal/mol  
 Epochs: 13%| | 4/30 [00:12<01:17, 2.98s/it]  
 Epoch 4 - Train Loss: 0.0612, Val Loss: 0.0422, RMSE: 40.89 kcal/mol  
 Epochs: 17%| | 5/30 [00:15<01:13, 2.94s/it]  
 Epoch 5 - Train Loss: 0.0344, Val Loss: 0.0289, RMSE: 33.85 kcal/mol  
 Epochs: 20%| | 6/30 [00:18<01:10, 2.93s/it]  
 Epoch 6 - Train Loss: 0.0262, Val Loss: 0.0240, RMSE: 30.83 kcal/mol  
 Epochs: 23%| | 7/30 [00:20<01:06, 2.87s/it]  
 Epoch 7 - Train Loss: 0.0209, Val Loss: 0.0194, RMSE: 27.78 kcal/mol  
 Epochs: 27%| | 8/30 [00:23<01:02, 2.84s/it]  
 Epoch 8 - Train Loss: 0.0166, Val Loss: 0.0155, RMSE: 24.78 kcal/mol  
 Epochs: 30%| | 9/30 [00:26<00:59, 2.83s/it]



Epoch 9 - Train Loss: 0.0134, Val Loss: 0.0128, RMSE: 22.51 kcal/mol  
Epochs: 33%| | 10/30 [00:29<00:56, 2.83s/it]

Epoch 10 - Train Loss: 0.0108, Val Loss: 0.0104, RMSE: 20.36 kcal/mol  
Epochs: 37%| | 11/30 [00:32<00:55, 2.93s/it]

Epoch 11 - Train Loss: 0.0089, Val Loss: 0.0088, RMSE: 18.72 kcal/mol  
Epochs: 40%| | 12/30 [00:35<00:55, 3.06s/it]

Epoch 12 - Train Loss: 0.0074, Val Loss: 0.0076, RMSE: 17.38 kcal/mol  
Epochs: 43%| | 13/30 [00:39<00:54, 3.20s/it]

Epoch 13 - Train Loss: 0.0063, Val Loss: 0.0067, RMSE: 16.29 kcal/mol  
Epochs: 47%| | 14/30 [00:42<00:52, 3.28s/it]

Epoch 14 - Train Loss: 0.0054, Val Loss: 0.0060, RMSE: 15.38 kcal/mol  
Epochs: 50%| | 15/30 [00:45<00:48, 3.22s/it]

Epoch 15 - Train Loss: 0.0048, Val Loss: 0.0054, RMSE: 14.70 kcal/mol  
Epochs: 53%| | 16/30 [00:48<00:43, 3.08s/it]

Epoch 16 - Train Loss: 0.0043, Val Loss: 0.0050, RMSE: 14.16 kcal/mol  
Epochs: 57%| | 17/30 [00:51<00:39, 3.01s/it]

Epoch 17 - Train Loss: 0.0040, Val Loss: 0.0047, RMSE: 13.73 kcal/mol  
Epochs: 60%| | 18/30 [00:54<00:35, 2.93s/it]

Epoch 18 - Train Loss: 0.0037, Val Loss: 0.0045, RMSE: 13.37 kcal/mol  
Epochs: 63%| | 19/30 [00:57<00:31, 2.91s/it]

Epoch 19 - Train Loss: 0.0036, Val Loss: 0.0043, RMSE: 13.00 kcal/mol  
Epochs: 67%| | 20/30 [00:59<00:28, 2.85s/it]

Epoch 20 - Train Loss: 0.0034, Val Loss: 0.0041, RMSE: 12.70 kcal/mol  
Epochs: 70%| | 21/30 [01:02<00:25, 2.83s/it]

Epoch 21 - Train Loss: 0.0032, Val Loss: 0.0039, RMSE: 12.41 kcal/mol  
Epochs: 73%| | 22/30 [01:05<00:22, 2.84s/it]

Epoch 22 - Train Loss: 0.0030, Val Loss: 0.0037, RMSE: 12.16 kcal/mol  
Epochs: 77%| | 23/30 [01:08<00:19, 2.81s/it]

Epoch 23 - Train Loss: 0.0029, Val Loss: 0.0036, RMSE: 11.92 kcal/mol  
Epochs: 80%| | 24/30 [01:10<00:16, 2.80s/it]

Epoch 24 - Train Loss: 0.0028, Val Loss: 0.0034, RMSE: 11.67 kcal/mol  
Epochs: 83%| | 25/30 [01:13<00:13, 2.80s/it]

```

Epoch 25 - Train Loss: 0.0027, Val Loss: 0.0033, RMSE: 11.44 kcal/mol
Epochs: 87%|                               | 26/30 [01:16<00:11, 2.79s/it]
Epoch 26 - Train Loss: 0.0026, Val Loss: 0.0032, RMSE: 11.25 kcal/mol
Epochs: 90%|                               | 27/30 [01:19<00:08, 2.78s/it]
Epoch 27 - Train Loss: 0.0025, Val Loss: 0.0031, RMSE: 11.09 kcal/mol
Epochs: 93%|                               | 28/30 [01:21<00:05, 2.76s/it]
Epoch 28 - Train Loss: 0.0025, Val Loss: 0.0030, RMSE: 10.94 kcal/mol
Epochs: 97%|                               | 29/30 [01:24<00:02, 2.76s/it]
Epoch 29 - Train Loss: 0.0024, Val Loss: 0.0029, RMSE: 10.81 kcal/mol
Epochs: 100%|                             | 30/30 [01:27<00:00, 2.93s/it]
Epoch 30 - Train Loss: 0.0023, Val Loss: 0.0029, RMSE: 10.69 kcal/mol

```

```

-----
ImportError                                Traceback (most recent call last)
File ~/opt/anaconda3/envs/ani_env/lib/python3.8/site-packages/IPython/core/
↳ formatters.py:340, in BaseFormatter.__call__(self, obj)
    338     pass
    339 else:
--> 340     return printer(obj)
    341 # Finally look for special method names
    342 method = get_real_method(obj, self.print_method)

File ~/opt/anaconda3/envs/ani_env/lib/python3.8/site-packages/IPython/core/
↳ pylabtools.py:152, in print_figure(fig, fmt, bbox_inches, base64, **kwargs)
    149     from matplotlib.backend_bases import FigureCanvasBase
    150     FigureCanvasBase(fig)
--> 152 fig.canvas.print_figure(bytes_io, **kw)
    153 data = bytes_io.getvalue()
    154 if fmt == 'svg':

File ~/opt/anaconda3/envs/ani_env/lib/python3.8/site-packages/matplotlib/
↳ backend_bases.py:2091, in print_figure(self, filename, dpi, facecolor,
↳ edgecolor, orientation, format, bbox_inches, **kwargs)
    2084 @property
    2085 def device_pixel_ratio(self):
    2086     """
    2087     The ratio of physical to logical pixels used for the canvas on_
↳ screen.
    2088
    2089     By default, this is 1, meaning physical and logical pixels are the_
↳ same

```

```
[23]: import json

# converting to json to save the results of the model for the future
json_results = [
    {
        "dropout": float(res["dropout"]),
        "l2": float(res["l2"]),
        "val_rmse": float(res["val_rmse"])
    }
    for res in results
]

with open("dropout_l2_rmse_results.json", "w") as f:
    json.dump(json_results, f, indent=4)

print("Results exported to 'dropout_l2_rmse_results.json'")
```

Results exported to 'dropout\_l2\_rmse\_results.json'

```
[11]: with open("dropout_l2_rmse_results.json", "r") as f:
        loaded_results = json.load(f)
```

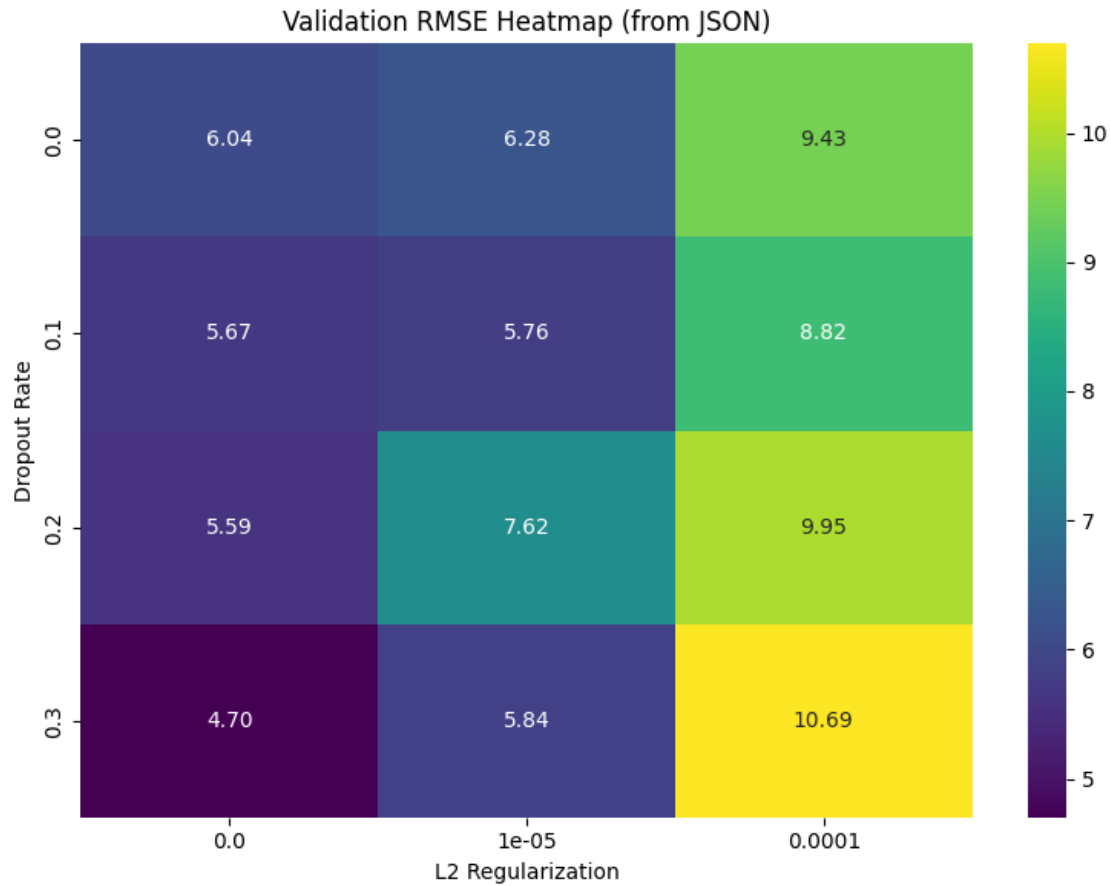
```
[12]: import pandas as pd
import seaborn as sns
!pip install matplotlib
import matplotlib
import matplotlib.pyplot as plt

df_loaded = pd.DataFrame(loaded_results)
df_loaded['dropout'] = df_loaded['dropout'].astype(float)
heatmap_data = df_loaded.pivot(index='dropout', columns='l2', values='val_rmse')

plt.figure(figsize=(8, 6))
sns.heatmap(heatmap_data, annot=True, fmt=".2f", cmap="viridis")
plt.title("Validation RMSE Heatmap (from JSON)")
plt.xlabel("L2 Regularization")
plt.ylabel("Dropout Rate")
plt.tight_layout()
plt.show()
```

Requirement already satisfied: matplotlib in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (3.7.5)  
Requirement already satisfied: contourpy>=1.0.1 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from  
matplotlib) (1.1.1)  
Requirement already satisfied: cycler>=0.10 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from

matplotlib) (0.12.1)  
Requirement already satisfied: fonttools>=4.22.0 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from  
matplotlib) (4.57.0)  
Requirement already satisfied: kiwisolver>=1.0.1 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from  
matplotlib) (1.4.4)  
Requirement already satisfied: numpy<2,>=1.20 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from  
matplotlib) (1.24.3)  
Requirement already satisfied: packaging>=20.0 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from  
matplotlib) (24.1)  
Requirement already satisfied: pillow>=6.2.0 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from  
matplotlib) (10.4.0)  
Requirement already satisfied: pyparsing>=2.3.1 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from  
matplotlib) (3.1.4)  
Requirement already satisfied: python-dateutil>=2.7 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from  
matplotlib) (2.9.0.post0)  
Requirement already satisfied: importlib-resources>=3.2.0 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from  
matplotlib) (6.4.0)  
Requirement already satisfied: zipp>=3.1.0 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from  
importlib-resources>=3.2.0->matplotlib) (3.20.2)  
Requirement already satisfied: six>=1.5 in  
/Users/saadhvi/opt/anaconda3/envs/ani\_env/lib/python3.8/site-packages (from  
python-dateutil>=2.7->matplotlib) (1.16.0)



[ ]:

```
[20]: num_rows = len(df_loaded['dropout'].unique())
num_cols = len(df_loaded['l2'].unique())

fig_loss, axes_loss = plt.subplots(num_rows, num_cols, figsize=(15, 10),
    ↪sharex=True, sharey=True)
fig_rmse, axes_rmse = plt.subplots(num_rows, num_cols, figsize=(15, 10),
    ↪sharex=True, sharey=True)

dropout_list = sorted(df_loaded['dropout'].unique())
l2_list = sorted(df_loaded['l2'].unique())

for i, dropout in enumerate(dropout_list):
    for j, l2 in enumerate(l2_list):
        print(f"\nRetraining model: dropout={dropout}, L2={l2}")
        model = build_model(dropout, l2, device)
        trainer = ANITrainer(model, epoch=30, l2=l2)
        train_losses, val_losses, val_rmse = trainer.train()
```

```

        train_subset, val_subset, early_stop=True, draw_curve=False
    )

    # Plot Loss
    ax_loss = axes_loss[i][j]
    ax_loss.plot(train_losses, label="Train Loss")
    ax_loss.plot(val_losses, label="Val Loss")
    ax_loss.set_yscale("log")
    ax_loss.set_title(f"dropout={dropout}, L2={l2}")
    ax_loss.legend()

    # Plot RMSE
    ax_rmse = axes_rmse[i][j]
    ax_rmse.plot(val_rmses, color='red', label="Val RMSE")
    ax_rmse.set_title(f"dropout={dropout}, L2={l2}")
    ax_rmse.set_ylabel("RMSE (kcal/mol)")
    ax_rmse.set_xlabel("Epoch")
    ax_rmse.legend()

    # Finalize layout
    fig_loss.suptitle("Train & Val Loss", fontsize=16)
    fig_rmse.suptitle("Val RMSE Curves", fontsize=16)
    fig_loss.tight_layout(rect=[0, 0, 1, 0.95])
    fig_rmse.tight_layout(rect=[0, 0, 1, 0.95])
    plt.show()

```

Retraining model: dropout=0.0, L2=0.0

```

Epochs:   3%|                                     | 1/30 [00:03<01:50,  3.80s/it]
Epoch 1 - Train Loss: 1.3789, Val Loss: 0.0498, RMSE: 44.26 kcal/mol
Epochs:   7%|                                     | 2/30 [00:06<01:35,  3.42s/it]
Epoch 2 - Train Loss: 0.1062, Val Loss: 0.0327, RMSE: 35.81 kcal/mol
Epochs:  10%|                                     | 3/30 [00:10<01:34,  3.52s/it]
Epoch 3 - Train Loss: 0.0488, Val Loss: 0.0244, RMSE: 30.94 kcal/mol
Epochs:  13%|                                     | 4/30 [00:14<01:31,  3.51s/it]
Epoch 4 - Train Loss: 0.0283, Val Loss: 0.0209, RMSE: 28.62 kcal/mol
Epochs:  17%|                                     | 5/30 [00:18<01:36,  3.87s/it]
Epoch 5 - Train Loss: 0.0207, Val Loss: 0.0168, RMSE: 25.68 kcal/mol
Epochs:  20%|                                     | 6/30 [00:21<01:28,  3.69s/it]
Epoch 6 - Train Loss: 0.0168, Val Loss: 0.0147, RMSE: 24.03 kcal/mol
Epochs:  23%|                                     | 7/30 [00:25<01:23,  3.61s/it]

```

Epoch 7 - Train Loss: 0.0142, Val Loss: 0.0126, RMSE: 22.22 kcal/mol  
Epochs: 27%| | 8/30 [00:28<01:15, 3.45s/it]

Epoch 8 - Train Loss: 0.0121, Val Loss: 0.0107, RMSE: 20.49 kcal/mol  
Epochs: 30%| | 9/30 [00:31<01:08, 3.27s/it]

Epoch 9 - Train Loss: 0.0098, Val Loss: 0.0083, RMSE: 18.08 kcal/mol  
Epochs: 33%| | 10/30 [00:34<01:03, 3.20s/it]

Epoch 10 - Train Loss: 0.0071, Val Loss: 0.0058, RMSE: 15.12 kcal/mol  
Epochs: 37%| | 11/30 [00:37<01:01, 3.24s/it]

Epoch 11 - Train Loss: 0.0047, Val Loss: 0.0041, RMSE: 12.63 kcal/mol  
Epochs: 40%| | 12/30 [00:41<00:58, 3.28s/it]

Epoch 12 - Train Loss: 0.0031, Val Loss: 0.0031, RMSE: 11.08 kcal/mol  
Epochs: 43%| | 13/30 [00:43<00:53, 3.13s/it]

Epoch 13 - Train Loss: 0.0022, Val Loss: 0.0026, RMSE: 10.10 kcal/mol  
Epochs: 47%| | 14/30 [00:46<00:49, 3.09s/it]

Epoch 14 - Train Loss: 0.0017, Val Loss: 0.0022, RMSE: 9.25 kcal/mol  
Epochs: 50%| | 15/30 [00:49<00:45, 3.05s/it]

Epoch 15 - Train Loss: 0.0014, Val Loss: 0.0019, RMSE: 8.57 kcal/mol  
Epochs: 53%| | 16/30 [00:52<00:41, 2.98s/it]

Epoch 16 - Train Loss: 0.0012, Val Loss: 0.0017, RMSE: 8.09 kcal/mol  
Epochs: 57%| | 17/30 [00:55<00:38, 2.92s/it]

Epoch 17 - Train Loss: 0.0010, Val Loss: 0.0015, RMSE: 7.71 kcal/mol  
Epochs: 60%| | 18/30 [00:58<00:34, 2.90s/it]

Epoch 18 - Train Loss: 0.0009, Val Loss: 0.0013, RMSE: 7.30 kcal/mol  
Epochs: 63%| | 19/30 [01:01<00:31, 2.86s/it]

Epoch 19 - Train Loss: 0.0008, Val Loss: 0.0012, RMSE: 6.89 kcal/mol  
Epochs: 67%| | 20/30 [01:03<00:28, 2.84s/it]

Epoch 20 - Train Loss: 0.0007, Val Loss: 0.0011, RMSE: 6.53 kcal/mol  
Epochs: 70%| | 21/30 [01:06<00:25, 2.82s/it]

Epoch 21 - Train Loss: 0.0007, Val Loss: 0.0010, RMSE: 6.29 kcal/mol  
Epochs: 73%| | 22/30 [01:09<00:22, 2.83s/it]

Epoch 22 - Train Loss: 0.0006, Val Loss: 0.0009, RMSE: 6.11 kcal/mol  
Epochs: 77%| | 23/30 [01:12<00:19, 2.81s/it]

Epoch 23 - Train Loss: 0.0006, Val Loss: 0.0009, RMSE: 5.96 kcal/mol  
 Epochs: 80%| | 24/30 [01:15<00:16, 2.80s/it]  
 Epoch 24 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.83 kcal/mol  
 Epochs: 83%| | 25/30 [01:17<00:14, 2.83s/it]  
 Epoch 25 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.70 kcal/mol  
 Epochs: 87%| | 26/30 [01:20<00:11, 2.83s/it]  
 Epoch 26 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.58 kcal/mol  
 Epochs: 90%| | 27/30 [01:23<00:08, 2.81s/it]  
 Epoch 27 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.46 kcal/mol  
 Epochs: 93%| | 28/30 [01:27<00:06, 3.09s/it]  
 Epoch 28 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.36 kcal/mol  
 Epochs: 97%| | 29/30 [01:30<00:03, 3.03s/it]  
 Epoch 29 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.25 kcal/mol  
 Epochs: 100%| | 30/30 [01:33<00:00, 3.10s/it]  
 Epoch 30 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.16 kcal/mol

Retraining model: dropout=0.0, L2=1e-05

Epochs: 3%| | 1/30 [00:04<02:02, 4.21s/it]  
 Epoch 1 - Train Loss: 1.0657, Val Loss: 0.0788, RMSE: 55.62 kcal/mol  
 Epochs: 7%| | 2/30 [00:07<01:36, 3.44s/it]  
 Epoch 2 - Train Loss: 0.1107, Val Loss: 0.0561, RMSE: 46.94 kcal/mol  
 Epochs: 10%| | 3/30 [00:10<01:28, 3.28s/it]  
 Epoch 3 - Train Loss: 0.0485, Val Loss: 0.0370, RMSE: 38.12 kcal/mol  
 Epochs: 13%| | 4/30 [00:13<01:20, 3.09s/it]  
 Epoch 4 - Train Loss: 0.0280, Val Loss: 0.0235, RMSE: 30.40 kcal/mol  
 Epochs: 17%| | 5/30 [00:15<01:14, 2.99s/it]  
 Epoch 5 - Train Loss: 0.0190, Val Loss: 0.0143, RMSE: 23.69 kcal/mol  
 Epochs: 20%| | 6/30 [00:18<01:09, 2.91s/it]  
 Epoch 6 - Train Loss: 0.0138, Val Loss: 0.0115, RMSE: 21.21 kcal/mol  
 Epochs: 23%| | 7/30 [00:21<01:06, 2.89s/it]  
 Epoch 7 - Train Loss: 0.0111, Val Loss: 0.0098, RMSE: 19.65 kcal/mol  
 Epochs: 27%| | 8/30 [00:24<01:04, 2.91s/it]



Epoch 8 - Train Loss: 0.0093, Val Loss: 0.0082, RMSE: 17.98 kcal/mol  
Epochs: 30%| | 9/30 [00:27<01:00, 2.90s/it]

Epoch 9 - Train Loss: 0.0075, Val Loss: 0.0064, RMSE: 15.93 kcal/mol  
Epochs: 33%| | 10/30 [00:30<00:57, 2.86s/it]

Epoch 10 - Train Loss: 0.0056, Val Loss: 0.0050, RMSE: 13.97 kcal/mol  
Epochs: 37%| | 11/30 [00:32<00:53, 2.83s/it]

Epoch 11 - Train Loss: 0.0040, Val Loss: 0.0038, RMSE: 12.26 kcal/mol  
Epochs: 40%| | 12/30 [00:35<00:51, 2.87s/it]

Epoch 12 - Train Loss: 0.0029, Val Loss: 0.0031, RMSE: 10.99 kcal/mol  
Epochs: 43%| | 13/30 [00:38<00:47, 2.82s/it]

Epoch 13 - Train Loss: 0.0022, Val Loss: 0.0027, RMSE: 10.39 kcal/mol  
Epochs: 47%| | 14/30 [00:41<00:44, 2.80s/it]

Epoch 14 - Train Loss: 0.0017, Val Loss: 0.0022, RMSE: 9.35 kcal/mol  
Epochs: 50%| | 15/30 [00:43<00:41, 2.75s/it]

Epoch 15 - Train Loss: 0.0014, Val Loss: 0.0019, RMSE: 8.73 kcal/mol  
Epochs: 53%| | 16/30 [00:46<00:38, 2.77s/it]

Epoch 16 - Train Loss: 0.0012, Val Loss: 0.0018, RMSE: 8.35 kcal/mol  
Epochs: 57%| | 17/30 [00:49<00:35, 2.75s/it]

Epoch 17 - Train Loss: 0.0010, Val Loss: 0.0016, RMSE: 7.94 kcal/mol  
Epochs: 60%| | 18/30 [00:52<00:32, 2.75s/it]

Epoch 18 - Train Loss: 0.0009, Val Loss: 0.0014, RMSE: 7.56 kcal/mol  
Epochs: 63%| | 19/30 [00:54<00:30, 2.75s/it]

Epoch 19 - Train Loss: 0.0008, Val Loss: 0.0013, RMSE: 7.31 kcal/mol  
Epochs: 67%| | 20/30 [00:57<00:27, 2.75s/it]

Epoch 20 - Train Loss: 0.0008, Val Loss: 0.0012, RMSE: 7.05 kcal/mol  
Epochs: 70%| | 21/30 [01:00<00:24, 2.75s/it]

Epoch 21 - Train Loss: 0.0007, Val Loss: 0.0012, RMSE: 6.84 kcal/mol  
Epochs: 73%| | 22/30 [01:03<00:21, 2.74s/it]

Epoch 22 - Train Loss: 0.0007, Val Loss: 0.0011, RMSE: 6.69 kcal/mol  
Epochs: 77%| | 23/30 [01:05<00:19, 2.76s/it]

Epoch 23 - Train Loss: 0.0006, Val Loss: 0.0011, RMSE: 6.56 kcal/mol  
Epochs: 80%| | 24/30 [01:08<00:16, 2.74s/it]

Epoch 24 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.45 kcal/mol  
 Epochs: 83%| | 25/30 [01:11<00:13, 2.74s/it]  
 Epoch 25 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.33 kcal/mol  
 Epochs: 87%| | 26/30 [01:14<00:10, 2.72s/it]  
 Epoch 26 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.21 kcal/mol  
 Epochs: 90%| | 27/30 [01:16<00:08, 2.73s/it]  
 Epoch 27 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 6.09 kcal/mol  
 Epochs: 93%| | 28/30 [01:19<00:05, 2.74s/it]  
 Epoch 28 - Train Loss: 0.0005, Val Loss: 0.0010, RMSE: 6.20 kcal/mol  
 Epochs: 97%| | 29/30 [01:22<00:02, 2.73s/it]  
 Epoch 29 - Train Loss: 0.0005, Val Loss: 0.0010, RMSE: 6.16 kcal/mol  
 Epochs: 100%| | 30/30 [01:24<00:00, 2.83s/it]  
 Epoch 30 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.96 kcal/mol

Retraining model: dropout=0.0, L2=0.0001

Epochs: 3%| | 1/30 [00:02<01:19, 2.73s/it]  
 Epoch 1 - Train Loss: 0.6512, Val Loss: 0.1411, RMSE: 74.55 kcal/mol  
 Epochs: 7%| | 2/30 [00:05<01:15, 2.70s/it]  
 Epoch 2 - Train Loss: 0.0850, Val Loss: 0.0326, RMSE: 35.79 kcal/mol  
 Epochs: 10%| | 3/30 [00:08<01:13, 2.71s/it]  
 Epoch 3 - Train Loss: 0.0270, Val Loss: 0.0284, RMSE: 33.41 kcal/mol  
 Epochs: 13%| | 4/30 [00:10<01:11, 2.73s/it]  
 Epoch 4 - Train Loss: 0.0221, Val Loss: 0.0158, RMSE: 24.90 kcal/mol  
 Epochs: 17%| | 5/30 [00:13<01:07, 2.72s/it]  
 Epoch 5 - Train Loss: 0.0152, Val Loss: 0.0138, RMSE: 23.26 kcal/mol  
 Epochs: 20%| | 6/30 [00:16<01:05, 2.73s/it]  
 Epoch 6 - Train Loss: 0.0125, Val Loss: 0.0110, RMSE: 20.83 kcal/mol  
 Epochs: 23%| | 7/30 [00:19<01:05, 2.84s/it]  
 Epoch 7 - Train Loss: 0.0106, Val Loss: 0.0095, RMSE: 19.28 kcal/mol  
 Epochs: 27%| | 8/30 [00:22<01:02, 2.83s/it]  
 Epoch 8 - Train Loss: 0.0091, Val Loss: 0.0082, RMSE: 17.98 kcal/mol  
 Epochs: 30%| | 9/30 [00:24<00:58, 2.80s/it]

Epoch 9 - Train Loss: 0.0077, Val Loss: 0.0071, RMSE: 16.65 kcal/mol  
Epochs: 33%| | 10/30 [00:27<00:55, 2.78s/it]

Epoch 10 - Train Loss: 0.0065, Val Loss: 0.0060, RMSE: 15.38 kcal/mol  
Epochs: 37%| | 11/30 [00:30<00:53, 2.79s/it]

Epoch 11 - Train Loss: 0.0055, Val Loss: 0.0051, RMSE: 14.18 kcal/mol  
Epochs: 40%| | 12/30 [00:33<00:50, 2.81s/it]

Epoch 12 - Train Loss: 0.0047, Val Loss: 0.0044, RMSE: 13.12 kcal/mol  
Epochs: 43%| | 13/30 [00:36<00:47, 2.79s/it]

Epoch 13 - Train Loss: 0.0040, Val Loss: 0.0039, RMSE: 12.40 kcal/mol  
Epochs: 47%| | 14/30 [00:38<00:44, 2.75s/it]

Epoch 14 - Train Loss: 0.0035, Val Loss: 0.0036, RMSE: 11.89 kcal/mol  
Epochs: 50%| | 15/30 [00:41<00:41, 2.80s/it]

Epoch 15 - Train Loss: 0.0031, Val Loss: 0.0034, RMSE: 11.55 kcal/mol  
Epochs: 53%| | 16/30 [00:44<00:38, 2.78s/it]

Epoch 16 - Train Loss: 0.0028, Val Loss: 0.0033, RMSE: 11.36 kcal/mol  
Epochs: 57%| | 17/30 [00:47<00:36, 2.78s/it]

Epoch 17 - Train Loss: 0.0027, Val Loss: 0.0031, RMSE: 11.09 kcal/mol  
Epochs: 60%| | 18/30 [00:49<00:33, 2.76s/it]

Epoch 18 - Train Loss: 0.0025, Val Loss: 0.0029, RMSE: 10.74 kcal/mol  
Epochs: 63%| | 19/30 [00:52<00:30, 2.76s/it]

Epoch 19 - Train Loss: 0.0024, Val Loss: 0.0027, RMSE: 10.37 kcal/mol  
Epochs: 67%| | 20/30 [00:55<00:27, 2.75s/it]

Epoch 20 - Train Loss: 0.0023, Val Loss: 0.0026, RMSE: 10.09 kcal/mol  
Epochs: 70%| | 21/30 [00:58<00:24, 2.76s/it]

Epoch 21 - Train Loss: 0.0022, Val Loss: 0.0025, RMSE: 9.92 kcal/mol  
Epochs: 73%| | 22/30 [01:00<00:22, 2.76s/it]

Epoch 22 - Train Loss: 0.0021, Val Loss: 0.0024, RMSE: 9.81 kcal/mol  
Epochs: 77%| | 23/30 [01:03<00:19, 2.74s/it]

Epoch 23 - Train Loss: 0.0020, Val Loss: 0.0024, RMSE: 9.74 kcal/mol  
Epochs: 80%| | 24/30 [01:06<00:16, 2.74s/it]

Epoch 24 - Train Loss: 0.0019, Val Loss: 0.0024, RMSE: 9.73 kcal/mol  
Epochs: 83%| | 25/30 [01:09<00:13, 2.73s/it]

Epoch 25 - Train Loss: 0.0019, Val Loss: 0.0024, RMSE: 9.73 kcal/mol  
 Epochs: 87%| | 26/30 [01:11<00:10, 2.74s/it]  
 Epoch 26 - Train Loss: 0.0019, Val Loss: 0.0024, RMSE: 9.72 kcal/mol  
 Epochs: 90%| | 27/30 [01:14<00:08, 2.74s/it]  
 Epoch 27 - Train Loss: 0.0018, Val Loss: 0.0024, RMSE: 9.69 kcal/mol  
 Epochs: 93%| | 28/30 [01:17<00:05, 2.73s/it]  
 Epoch 28 - Train Loss: 0.0018, Val Loss: 0.0023, RMSE: 9.66 kcal/mol  
 Epochs: 97%| | 29/30 [01:20<00:02, 2.73s/it]  
 Epoch 29 - Train Loss: 0.0017, Val Loss: 0.0023, RMSE: 9.60 kcal/mol  
 Epochs: 100%| | 30/30 [01:22<00:00, 2.76s/it]  
 Epoch 30 - Train Loss: 0.0017, Val Loss: 0.0023, RMSE: 9.55 kcal/mol

Retraining model: dropout=0.1, L2=0.0

Epochs: 3%| | 1/30 [00:03<01:40, 3.47s/it]  
 Epoch 1 - Train Loss: 0.6121, Val Loss: 0.0532, RMSE: 45.74 kcal/mol  
 Epochs: 7%| | 2/30 [00:06<01:24, 3.02s/it]  
 Epoch 2 - Train Loss: 0.0658, Val Loss: 0.0331, RMSE: 36.08 kcal/mol  
 Epochs: 10%| | 3/30 [00:08<01:18, 2.90s/it]  
 Epoch 3 - Train Loss: 0.0326, Val Loss: 0.0283, RMSE: 33.38 kcal/mol  
 Epochs: 13%| | 4/30 [00:11<01:13, 2.84s/it]  
 Epoch 4 - Train Loss: 0.0256, Val Loss: 0.0221, RMSE: 29.49 kcal/mol  
 Epochs: 17%| | 5/30 [00:14<01:10, 2.80s/it]  
 Epoch 5 - Train Loss: 0.0198, Val Loss: 0.0175, RMSE: 26.22 kcal/mol  
 Epochs: 20%| | 6/30 [00:17<01:06, 2.79s/it]  
 Epoch 6 - Train Loss: 0.0167, Val Loss: 0.0146, RMSE: 23.99 kcal/mol  
 Epochs: 23%| | 7/30 [00:19<01:03, 2.76s/it]  
 Epoch 7 - Train Loss: 0.0145, Val Loss: 0.0127, RMSE: 22.33 kcal/mol  
 Epochs: 27%| | 8/30 [00:22<01:00, 2.76s/it]  
 Epoch 8 - Train Loss: 0.0124, Val Loss: 0.0110, RMSE: 20.80 kcal/mol  
 Epochs: 30%| | 9/30 [00:25<00:57, 2.74s/it]  
 Epoch 9 - Train Loss: 0.0104, Val Loss: 0.0091, RMSE: 18.96 kcal/mol  
 Epochs: 33%| | 10/30 [00:28<00:54, 2.74s/it]

Epoch 10 - Train Loss: 0.0082, Val Loss: 0.0071, RMSE: 16.73 kcal/mol  
Epochs: 37%| | 11/30 [00:30<00:51, 2.73s/it]

Epoch 11 - Train Loss: 0.0061, Val Loss: 0.0054, RMSE: 14.61 kcal/mol  
Epochs: 40%| | 12/30 [00:33<00:49, 2.73s/it]

Epoch 12 - Train Loss: 0.0043, Val Loss: 0.0042, RMSE: 12.79 kcal/mol  
Epochs: 43%| | 13/30 [00:36<00:46, 2.73s/it]

Epoch 13 - Train Loss: 0.0030, Val Loss: 0.0033, RMSE: 11.44 kcal/mol  
Epochs: 47%| | 14/30 [00:39<00:43, 2.74s/it]

Epoch 14 - Train Loss: 0.0021, Val Loss: 0.0027, RMSE: 10.22 kcal/mol  
Epochs: 50%| | 15/30 [00:41<00:41, 2.73s/it]

Epoch 15 - Train Loss: 0.0017, Val Loss: 0.0024, RMSE: 9.74 kcal/mol  
Epochs: 53%| | 16/30 [00:44<00:38, 2.73s/it]

Epoch 16 - Train Loss: 0.0014, Val Loss: 0.0021, RMSE: 9.11 kcal/mol  
Epochs: 57%| | 17/30 [00:47<00:35, 2.73s/it]

Epoch 17 - Train Loss: 0.0012, Val Loss: 0.0018, RMSE: 8.48 kcal/mol  
Epochs: 60%| | 18/30 [00:49<00:32, 2.74s/it]

Epoch 18 - Train Loss: 0.0010, Val Loss: 0.0016, RMSE: 8.00 kcal/mol  
Epochs: 63%| | 19/30 [00:52<00:30, 2.74s/it]

Epoch 19 - Train Loss: 0.0009, Val Loss: 0.0015, RMSE: 7.58 kcal/mol  
Epochs: 67%| | 20/30 [00:55<00:27, 2.76s/it]

Epoch 20 - Train Loss: 0.0008, Val Loss: 0.0013, RMSE: 7.15 kcal/mol  
Epochs: 70%| | 21/30 [00:58<00:24, 2.77s/it]

Epoch 21 - Train Loss: 0.0007, Val Loss: 0.0012, RMSE: 6.78 kcal/mol  
Epochs: 73%| | 22/30 [01:01<00:22, 2.76s/it]

Epoch 22 - Train Loss: 0.0006, Val Loss: 0.0011, RMSE: 6.47 kcal/mol  
Epochs: 77%| | 23/30 [01:03<00:19, 2.75s/it]

Epoch 23 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.24 kcal/mol  
Epochs: 80%| | 24/30 [01:06<00:16, 2.74s/it]

Epoch 24 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 6.05 kcal/mol  
Epochs: 83%| | 25/30 [01:09<00:13, 2.74s/it]

Epoch 25 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.88 kcal/mol  
Epochs: 87%| | 26/30 [01:11<00:10, 2.74s/it]

Epoch 26 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.74 kcal/mol

Epochs: 90%| | 27/30 [01:14<00:08, 2.75s/it]

Epoch 27 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.61 kcal/mol

Epochs: 93%| | 28/30 [01:17<00:05, 2.80s/it]

Epoch 28 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.49 kcal/mol

Epochs: 97%| | 29/30 [01:21<00:02, 2.98s/it]

Epoch 29 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.38 kcal/mol

Epochs: 100%| | 30/30 [01:24<00:00, 2.81s/it]

Epoch 30 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.31 kcal/mol

Retraining model: dropout=0.1, L2=1e-05

Epochs: 3%| | 1/30 [00:04<02:04, 4.29s/it]

Epoch 1 - Train Loss: 0.2069, Val Loss: 0.0684, RMSE: 51.89 kcal/mol

Epochs: 7%| | 2/30 [00:07<01:47, 3.85s/it]

Epoch 2 - Train Loss: 0.0491, Val Loss: 0.0311, RMSE: 34.98 kcal/mol

Epochs: 10%| | 3/30 [00:11<01:42, 3.79s/it]

Epoch 3 - Train Loss: 0.0284, Val Loss: 0.0227, RMSE: 29.90 kcal/mol

Epochs: 13%| | 4/30 [00:14<01:28, 3.39s/it]

Epoch 4 - Train Loss: 0.0189, Val Loss: 0.0172, RMSE: 25.95 kcal/mol

Epochs: 17%| | 5/30 [00:17<01:18, 3.15s/it]

Epoch 5 - Train Loss: 0.0149, Val Loss: 0.0131, RMSE: 22.65 kcal/mol

Epochs: 20%| | 6/30 [00:20<01:13, 3.08s/it]

Epoch 6 - Train Loss: 0.0118, Val Loss: 0.0104, RMSE: 20.25 kcal/mol

Epochs: 23%| | 7/30 [00:22<01:09, 3.01s/it]

Epoch 7 - Train Loss: 0.0090, Val Loss: 0.0071, RMSE: 16.74 kcal/mol

Epochs: 27%| | 8/30 [00:25<01:04, 2.94s/it]

Epoch 8 - Train Loss: 0.0058, Val Loss: 0.0049, RMSE: 13.93 kcal/mol

Epochs: 30%| | 9/30 [00:29<01:05, 3.13s/it]

Epoch 9 - Train Loss: 0.0035, Val Loss: 0.0036, RMSE: 11.93 kcal/mol

Epochs: 33%| | 10/30 [00:33<01:07, 3.38s/it]

Epoch 10 - Train Loss: 0.0023, Val Loss: 0.0027, RMSE: 10.29 kcal/mol

Epochs: 37%| | 11/30 [00:37<01:12, 3.81s/it]

Epoch 11 - Train Loss: 0.0017, Val Loss: 0.0023, RMSE: 9.48 kcal/mol  
Epochs: 40%| | 12/30 [00:42<01:14, 4.11s/it]

Epoch 12 - Train Loss: 0.0014, Val Loss: 0.0020, RMSE: 8.92 kcal/mol  
Epochs: 43%| | 13/30 [00:46<01:09, 4.06s/it]

Epoch 13 - Train Loss: 0.0012, Val Loss: 0.0017, RMSE: 8.20 kcal/mol  
Epochs: 47%| | 14/30 [00:51<01:06, 4.16s/it]

Epoch 14 - Train Loss: 0.0010, Val Loss: 0.0015, RMSE: 7.65 kcal/mol  
Epochs: 50%| | 15/30 [00:55<01:05, 4.34s/it]

Epoch 15 - Train Loss: 0.0008, Val Loss: 0.0013, RMSE: 7.29 kcal/mol  
Epochs: 53%| | 16/30 [01:01<01:07, 4.86s/it]

Epoch 16 - Train Loss: 0.0008, Val Loss: 0.0012, RMSE: 7.03 kcal/mol  
Epochs: 57%| | 17/30 [01:06<01:03, 4.89s/it]

Epoch 17 - Train Loss: 0.0007, Val Loss: 0.0012, RMSE: 6.86 kcal/mol  
Epochs: 60%| | 18/30 [01:11<00:58, 4.88s/it]

Epoch 18 - Train Loss: 0.0007, Val Loss: 0.0011, RMSE: 6.62 kcal/mol  
Epochs: 63%| | 19/30 [01:15<00:50, 4.63s/it]

Epoch 19 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.42 kcal/mol  
Epochs: 67%| | 20/30 [01:19<00:43, 4.34s/it]

Epoch 20 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.26 kcal/mol  
Epochs: 70%| | 21/30 [01:23<00:37, 4.14s/it]

Epoch 21 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.15 kcal/mol  
Epochs: 73%| | 22/30 [01:26<00:32, 4.02s/it]

Epoch 22 - Train Loss: 0.0006, Val Loss: 0.0009, RMSE: 6.05 kcal/mol  
Epochs: 77%| | 23/30 [01:30<00:27, 3.87s/it]

Epoch 23 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.25 kcal/mol  
Epochs: 80%| | 24/30 [01:33<00:22, 3.78s/it]

Epoch 24 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.91 kcal/mol  
Epochs: 83%| | 25/30 [01:37<00:18, 3.68s/it]

Epoch 25 - Train Loss: 0.0005, Val Loss: 0.0010, RMSE: 6.17 kcal/mol  
Epochs: 87%| | 26/30 [01:40<00:14, 3.63s/it]

Epoch 26 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.73 kcal/mol  
Epochs: 90%| | 27/30 [01:44<00:10, 3.56s/it]

Epoch 27 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.66 kcal/mol

Epochs: 93%| | 28/30 [01:47<00:07, 3.52s/it]

Epoch 28 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.75 kcal/mol

Epochs: 97%| | 29/30 [01:51<00:03, 3.50s/it]

Epoch 29 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 6.08 kcal/mol

Epochs: 100%| | 30/30 [01:54<00:00, 3.82s/it]

Epoch 30 - Train Loss: 0.0005, Val Loss: 0.0010, RMSE: 6.25 kcal/mol

Retraining model: dropout=0.1, L2=0.0001

Epochs: 3%| | 1/30 [00:04<02:24, 4.97s/it]

Epoch 1 - Train Loss: 0.1218, Val Loss: 0.0465, RMSE: 42.69 kcal/mol

Epochs: 7%| | 2/30 [00:08<01:52, 4.01s/it]

Epoch 2 - Train Loss: 0.0313, Val Loss: 0.0133, RMSE: 22.83 kcal/mol

Epochs: 10%| | 3/30 [00:11<01:39, 3.70s/it]

Epoch 3 - Train Loss: 0.0141, Val Loss: 0.0094, RMSE: 19.20 kcal/mol

Epochs: 13%| | 4/30 [00:15<01:33, 3.58s/it]

Epoch 4 - Train Loss: 0.0094, Val Loss: 0.0076, RMSE: 17.25 kcal/mol

Epochs: 17%| | 5/30 [00:18<01:25, 3.40s/it]

Epoch 5 - Train Loss: 0.0072, Val Loss: 0.0062, RMSE: 15.68 kcal/mol

Epochs: 20%| | 6/30 [00:20<01:17, 3.22s/it]

Epoch 6 - Train Loss: 0.0059, Val Loss: 0.0053, RMSE: 14.44 kcal/mol

Epochs: 23%| | 7/30 [00:23<01:10, 3.08s/it]

Epoch 7 - Train Loss: 0.0049, Val Loss: 0.0048, RMSE: 13.74 kcal/mol

Epochs: 27%| | 8/30 [00:26<01:05, 2.97s/it]

Epoch 8 - Train Loss: 0.0043, Val Loss: 0.0044, RMSE: 13.13 kcal/mol

Epochs: 30%| | 9/30 [00:29<01:00, 2.89s/it]

Epoch 9 - Train Loss: 0.0037, Val Loss: 0.0036, RMSE: 12.01 kcal/mol

Epochs: 33%| | 10/30 [00:32<00:57, 2.86s/it]

Epoch 10 - Train Loss: 0.0030, Val Loss: 0.0032, RMSE: 11.19 kcal/mol

Epochs: 37%| | 11/30 [00:34<00:53, 2.84s/it]

Epoch 11 - Train Loss: 0.0025, Val Loss: 0.0029, RMSE: 10.70 kcal/mol

Epochs: 40%| | 12/30 [00:37<00:51, 2.83s/it]



Epoch 12 - Train Loss: 0.0022, Val Loss: 0.0026, RMSE: 10.23 kcal/mol  
Epochs: 43%| | 13/30 [00:40<00:47, 2.82s/it]

Epoch 13 - Train Loss: 0.0019, Val Loss: 0.0025, RMSE: 9.89 kcal/mol  
Epochs: 47%| | 14/30 [00:43<00:44, 2.80s/it]

Epoch 14 - Train Loss: 0.0019, Val Loss: 0.0024, RMSE: 9.69 kcal/mol  
Epochs: 50%| | 15/30 [00:45<00:41, 2.79s/it]

Epoch 15 - Train Loss: 0.0017, Val Loss: 0.0023, RMSE: 9.58 kcal/mol  
Epochs: 53%| | 16/30 [00:48<00:38, 2.77s/it]

Epoch 16 - Train Loss: 0.0016, Val Loss: 0.0023, RMSE: 9.54 kcal/mol  
Epochs: 57%| | 17/30 [00:51<00:36, 2.77s/it]

Epoch 17 - Train Loss: 0.0016, Val Loss: 0.0022, RMSE: 9.39 kcal/mol  
Epochs: 60%| | 18/30 [00:54<00:33, 2.75s/it]

Epoch 18 - Train Loss: 0.0015, Val Loss: 0.0022, RMSE: 9.26 kcal/mol  
Epochs: 63%| | 19/30 [00:56<00:30, 2.77s/it]

Epoch 19 - Train Loss: 0.0015, Val Loss: 0.0019, RMSE: 8.70 kcal/mol  
Epochs: 67%| | 20/30 [00:59<00:27, 2.76s/it]

Epoch 20 - Train Loss: 0.0020, Val Loss: 0.0021, RMSE: 9.07 kcal/mol  
Epochs: 70%| | 21/30 [01:02<00:24, 2.75s/it]

Epoch 21 - Train Loss: 0.0019, Val Loss: 0.0026, RMSE: 10.25 kcal/mol  
Epochs: 73%| | 22/30 [01:05<00:22, 2.76s/it]

Epoch 22 - Train Loss: 0.0018, Val Loss: 0.0021, RMSE: 9.15 kcal/mol  
Epochs: 77%| | 23/30 [01:08<00:19, 2.82s/it]

Epoch 23 - Train Loss: 0.0016, Val Loss: 0.0018, RMSE: 8.57 kcal/mol  
Epochs: 80%| | 24/30 [01:10<00:16, 2.80s/it]

Epoch 24 - Train Loss: 0.0014, Val Loss: 0.0019, RMSE: 8.79 kcal/mol  
Epochs: 83%| | 25/30 [01:13<00:13, 2.78s/it]

Epoch 25 - Train Loss: 0.0015, Val Loss: 0.0020, RMSE: 8.93 kcal/mol  
Epochs: 87%| | 26/30 [01:16<00:11, 2.77s/it]

Epoch 26 - Train Loss: 0.0014, Val Loss: 0.0017, RMSE: 8.28 kcal/mol  
Epochs: 90%| | 27/30 [01:19<00:08, 2.77s/it]

Epoch 27 - Train Loss: 0.0013, Val Loss: 0.0017, RMSE: 8.33 kcal/mol  
Epochs: 93%| | 28/30 [01:21<00:05, 2.76s/it]

Epoch 28 - Train Loss: 0.0014, Val Loss: 0.0017, RMSE: 8.25 kcal/mol

Epochs: 97%| | 29/30 [01:24<00:02, 2.76s/it]

Epoch 29 - Train Loss: 0.0012, Val Loss: 0.0017, RMSE: 8.24 kcal/mol

Epochs: 100%| | 30/30 [01:27<00:00, 2.91s/it]

Epoch 30 - Train Loss: 0.0012, Val Loss: 0.0019, RMSE: 8.69 kcal/mol

Retraining model: dropout=0.2, L2=0.0

Epochs: 3%| | 1/30 [00:03<01:43, 3.59s/it]

Epoch 1 - Train Loss: 0.1259, Val Loss: 0.0435, RMSE: 41.39 kcal/mol

Epochs: 7%| | 2/30 [00:06<01:26, 3.08s/it]

Epoch 2 - Train Loss: 0.0334, Val Loss: 0.0242, RMSE: 30.86 kcal/mol

Epochs: 10%| | 3/30 [00:09<01:20, 2.96s/it]

Epoch 3 - Train Loss: 0.0210, Val Loss: 0.0161, RMSE: 25.11 kcal/mol

Epochs: 13%| | 4/30 [00:11<01:15, 2.89s/it]

Epoch 4 - Train Loss: 0.0150, Val Loss: 0.0119, RMSE: 21.63 kcal/mol

Epochs: 17%| | 5/30 [00:14<01:12, 2.89s/it]

Epoch 5 - Train Loss: 0.0114, Val Loss: 0.0095, RMSE: 19.29 kcal/mol

Epochs: 20%| | 6/30 [00:17<01:08, 2.84s/it]

Epoch 6 - Train Loss: 0.0081, Val Loss: 0.0062, RMSE: 15.58 kcal/mol

Epochs: 23%| | 7/30 [00:20<01:04, 2.80s/it]

Epoch 7 - Train Loss: 0.0050, Val Loss: 0.0045, RMSE: 13.36 kcal/mol

Epochs: 27%| | 8/30 [00:23<01:01, 2.79s/it]

Epoch 8 - Train Loss: 0.0032, Val Loss: 0.0035, RMSE: 11.75 kcal/mol

Epochs: 30%| | 9/30 [00:25<00:57, 2.75s/it]

Epoch 9 - Train Loss: 0.0022, Val Loss: 0.0026, RMSE: 10.23 kcal/mol

Epochs: 33%| | 10/30 [00:28<00:54, 2.74s/it]

Epoch 10 - Train Loss: 0.0016, Val Loss: 0.0022, RMSE: 9.42 kcal/mol

Epochs: 37%| | 11/30 [00:31<00:53, 2.82s/it]

Epoch 11 - Train Loss: 0.0013, Val Loss: 0.0019, RMSE: 8.60 kcal/mol

Epochs: 40%| | 12/30 [00:34<00:50, 2.79s/it]

Epoch 12 - Train Loss: 0.0011, Val Loss: 0.0016, RMSE: 7.90 kcal/mol

Epochs: 43%| | 13/30 [00:36<00:47, 2.78s/it]

Epoch 13 - Train Loss: 0.0009, Val Loss: 0.0014, RMSE: 7.39 kcal/mol  
Epochs: 47%| | 14/30 [00:39<00:44, 2.76s/it]

Epoch 14 - Train Loss: 0.0008, Val Loss: 0.0012, RMSE: 6.96 kcal/mol  
Epochs: 50%| | 15/30 [00:42<00:41, 2.76s/it]

Epoch 15 - Train Loss: 0.0007, Val Loss: 0.0011, RMSE: 6.59 kcal/mol  
Epochs: 53%| | 16/30 [00:45<00:38, 2.75s/it]

Epoch 16 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.34 kcal/mol  
Epochs: 57%| | 17/30 [00:47<00:35, 2.73s/it]

Epoch 17 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 6.09 kcal/mol  
Epochs: 60%| | 18/30 [00:50<00:32, 2.73s/it]

Epoch 18 - Train Loss: 0.0005, Val Loss: 0.0009, RMSE: 5.82 kcal/mol  
Epochs: 63%| | 19/30 [00:53<00:30, 2.73s/it]

Epoch 19 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.63 kcal/mol  
Epochs: 67%| | 20/30 [00:55<00:27, 2.73s/it]

Epoch 20 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.43 kcal/mol  
Epochs: 70%| | 21/30 [00:58<00:24, 2.74s/it]

Epoch 21 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.30 kcal/mol  
Epochs: 73%| | 22/30 [01:03<00:25, 3.21s/it]

Epoch 22 - Train Loss: 0.0003, Val Loss: 0.0007, RMSE: 5.21 kcal/mol  
Epochs: 77%| | 23/30 [01:05<00:21, 3.07s/it]

Epoch 23 - Train Loss: 0.0003, Val Loss: 0.0007, RMSE: 5.15 kcal/mol  
Epochs: 80%| | 24/30 [01:08<00:17, 2.97s/it]

Epoch 24 - Train Loss: 0.0003, Val Loss: 0.0006, RMSE: 5.06 kcal/mol  
Epochs: 83%| | 25/30 [01:11<00:14, 2.91s/it]

Epoch 25 - Train Loss: 0.0003, Val Loss: 0.0006, RMSE: 4.91 kcal/mol  
Epochs: 87%| | 26/30 [01:14<00:11, 2.85s/it]

Epoch 26 - Train Loss: 0.0003, Val Loss: 0.0007, RMSE: 5.09 kcal/mol  
Epochs: 90%| | 27/30 [01:16<00:08, 2.82s/it]

Epoch 27 - Train Loss: 0.0004, Val Loss: 0.0006, RMSE: 5.07 kcal/mol  
Epochs: 93%| | 28/30 [01:19<00:05, 2.81s/it]

Epoch 28 - Train Loss: 0.0003, Val Loss: 0.0007, RMSE: 5.41 kcal/mol  
Epochs: 97%| | 29/30 [01:22<00:02, 2.78s/it]

Epoch 29 - Train Loss: 0.0003, Val Loss: 0.0006, RMSE: 4.69 kcal/mol

Epochs: 100%| | 30/30 [01:25<00:00, 2.83s/it]

Epoch 30 - Train Loss: 0.0002, Val Loss: 0.0005, RMSE: 4.59 kcal/mol

Retraining model: dropout=0.2, L2=1e-05

Epochs: 3%| | 1/30 [00:03<01:54, 3.95s/it]

Epoch 1 - Train Loss: 1.2875, Val Loss: 0.1473, RMSE: 76.04 kcal/mol

Epochs: 7%| | 2/30 [00:06<01:34, 3.36s/it]

Epoch 2 - Train Loss: 0.1582, Val Loss: 0.0537, RMSE: 45.92 kcal/mol

Epochs: 10%| | 3/30 [00:09<01:23, 3.09s/it]

Epoch 3 - Train Loss: 0.0557, Val Loss: 0.0355, RMSE: 37.36 kcal/mol

Epochs: 13%| | 4/30 [00:12<01:18, 3.01s/it]

Epoch 4 - Train Loss: 0.0332, Val Loss: 0.0276, RMSE: 32.94 kcal/mol

Epochs: 17%| | 5/30 [00:15<01:14, 2.96s/it]

Epoch 5 - Train Loss: 0.0230, Val Loss: 0.0199, RMSE: 27.99 kcal/mol

Epochs: 20%| | 6/30 [00:18<01:09, 2.89s/it]

Epoch 6 - Train Loss: 0.0184, Val Loss: 0.0158, RMSE: 24.91 kcal/mol

Epochs: 23%| | 7/30 [00:20<01:05, 2.85s/it]

Epoch 7 - Train Loss: 0.0152, Val Loss: 0.0134, RMSE: 22.95 kcal/mol

Epochs: 27%| | 8/30 [00:23<01:02, 2.86s/it]

Epoch 8 - Train Loss: 0.0128, Val Loss: 0.0116, RMSE: 21.36 kcal/mol

Epochs: 30%| | 9/30 [00:26<00:59, 2.82s/it]

Epoch 9 - Train Loss: 0.0107, Val Loss: 0.0092, RMSE: 18.96 kcal/mol

Epochs: 33%| | 10/30 [00:29<00:55, 2.79s/it]

Epoch 10 - Train Loss: 0.0084, Val Loss: 0.0071, RMSE: 16.65 kcal/mol

Epochs: 37%| | 11/30 [00:32<00:52, 2.77s/it]

Epoch 11 - Train Loss: 0.0064, Val Loss: 0.0054, RMSE: 14.50 kcal/mol

Epochs: 40%| | 12/30 [00:34<00:49, 2.78s/it]

Epoch 12 - Train Loss: 0.0047, Val Loss: 0.0045, RMSE: 13.25 kcal/mol

Epochs: 43%| | 13/30 [00:37<00:47, 2.78s/it]

Epoch 13 - Train Loss: 0.0036, Val Loss: 0.0037, RMSE: 11.97 kcal/mol

Epochs: 47%| | 14/30 [00:40<00:44, 2.78s/it]

Epoch 14 - Train Loss: 0.0028, Val Loss: 0.0030, RMSE: 10.81 kcal/mol  
Epochs: 50%| | 15/30 [00:43<00:41, 2.80s/it]

Epoch 15 - Train Loss: 0.0022, Val Loss: 0.0026, RMSE: 10.05 kcal/mol  
Epochs: 53%| | 16/30 [00:46<00:39, 2.81s/it]

Epoch 16 - Train Loss: 0.0019, Val Loss: 0.0023, RMSE: 9.53 kcal/mol  
Epochs: 57%| | 17/30 [00:48<00:36, 2.78s/it]

Epoch 17 - Train Loss: 0.0016, Val Loss: 0.0021, RMSE: 9.14 kcal/mol  
Epochs: 60%| | 18/30 [00:51<00:33, 2.77s/it]

Epoch 18 - Train Loss: 0.0014, Val Loss: 0.0019, RMSE: 8.57 kcal/mol  
Epochs: 63%| | 19/30 [00:54<00:30, 2.77s/it]

Epoch 19 - Train Loss: 0.0012, Val Loss: 0.0017, RMSE: 8.17 kcal/mol  
Epochs: 67%| | 20/30 [00:57<00:27, 2.77s/it]

Epoch 20 - Train Loss: 0.0011, Val Loss: 0.0016, RMSE: 7.85 kcal/mol  
Epochs: 70%| | 21/30 [00:59<00:24, 2.76s/it]

Epoch 21 - Train Loss: 0.0010, Val Loss: 0.0015, RMSE: 7.61 kcal/mol  
Epochs: 73%| | 22/30 [01:02<00:22, 2.76s/it]

Epoch 22 - Train Loss: 0.0010, Val Loss: 0.0014, RMSE: 7.40 kcal/mol  
Epochs: 77%| | 23/30 [01:05<00:19, 2.77s/it]

Epoch 23 - Train Loss: 0.0009, Val Loss: 0.0013, RMSE: 7.18 kcal/mol  
Epochs: 80%| | 24/30 [01:08<00:16, 2.76s/it]

Epoch 24 - Train Loss: 0.0008, Val Loss: 0.0012, RMSE: 6.93 kcal/mol  
Epochs: 83%| | 25/30 [01:10<00:13, 2.75s/it]

Epoch 25 - Train Loss: 0.0008, Val Loss: 0.0011, RMSE: 6.69 kcal/mol  
Epochs: 87%| | 26/30 [01:13<00:11, 2.77s/it]

Epoch 26 - Train Loss: 0.0007, Val Loss: 0.0011, RMSE: 6.58 kcal/mol  
Epochs: 90%| | 27/30 [01:16<00:08, 2.76s/it]

Epoch 27 - Train Loss: 0.0007, Val Loss: 0.0010, RMSE: 6.40 kcal/mol  
Epochs: 93%| | 28/30 [01:19<00:05, 2.76s/it]

Epoch 28 - Train Loss: 0.0007, Val Loss: 0.0010, RMSE: 6.31 kcal/mol  
Epochs: 97%| | 29/30 [01:21<00:02, 2.77s/it]

Epoch 29 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.19 kcal/mol  
Epochs: 100%| | 30/30 [01:24<00:00, 2.82s/it]

Epoch 30 - Train Loss: 0.0006, Val Loss: 0.0009, RMSE: 6.07 kcal/mol

Retraining model: dropout=0.2, L2=0.0001

Epochs: 3%| | 1/30 [00:03<01:43, 3.57s/it]

Epoch 1 - Train Loss: 0.1069, Val Loss: 0.0549, RMSE: 46.47 kcal/mol

Epochs: 7%| | 2/30 [00:06<01:25, 3.06s/it]

Epoch 2 - Train Loss: 0.0348, Val Loss: 0.0266, RMSE: 32.38 kcal/mol

Epochs: 10%| | 3/30 [00:09<01:18, 2.92s/it]

Epoch 3 - Train Loss: 0.0237, Val Loss: 0.0190, RMSE: 27.30 kcal/mol

Epochs: 13%| | 4/30 [00:11<01:13, 2.84s/it]

Epoch 4 - Train Loss: 0.0184, Val Loss: 0.0169, RMSE: 25.81 kcal/mol

Epochs: 17%| | 5/30 [00:14<01:10, 2.80s/it]

Epoch 5 - Train Loss: 0.0155, Val Loss: 0.0143, RMSE: 23.73 kcal/mol

Epochs: 20%| | 6/30 [00:17<01:06, 2.78s/it]

Epoch 6 - Train Loss: 0.0133, Val Loss: 0.0115, RMSE: 21.25 kcal/mol

Epochs: 23%| | 7/30 [00:20<01:04, 2.80s/it]

Epoch 7 - Train Loss: 0.0109, Val Loss: 0.0092, RMSE: 19.00 kcal/mol

Epochs: 27%| | 8/30 [00:22<01:01, 2.78s/it]

Epoch 8 - Train Loss: 0.0084, Val Loss: 0.0072, RMSE: 16.84 kcal/mol

Epochs: 30%| | 9/30 [00:25<00:58, 2.78s/it]

Epoch 9 - Train Loss: 0.0063, Val Loss: 0.0054, RMSE: 14.58 kcal/mol

Epochs: 33%| | 10/30 [00:28<00:55, 2.77s/it]

Epoch 10 - Train Loss: 0.0046, Val Loss: 0.0045, RMSE: 13.30 kcal/mol

Epochs: 37%| | 11/30 [00:31<00:52, 2.76s/it]

Epoch 11 - Train Loss: 0.0036, Val Loss: 0.0036, RMSE: 11.89 kcal/mol

Epochs: 40%| | 12/30 [00:33<00:49, 2.75s/it]

Epoch 12 - Train Loss: 0.0029, Val Loss: 0.0033, RMSE: 11.32 kcal/mol

Epochs: 43%| | 13/30 [00:36<00:46, 2.73s/it]

Epoch 13 - Train Loss: 0.0026, Val Loss: 0.0029, RMSE: 10.76 kcal/mol

Epochs: 47%| | 14/30 [00:39<00:43, 2.74s/it]

Epoch 14 - Train Loss: 0.0024, Val Loss: 0.0027, RMSE: 10.36 kcal/mol

Epochs: 50%| | 15/30 [00:42<00:42, 2.81s/it]

Epoch 15 - Train Loss: 0.0021, Val Loss: 0.0025, RMSE: 9.94 kcal/mol  
Epochs: 53%| | 16/30 [00:45<00:42, 3.01s/it]

Epoch 16 - Train Loss: 0.0020, Val Loss: 0.0025, RMSE: 10.03 kcal/mol  
Epochs: 57%| | 17/30 [00:48<00:40, 3.09s/it]

Epoch 17 - Train Loss: 0.0020, Val Loss: 0.0024, RMSE: 9.68 kcal/mol  
Epochs: 60%| | 18/30 [00:52<00:39, 3.30s/it]

Epoch 18 - Train Loss: 0.0017, Val Loss: 0.0021, RMSE: 9.10 kcal/mol  
Epochs: 63%| | 19/30 [00:56<00:37, 3.39s/it]

Epoch 19 - Train Loss: 0.0018, Val Loss: 0.0025, RMSE: 10.04 kcal/mol  
Epochs: 67%| | 20/30 [00:59<00:33, 3.40s/it]

Epoch 20 - Train Loss: 0.0018, Val Loss: 0.0020, RMSE: 8.94 kcal/mol  
Epochs: 70%| | 21/30 [01:02<00:28, 3.21s/it]

Epoch 21 - Train Loss: 0.0014, Val Loss: 0.0018, RMSE: 8.56 kcal/mol  
Epochs: 73%| | 22/30 [01:05<00:25, 3.13s/it]

Epoch 22 - Train Loss: 0.0016, Val Loss: 0.0018, RMSE: 8.41 kcal/mol  
Epochs: 77%| | 23/30 [01:08<00:21, 3.02s/it]

Epoch 23 - Train Loss: 0.0017, Val Loss: 0.0018, RMSE: 8.49 kcal/mol  
Epochs: 80%| | 24/30 [01:10<00:17, 2.93s/it]

Epoch 24 - Train Loss: 0.0015, Val Loss: 0.0019, RMSE: 8.62 kcal/mol  
Epochs: 83%| | 25/30 [01:13<00:14, 2.88s/it]

Epoch 25 - Train Loss: 0.0015, Val Loss: 0.0018, RMSE: 8.38 kcal/mol  
Epochs: 87%| | 26/30 [01:16<00:11, 2.84s/it]

Epoch 26 - Train Loss: 0.0013, Val Loss: 0.0017, RMSE: 8.27 kcal/mol  
Epochs: 90%| | 27/30 [01:19<00:08, 2.84s/it]

Epoch 27 - Train Loss: 0.0014, Val Loss: 0.0020, RMSE: 8.83 kcal/mol  
Epochs: 93%| | 28/30 [01:22<00:05, 2.83s/it]

Epoch 28 - Train Loss: 0.0017, Val Loss: 0.0017, RMSE: 8.16 kcal/mol  
Epochs: 97%| | 29/30 [01:24<00:02, 2.80s/it]

Epoch 29 - Train Loss: 0.0015, Val Loss: 0.0019, RMSE: 8.69 kcal/mol  
Epochs: 100%| | 30/30 [01:27<00:00, 2.92s/it]

Epoch 30 - Train Loss: 0.0013, Val Loss: 0.0016, RMSE: 8.05 kcal/mol

Retraining model: dropout=0.3, L2=0.0

Epochs: 3%| | 1/30 [00:03<01:48, 3.74s/it]  
Epoch 1 - Train Loss: 0.1650, Val Loss: 0.0511, RMSE: 44.85 kcal/mol  
Epochs: 7%| | 2/30 [00:06<01:27, 3.12s/it]  
Epoch 2 - Train Loss: 0.0275, Val Loss: 0.0201, RMSE: 28.11 kcal/mol  
Epochs: 10%| | 3/30 [00:09<01:19, 2.95s/it]  
Epoch 3 - Train Loss: 0.0154, Val Loss: 0.0123, RMSE: 21.96 kcal/mol  
Epochs: 13%| | 4/30 [00:11<01:15, 2.90s/it]  
Epoch 4 - Train Loss: 0.0106, Val Loss: 0.0084, RMSE: 18.16 kcal/mol  
Epochs: 17%| | 5/30 [00:14<01:10, 2.82s/it]  
Epoch 5 - Train Loss: 0.0075, Val Loss: 0.0058, RMSE: 15.06 kcal/mol  
Epochs: 20%| | 6/30 [00:17<01:06, 2.79s/it]  
Epoch 6 - Train Loss: 0.0048, Val Loss: 0.0041, RMSE: 12.77 kcal/mol  
Epochs: 23%| | 7/30 [00:20<01:03, 2.76s/it]  
Epoch 7 - Train Loss: 0.0031, Val Loss: 0.0030, RMSE: 10.93 kcal/mol  
Epochs: 27%| | 8/30 [00:22<01:00, 2.75s/it]  
Epoch 8 - Train Loss: 0.0021, Val Loss: 0.0024, RMSE: 9.73 kcal/mol  
Epochs: 30%| | 9/30 [00:25<00:57, 2.75s/it]  
Epoch 9 - Train Loss: 0.0016, Val Loss: 0.0020, RMSE: 8.83 kcal/mol  
Epochs: 33%| | 10/30 [00:28<00:54, 2.74s/it]  
Epoch 10 - Train Loss: 0.0013, Val Loss: 0.0017, RMSE: 8.25 kcal/mol  
Epochs: 37%| | 11/30 [00:31<00:51, 2.73s/it]  
Epoch 11 - Train Loss: 0.0010, Val Loss: 0.0015, RMSE: 7.60 kcal/mol  
Epochs: 40%| | 12/30 [00:33<00:49, 2.75s/it]  
Epoch 12 - Train Loss: 0.0009, Val Loss: 0.0013, RMSE: 7.17 kcal/mol  
Epochs: 43%| | 13/30 [00:36<00:46, 2.74s/it]  
Epoch 13 - Train Loss: 0.0008, Val Loss: 0.0012, RMSE: 6.82 kcal/mol  
Epochs: 47%| | 14/30 [00:39<00:43, 2.74s/it]  
Epoch 14 - Train Loss: 0.0007, Val Loss: 0.0010, RMSE: 6.45 kcal/mol  
Epochs: 50%| | 15/30 [00:42<00:41, 2.74s/it]  
Epoch 15 - Train Loss: 0.0006, Val Loss: 0.0010, RMSE: 6.17 kcal/mol  
Epochs: 53%| | 16/30 [00:44<00:38, 2.75s/it]



Epoch 16 - Train Loss: 0.0006, Val Loss: 0.0009, RMSE: 5.95 kcal/mol  
Epochs: 57%| | 17/30 [00:47<00:35, 2.75s/it]

Epoch 17 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.79 kcal/mol  
Epochs: 60%| | 18/30 [00:50<00:32, 2.73s/it]

Epoch 18 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.74 kcal/mol  
Epochs: 63%| | 19/30 [00:52<00:30, 2.74s/it]

Epoch 19 - Train Loss: 0.0005, Val Loss: 0.0008, RMSE: 5.75 kcal/mol  
Epochs: 67%| | 20/30 [00:55<00:27, 2.74s/it]

Epoch 20 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.68 kcal/mol  
Epochs: 70%| | 21/30 [00:58<00:24, 2.74s/it]

Epoch 21 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.50 kcal/mol  
Epochs: 73%| | 22/30 [01:01<00:22, 2.78s/it]

Epoch 22 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.78 kcal/mol  
Epochs: 77%| | 23/30 [01:04<00:19, 2.79s/it]

Epoch 23 - Train Loss: 0.0004, Val Loss: 0.0006, RMSE: 5.02 kcal/mol  
Epochs: 80%| | 24/30 [01:06<00:16, 2.76s/it]

Epoch 24 - Train Loss: 0.0004, Val Loss: 0.0010, RMSE: 6.15 kcal/mol  
Epochs: 83%| | 25/30 [01:09<00:13, 2.76s/it]

Epoch 25 - Train Loss: 0.0004, Val Loss: 0.0007, RMSE: 5.23 kcal/mol  
Epochs: 87%| | 26/30 [01:12<00:11, 2.78s/it]

Epoch 26 - Train Loss: 0.0004, Val Loss: 0.0008, RMSE: 5.52 kcal/mol  
Epochs: 90%| | 27/30 [01:15<00:08, 2.80s/it]

Epoch 27 - Train Loss: 0.0004, Val Loss: 0.0006, RMSE: 4.92 kcal/mol  
Epochs: 93%| | 28/30 [01:18<00:05, 2.79s/it]

Epoch 28 - Train Loss: 0.0003, Val Loss: 0.0006, RMSE: 4.77 kcal/mol  
Epochs: 97%| | 29/30 [01:20<00:02, 2.78s/it]

Epoch 29 - Train Loss: 0.0003, Val Loss: 0.0006, RMSE: 4.82 kcal/mol  
Epochs: 100%| | 30/30 [01:23<00:00, 2.78s/it]

Epoch 30 - Train Loss: 0.0003, Val Loss: 0.0006, RMSE: 4.79 kcal/mol

Retraining model: dropout=0.3, L2=1e-05

Epochs: 3%| | 1/30 [00:03<01:47, 3.71s/it]

Epoch 1 - Train Loss: 0.5001, Val Loss: 0.2499, RMSE: 99.26 kcal/mol  
Epochs: 7%| | 2/30 [00:06<01:27, 3.14s/it]

Epoch 2 - Train Loss: 0.1851, Val Loss: 0.1332, RMSE: 72.40 kcal/mol  
Epochs: 10%| | 3/30 [00:09<01:19, 2.95s/it]

Epoch 3 - Train Loss: 0.0973, Val Loss: 0.0602, RMSE: 48.66 kcal/mol  
Epochs: 13%| | 4/30 [00:12<01:15, 2.92s/it]

Epoch 4 - Train Loss: 0.0476, Val Loss: 0.0356, RMSE: 37.38 kcal/mol  
Epochs: 17%| | 5/30 [00:14<01:12, 2.92s/it]

Epoch 5 - Train Loss: 0.0305, Val Loss: 0.0232, RMSE: 30.21 kcal/mol  
Epochs: 20%| | 6/30 [00:17<01:09, 2.90s/it]

Epoch 6 - Train Loss: 0.0207, Val Loss: 0.0164, RMSE: 25.40 kcal/mol  
Epochs: 23%| | 7/30 [00:20<01:05, 2.85s/it]

Epoch 7 - Train Loss: 0.0147, Val Loss: 0.0119, RMSE: 21.63 kcal/mol  
Epochs: 27%| | 8/30 [00:23<01:05, 2.98s/it]

Epoch 8 - Train Loss: 0.0103, Val Loss: 0.0086, RMSE: 18.38 kcal/mol  
Epochs: 30%| | 9/30 [00:27<01:04, 3.07s/it]

Epoch 9 - Train Loss: 0.0071, Val Loss: 0.0069, RMSE: 16.38 kcal/mol  
Epochs: 33%| | 10/30 [00:30<01:02, 3.15s/it]

Epoch 10 - Train Loss: 0.0051, Val Loss: 0.0053, RMSE: 14.41 kcal/mol  
Epochs: 37%| | 11/30 [00:33<01:00, 3.18s/it]

Epoch 11 - Train Loss: 0.0039, Val Loss: 0.0042, RMSE: 12.89 kcal/mol  
Epochs: 40%| | 12/30 [00:37<00:58, 3.23s/it]

Epoch 12 - Train Loss: 0.0030, Val Loss: 0.0037, RMSE: 12.00 kcal/mol  
Epochs: 43%| | 13/30 [00:40<00:55, 3.25s/it]

Epoch 13 - Train Loss: 0.0025, Val Loss: 0.0034, RMSE: 11.49 kcal/mol  
Epochs: 47%| | 14/30 [00:43<00:51, 3.25s/it]

Epoch 14 - Train Loss: 0.0021, Val Loss: 0.0029, RMSE: 10.66 kcal/mol  
Epochs: 50%| | 15/30 [00:46<00:49, 3.28s/it]

Epoch 15 - Train Loss: 0.0018, Val Loss: 0.0026, RMSE: 10.04 kcal/mol  
Epochs: 53%| | 16/30 [00:50<00:45, 3.28s/it]

Epoch 16 - Train Loss: 0.0015, Val Loss: 0.0023, RMSE: 9.60 kcal/mol  
Epochs: 57%| | 17/30 [00:53<00:42, 3.30s/it]

Epoch 17 - Train Loss: 0.0014, Val Loss: 0.0021, RMSE: 9.17 kcal/mol  
Epochs: 60%| | 18/30 [00:56<00:39, 3.32s/it]

Epoch 18 - Train Loss: 0.0013, Val Loss: 0.0020, RMSE: 8.83 kcal/mol  
Epochs: 63%| | 19/30 [01:00<00:36, 3.30s/it]

Epoch 19 - Train Loss: 0.0012, Val Loss: 0.0019, RMSE: 8.66 kcal/mol  
Epochs: 67%| | 20/30 [01:04<00:34, 3.48s/it]

Epoch 20 - Train Loss: 0.0011, Val Loss: 0.0019, RMSE: 8.58 kcal/mol  
Epochs: 70%| | 21/30 [01:07<00:30, 3.42s/it]

Epoch 21 - Train Loss: 0.0010, Val Loss: 0.0018, RMSE: 8.46 kcal/mol  
Epochs: 73%| | 22/30 [01:10<00:27, 3.41s/it]

Epoch 22 - Train Loss: 0.0010, Val Loss: 0.0017, RMSE: 8.22 kcal/mol  
Epochs: 77%| | 23/30 [01:14<00:23, 3.41s/it]

Epoch 23 - Train Loss: 0.0009, Val Loss: 0.0016, RMSE: 7.88 kcal/mol  
Epochs: 80%| | 24/30 [01:17<00:20, 3.40s/it]

Epoch 24 - Train Loss: 0.0008, Val Loss: 0.0014, RMSE: 7.45 kcal/mol  
Epochs: 83%| | 25/30 [01:20<00:17, 3.41s/it]

Epoch 25 - Train Loss: 0.0007, Val Loss: 0.0013, RMSE: 7.08 kcal/mol  
Epochs: 87%| | 26/30 [01:24<00:13, 3.39s/it]

Epoch 26 - Train Loss: 0.0007, Val Loss: 0.0012, RMSE: 6.92 kcal/mol  
Epochs: 90%| | 27/30 [01:27<00:10, 3.38s/it]

Epoch 27 - Train Loss: 0.0006, Val Loss: 0.0012, RMSE: 6.76 kcal/mol  
Epochs: 93%| | 28/30 [01:31<00:06, 3.40s/it]

Epoch 28 - Train Loss: 0.0006, Val Loss: 0.0011, RMSE: 6.62 kcal/mol  
Epochs: 97%| | 29/30 [01:34<00:03, 3.31s/it]

Epoch 29 - Train Loss: 0.0006, Val Loss: 0.0011, RMSE: 6.49 kcal/mol  
Epochs: 100%| | 30/30 [01:37<00:00, 3.25s/it]

Epoch 30 - Train Loss: 0.0006, Val Loss: 0.0011, RMSE: 6.50 kcal/mol

Retraining model: dropout=0.3, L2=0.0001

Epochs: 3%| | 1/30 [00:04<02:03, 4.26s/it]

Epoch 1 - Train Loss: 0.9202, Val Loss: 0.1270, RMSE: 70.76 kcal/mol  
Epochs: 7%| | 2/30 [00:07<01:43, 3.68s/it]

Epoch 2 - Train Loss: 0.1434, Val Loss: 0.0753, RMSE: 54.49 kcal/mol  
Epochs: 10%| | 3/30 [00:10<01:35, 3.55s/it]

Epoch 3 - Train Loss: 0.0763, Val Loss: 0.0648, RMSE: 50.58 kcal/mol  
Epochs: 13%| | 4/30 [00:18<02:16, 5.25s/it]

Epoch 4 - Train Loss: 0.0569, Val Loss: 0.0459, RMSE: 42.53 kcal/mol  
Epochs: 17%| | 5/30 [00:27<02:40, 6.42s/it]

Epoch 5 - Train Loss: 0.0418, Val Loss: 0.0336, RMSE: 36.37 kcal/mol  
Epochs: 20%| | 6/30 [00:32<02:20, 5.86s/it]

Epoch 6 - Train Loss: 0.0323, Val Loss: 0.0279, RMSE: 33.15 kcal/mol  
Epochs: 23%| | 7/30 [00:36<02:04, 5.42s/it]

Epoch 7 - Train Loss: 0.0264, Val Loss: 0.0232, RMSE: 30.18 kcal/mol  
Epochs: 27%| | 8/30 [00:40<01:48, 4.94s/it]

Epoch 8 - Train Loss: 0.0216, Val Loss: 0.0190, RMSE: 27.34 kcal/mol  
Epochs: 30%| | 9/30 [00:45<01:43, 4.93s/it]

Epoch 9 - Train Loss: 0.0177, Val Loss: 0.0153, RMSE: 24.53 kcal/mol  
Epochs: 33%| | 10/30 [00:49<01:33, 4.67s/it]

Epoch 10 - Train Loss: 0.0143, Val Loss: 0.0126, RMSE: 22.21 kcal/mol  
Epochs: 37%| | 11/30 [00:56<01:45, 5.53s/it]

Epoch 11 - Train Loss: 0.0113, Val Loss: 0.0101, RMSE: 19.87 kcal/mol  
Epochs: 40%| | 12/30 [01:07<02:05, 6.99s/it]

Epoch 12 - Train Loss: 0.0088, Val Loss: 0.0083, RMSE: 18.00 kcal/mol  
Epochs: 43%| | 13/30 [01:13<01:55, 6.78s/it]

Epoch 13 - Train Loss: 0.0069, Val Loss: 0.0071, RMSE: 16.73 kcal/mol  
Epochs: 47%| | 14/30 [01:18<01:40, 6.25s/it]

Epoch 14 - Train Loss: 0.0057, Val Loss: 0.0063, RMSE: 15.70 kcal/mol  
Epochs: 50%| | 15/30 [01:27<01:43, 6.91s/it]

Epoch 15 - Train Loss: 0.0049, Val Loss: 0.0057, RMSE: 14.89 kcal/mol  
Epochs: 53%| | 16/30 [01:32<01:32, 6.59s/it]

Epoch 16 - Train Loss: 0.0043, Val Loss: 0.0052, RMSE: 14.25 kcal/mol  
Epochs: 57%| | 17/30 [01:38<01:22, 6.32s/it]

Epoch 17 - Train Loss: 0.0039, Val Loss: 0.0048, RMSE: 13.71 kcal/mol  
Epochs: 60%| | 18/30 [01:42<01:06, 5.57s/it]

Epoch 18 - Train Loss: 0.0036, Val Loss: 0.0044, RMSE: 13.15 kcal/mol  
Epochs: 63%| | 19/30 [01:45<00:53, 4.91s/it]

Epoch 19 - Train Loss: 0.0033, Val Loss: 0.0040, RMSE: 12.55 kcal/mol  
Epochs: 67%| | 20/30 [01:49<00:44, 4.44s/it]

Epoch 20 - Train Loss: 0.0031, Val Loss: 0.0038, RMSE: 12.16 kcal/mol  
Epochs: 70%| | 21/30 [01:52<00:37, 4.15s/it]

Epoch 21 - Train Loss: 0.0029, Val Loss: 0.0037, RMSE: 11.98 kcal/mol  
Epochs: 73%| | 22/30 [01:56<00:31, 3.93s/it]

Epoch 22 - Train Loss: 0.0028, Val Loss: 0.0035, RMSE: 11.74 kcal/mol  
Epochs: 77%| | 23/30 [01:59<00:26, 3.78s/it]

Epoch 23 - Train Loss: 0.0026, Val Loss: 0.0034, RMSE: 11.60 kcal/mol  
Epochs: 80%| | 24/30 [02:02<00:21, 3.64s/it]

Epoch 24 - Train Loss: 0.0026, Val Loss: 0.0034, RMSE: 11.49 kcal/mol  
Epochs: 83%| | 25/30 [02:05<00:16, 3.39s/it]

Epoch 25 - Train Loss: 0.0025, Val Loss: 0.0033, RMSE: 11.46 kcal/mol  
Epochs: 87%| | 26/30 [02:08<00:13, 3.33s/it]

Epoch 26 - Train Loss: 0.0024, Val Loss: 0.0033, RMSE: 11.45 kcal/mol  
Epochs: 90%| | 27/30 [02:12<00:10, 3.49s/it]

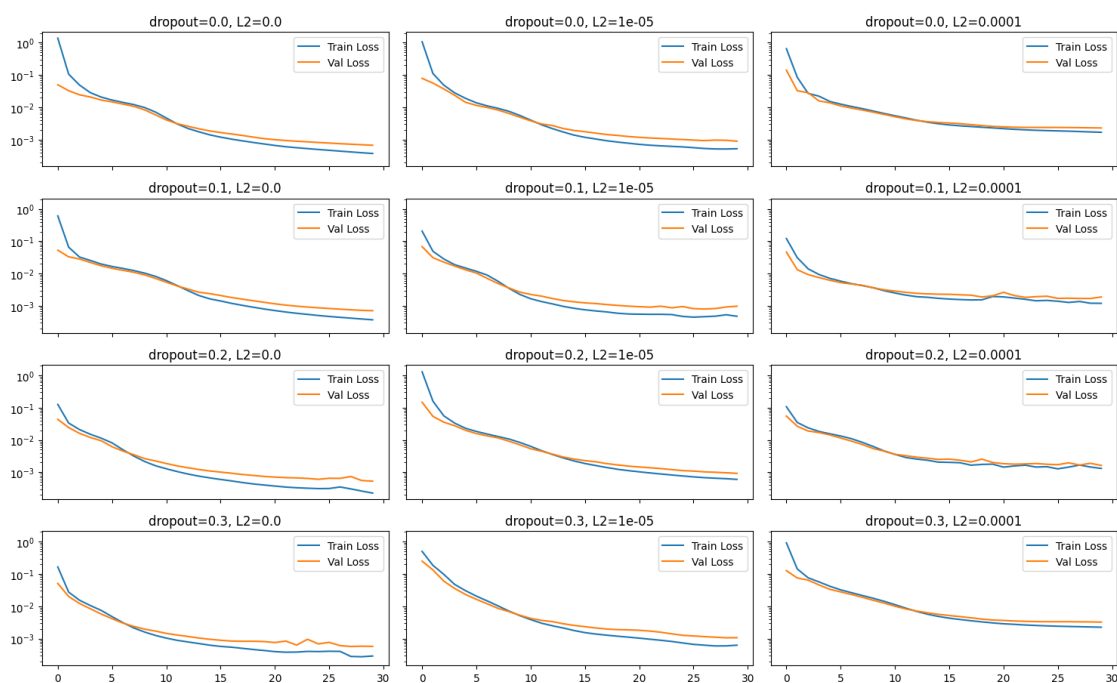
Epoch 27 - Train Loss: 0.0024, Val Loss: 0.0033, RMSE: 11.45 kcal/mol  
Epochs: 93%| | 28/30 [02:16<00:07, 3.59s/it]

Epoch 28 - Train Loss: 0.0023, Val Loss: 0.0033, RMSE: 11.41 kcal/mol  
Epochs: 97%| | 29/30 [02:19<00:03, 3.46s/it]

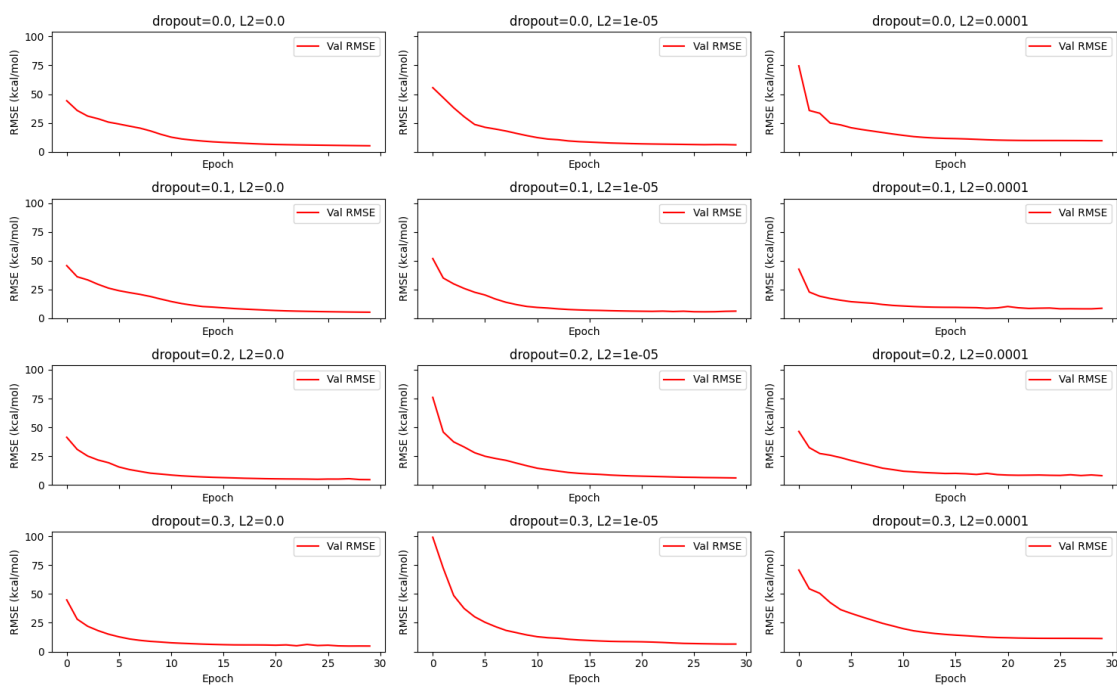
Epoch 29 - Train Loss: 0.0023, Val Loss: 0.0033, RMSE: 11.38 kcal/mol  
Epochs: 100%| | 30/30 [02:22<00:00, 4.76s/it]

Epoch 30 - Train Loss: 0.0023, Val Loss: 0.0032, RMSE: 11.29 kcal/mol

Train & Val Loss (Reloaded from JSON)



Val RMSE Curves (Reloaded from JSON)



```
[34]: from sklearn.model_selection import KFold
import numpy as np
import torch

k = 5
dropout = 0.3
l2 = 0.0
num_epochs = 30
batch_size = 512

indexed_dataset = list(get_data_subset(train_data, ''))

kf = KFold(n_splits=k, shuffle=True)
rmse_scores = []

for fold, (train_idx, val_idx) in enumerate(kf.split(indexed_dataset)):
    print(f"\n--- Fold {fold + 1} ---")

    train_samples = [indexed_dataset[i] for i in train_idx]
    val_samples = [indexed_dataset[i] for i in val_idx]

    train_subset = torchani.data.TransformableIterable(train_samples)
    val_subset = torchani.data.TransformableIterable(val_samples)

    model = build_model(dropout=dropout, l2=l2, device=device)

    trainer = ANITrainer(model, epoch=num_epochs, l2=l2, batch_size=batch_size)
    _, _, val_rmses = trainer.train(train_subset, val_subset, early_stop=True,
    ↪draw_curve=False)

    final_rmse = val_rmses[-1]
    rmse_scores.append(final_rmse)
    print(f"Final RMSE for fold {fold + 1}: {final_rmse:.4f} kcal/mol")

mean_rmse = np.mean(rmse_scores)
std_rmse = np.std(rmse_scores)
print(f"\nAverage RMSE over {k} folds: {mean_rmse:.4f} ± {std_rmse:.4f} kcal/
    ↪mol")
```

--- Fold 1 ---

Epochs: 3% | 1/30 [00:11<05:35, 11.58s/it]

Epoch 1 - Train Loss: 2.3360, Val Loss: 0.0219, RMSE: 32.92 kcal/mol

Epochs: 7% | 2/30 [00:21<04:51, 10.42s/it]

Epoch 2 - Train Loss: 0.0678, Val Loss: 0.0130, RMSE: 25.41 kcal/mol

Epochs: 10%| | 3/30 [00:29<04:14, 9.44s/it]  
Epoch 3 - Train Loss: 0.0417, Val Loss: 0.0084, RMSE: 20.39 kcal/mol  
Epochs: 13%| | 4/30 [00:39<04:15, 9.84s/it]  
Epoch 4 - Train Loss: 0.0257, Val Loss: 0.0047, RMSE: 15.29 kcal/mol  
Epochs: 17%| | 5/30 [00:54<04:45, 11.43s/it]  
Epoch 5 - Train Loss: 0.0152, Val Loss: 0.0029, RMSE: 11.97 kcal/mol  
Epochs: 20%| | 6/30 [01:08<04:58, 12.43s/it]  
Epoch 6 - Train Loss: 0.0098, Val Loss: 0.0017, RMSE: 9.13 kcal/mol  
Epochs: 23%| | 7/30 [01:17<04:23, 11.45s/it]  
Epoch 7 - Train Loss: 0.0059, Val Loss: 0.0012, RMSE: 7.74 kcal/mol  
Epochs: 27%| | 8/30 [01:24<03:34, 9.75s/it]  
Epoch 8 - Train Loss: 0.0042, Val Loss: 0.0010, RMSE: 6.92 kcal/mol  
Epochs: 30%| | 9/30 [01:30<03:01, 8.66s/it]  
Epoch 9 - Train Loss: 0.0033, Val Loss: 0.0008, RMSE: 6.28 kcal/mol  
Epochs: 33%| | 10/30 [01:37<02:41, 8.05s/it]  
Epoch 10 - Train Loss: 0.0026, Val Loss: 0.0007, RMSE: 5.84 kcal/mol  
Epochs: 37%| | 11/30 [01:43<02:23, 7.55s/it]  
Epoch 11 - Train Loss: 0.0022, Val Loss: 0.0006, RMSE: 5.53 kcal/mol  
Epochs: 40%| | 12/30 [01:50<02:13, 7.42s/it]  
Epoch 12 - Train Loss: 0.0019, Val Loss: 0.0006, RMSE: 5.27 kcal/mol  
Epochs: 43%| | 13/30 [01:57<02:01, 7.16s/it]  
Epoch 13 - Train Loss: 0.0017, Val Loss: 0.0005, RMSE: 5.06 kcal/mol  
Epochs: 47%| | 14/30 [02:03<01:50, 6.94s/it]  
Epoch 14 - Train Loss: 0.0015, Val Loss: 0.0005, RMSE: 4.89 kcal/mol  
Epochs: 50%| | 15/30 [02:09<01:40, 6.69s/it]  
Epoch 15 - Train Loss: 0.0014, Val Loss: 0.0005, RMSE: 4.74 kcal/mol  
Epochs: 53%| | 16/30 [02:16<01:32, 6.60s/it]  
Epoch 16 - Train Loss: 0.0013, Val Loss: 0.0004, RMSE: 4.60 kcal/mol  
Epochs: 57%| | 17/30 [02:22<01:23, 6.46s/it]  
Epoch 17 - Train Loss: 0.0012, Val Loss: 0.0004, RMSE: 4.48 kcal/mol  
Epochs: 60%| | 18/30 [02:28<01:15, 6.31s/it]  
Epoch 18 - Train Loss: 0.0011, Val Loss: 0.0004, RMSE: 4.38 kcal/mol



Epochs: 63%| | 19/30 [02:34<01:08, 6.20s/it]  
Epoch 19 - Train Loss: 0.0010, Val Loss: 0.0004, RMSE: 4.32 kcal/mol  
Epochs: 67%| | 20/30 [02:40<01:01, 6.20s/it]  
Epoch 20 - Train Loss: 0.0009, Val Loss: 0.0004, RMSE: 4.25 kcal/mol  
Epochs: 70%| | 21/30 [02:47<00:57, 6.37s/it]  
Epoch 21 - Train Loss: 0.0009, Val Loss: 0.0003, RMSE: 4.16 kcal/mol  
Epochs: 73%| | 22/30 [02:53<00:50, 6.36s/it]  
Epoch 22 - Train Loss: 0.0008, Val Loss: 0.0003, RMSE: 4.03 kcal/mol  
Epochs: 77%| | 23/30 [02:59<00:44, 6.35s/it]  
Epoch 23 - Train Loss: 0.0008, Val Loss: 0.0003, RMSE: 3.93 kcal/mol  
Epochs: 80%| | 24/30 [03:05<00:37, 6.32s/it]  
Epoch 24 - Train Loss: 0.0007, Val Loss: 0.0003, RMSE: 3.83 kcal/mol  
Epochs: 83%| | 25/30 [03:12<00:31, 6.40s/it]  
Epoch 25 - Train Loss: 0.0007, Val Loss: 0.0003, RMSE: 3.76 kcal/mol  
Epochs: 87%| | 26/30 [03:19<00:25, 6.45s/it]  
Epoch 26 - Train Loss: 0.0007, Val Loss: 0.0003, RMSE: 3.68 kcal/mol  
Epochs: 90%| | 27/30 [03:25<00:19, 6.53s/it]  
Epoch 27 - Train Loss: 0.0006, Val Loss: 0.0003, RMSE: 3.61 kcal/mol  
Epochs: 93%| | 28/30 [03:32<00:13, 6.54s/it]  
Epoch 28 - Train Loss: 0.0006, Val Loss: 0.0002, RMSE: 3.53 kcal/mol  
Epochs: 97%| | 29/30 [03:38<00:06, 6.36s/it]  
Epoch 29 - Train Loss: 0.0006, Val Loss: 0.0002, RMSE: 3.46 kcal/mol  
Epochs: 100%| | 30/30 [03:44<00:00, 7.49s/it]  
Epoch 30 - Train Loss: 0.0006, Val Loss: 0.0002, RMSE: 3.39 kcal/mol  
Final RMSE for fold 1: 3.3935 kcal/mol

--- Fold 2 ---

Epochs: 3%| | 1/30 [00:10<04:53, 10.13s/it]  
Epoch 1 - Train Loss: 1.6018, Val Loss: 0.0178, RMSE: 29.65 kcal/mol  
Epochs: 7%| | 2/30 [00:16<03:42, 7.95s/it]  
Epoch 2 - Train Loss: 0.0571, Val Loss: 0.0121, RMSE: 24.51 kcal/mol  
Epochs: 10%| | 3/30 [00:22<03:08, 6.98s/it]

Epoch 3 - Train Loss: 0.0362, Val Loss: 0.0079, RMSE: 19.76 kcal/mol  
Epochs: 13%| | 4/30 [00:28<02:50, 6.55s/it]

Epoch 4 - Train Loss: 0.0211, Val Loss: 0.0045, RMSE: 14.91 kcal/mol  
Epochs: 17%| | 5/30 [00:35<02:51, 6.87s/it]

Epoch 5 - Train Loss: 0.0116, Val Loss: 0.0026, RMSE: 11.29 kcal/mol  
Epochs: 20%| | 6/30 [00:44<03:04, 7.69s/it]

Epoch 6 - Train Loss: 0.0063, Val Loss: 0.0015, RMSE: 8.61 kcal/mol  
Epochs: 23%| | 7/30 [00:52<02:54, 7.61s/it]

Epoch 7 - Train Loss: 0.0039, Val Loss: 0.0010, RMSE: 7.17 kcal/mol  
Epochs: 27%| | 8/30 [01:04<03:19, 9.06s/it]

Epoch 8 - Train Loss: 0.0028, Val Loss: 0.0008, RMSE: 6.28 kcal/mol  
Epochs: 30%| | 9/30 [01:13<03:07, 8.93s/it]

Epoch 9 - Train Loss: 0.0023, Val Loss: 0.0007, RMSE: 5.69 kcal/mol  
Epochs: 33%| | 10/30 [01:22<03:03, 9.17s/it]

Epoch 10 - Train Loss: 0.0019, Val Loss: 0.0006, RMSE: 5.32 kcal/mol  
Epochs: 37%| | 11/30 [01:30<02:47, 8.79s/it]

Epoch 11 - Train Loss: 0.0017, Val Loss: 0.0005, RMSE: 5.07 kcal/mol  
Epochs: 40%| | 12/30 [01:37<02:23, 8.00s/it]

Epoch 12 - Train Loss: 0.0016, Val Loss: 0.0005, RMSE: 4.85 kcal/mol  
Epochs: 43%| | 13/30 [01:43<02:08, 7.59s/it]

Epoch 13 - Train Loss: 0.0014, Val Loss: 0.0004, RMSE: 4.66 kcal/mol  
Epochs: 47%| | 14/30 [01:50<01:56, 7.30s/it]

Epoch 14 - Train Loss: 0.0013, Val Loss: 0.0004, RMSE: 4.46 kcal/mol  
Epochs: 50%| | 15/30 [01:58<01:55, 7.69s/it]

Epoch 15 - Train Loss: 0.0012, Val Loss: 0.0004, RMSE: 4.31 kcal/mol  
Epochs: 53%| | 16/30 [02:05<01:44, 7.47s/it]

Epoch 16 - Train Loss: 0.0011, Val Loss: 0.0004, RMSE: 4.17 kcal/mol  
Epochs: 57%| | 17/30 [02:12<01:32, 7.10s/it]

Epoch 17 - Train Loss: 0.0010, Val Loss: 0.0003, RMSE: 3.99 kcal/mol  
Epochs: 60%| | 18/30 [02:18<01:21, 6.80s/it]

Epoch 18 - Train Loss: 0.0009, Val Loss: 0.0003, RMSE: 3.78 kcal/mol  
Epochs: 63%| | 19/30 [02:27<01:23, 7.58s/it]

Epoch 19 - Train Loss: 0.0008, Val Loss: 0.0003, RMSE: 3.61 kcal/mol  
Epochs: 67%| | 20/30 [02:34<01:14, 7.50s/it]  
Epoch 20 - Train Loss: 0.0008, Val Loss: 0.0002, RMSE: 3.51 kcal/mol  
Epochs: 70%| | 21/30 [02:41<01:04, 7.20s/it]  
Epoch 21 - Train Loss: 0.0007, Val Loss: 0.0002, RMSE: 3.42 kcal/mol  
Epochs: 73%| | 22/30 [02:47<00:55, 6.98s/it]  
Epoch 22 - Train Loss: 0.0007, Val Loss: 0.0002, RMSE: 3.35 kcal/mol  
Epochs: 77%| | 23/30 [02:55<00:49, 7.12s/it]  
Epoch 23 - Train Loss: 0.0006, Val Loss: 0.0002, RMSE: 3.29 kcal/mol  
Epochs: 80%| | 24/30 [03:03<00:43, 7.32s/it]  
Epoch 24 - Train Loss: 0.0006, Val Loss: 0.0002, RMSE: 3.27 kcal/mol  
Epochs: 83%| | 25/30 [03:09<00:34, 6.95s/it]  
Epoch 25 - Train Loss: 0.0006, Val Loss: 0.0002, RMSE: 3.24 kcal/mol  
Epochs: 87%| | 26/30 [03:15<00:26, 6.65s/it]  
Epoch 26 - Train Loss: 0.0006, Val Loss: 0.0002, RMSE: 3.21 kcal/mol  
Epochs: 90%| | 27/30 [03:21<00:19, 6.53s/it]  
Epoch 27 - Train Loss: 0.0006, Val Loss: 0.0002, RMSE: 3.20 kcal/mol  
Epochs: 93%| | 28/30 [03:27<00:12, 6.45s/it]  
Epoch 28 - Train Loss: 0.0005, Val Loss: 0.0002, RMSE: 3.15 kcal/mol  
Epochs: 97%| | 29/30 [03:34<00:06, 6.46s/it]  
Epoch 29 - Train Loss: 0.0005, Val Loss: 0.0002, RMSE: 3.10 kcal/mol  
Epochs: 100%| | 30/30 [03:40<00:00, 7.34s/it]  
Epoch 30 - Train Loss: 0.0005, Val Loss: 0.0002, RMSE: 3.05 kcal/mol  
Final RMSE for fold 2: 3.0455 kcal/mol

--- Fold 3 ---

Epochs: 3%| | 1/30 [00:09<04:24, 9.12s/it]  
Epoch 1 - Train Loss: 0.4296, Val Loss: 0.0150, RMSE: 27.20 kcal/mol  
Epochs: 7%| | 2/30 [00:15<03:22, 7.24s/it]  
Epoch 2 - Train Loss: 0.0462, Val Loss: 0.0081, RMSE: 19.94 kcal/mol  
Epochs: 10%| | 3/30 [00:21<03:02, 6.77s/it]  
Epoch 3 - Train Loss: 0.0231, Val Loss: 0.0033, RMSE: 12.70 kcal/mol

Epochs: 13%| | 4/30 [00:27<02:55, 6.75s/it]  
Epoch 4 - Train Loss: 0.0104, Val Loss: 0.0018, RMSE: 9.54 kcal/mol  
Epochs: 17%| | 5/30 [00:34<02:43, 6.52s/it]  
Epoch 5 - Train Loss: 0.0063, Val Loss: 0.0011, RMSE: 7.33 kcal/mol  
Epochs: 20%| | 6/30 [00:40<02:34, 6.42s/it]  
Epoch 6 - Train Loss: 0.0040, Val Loss: 0.0008, RMSE: 6.42 kcal/mol  
Epochs: 23%| | 7/30 [00:46<02:25, 6.31s/it]  
Epoch 7 - Train Loss: 0.0030, Val Loss: 0.0006, RMSE: 5.53 kcal/mol  
Epochs: 27%| | 8/30 [00:52<02:19, 6.36s/it]  
Epoch 8 - Train Loss: 0.0023, Val Loss: 0.0006, RMSE: 5.33 kcal/mol  
Epochs: 30%| | 9/30 [00:59<02:12, 6.29s/it]  
Epoch 9 - Train Loss: 0.0020, Val Loss: 0.0006, RMSE: 5.32 kcal/mol  
Epochs: 33%| | 10/30 [01:04<02:03, 6.16s/it]  
Epoch 10 - Train Loss: 0.0017, Val Loss: 0.0005, RMSE: 5.07 kcal/mol  
Epochs: 37%| | 11/30 [01:11<01:57, 6.17s/it]  
Epoch 11 - Train Loss: 0.0015, Val Loss: 0.0005, RMSE: 4.72 kcal/mol  
Epochs: 40%| | 12/30 [01:17<01:54, 6.35s/it]  
Epoch 12 - Train Loss: 0.0013, Val Loss: 0.0004, RMSE: 4.57 kcal/mol  
Epochs: 43%| | 13/30 [01:25<01:54, 6.73s/it]  
Epoch 13 - Train Loss: 0.0012, Val Loss: 0.0004, RMSE: 4.49 kcal/mol  
Epochs: 47%| | 14/30 [01:33<01:52, 7.06s/it]  
Epoch 14 - Train Loss: 0.0011, Val Loss: 0.0004, RMSE: 4.49 kcal/mol  
Epochs: 50%| | 15/30 [01:40<01:48, 7.25s/it]  
Epoch 15 - Train Loss: 0.0010, Val Loss: 0.0004, RMSE: 4.52 kcal/mol  
Epochs: 53%| | 16/30 [01:49<01:45, 7.52s/it]  
Epoch 16 - Train Loss: 0.0010, Val Loss: 0.0004, RMSE: 4.52 kcal/mol  
Epochs: 57%| | 17/30 [01:56<01:36, 7.40s/it]  
Epoch 17 - Train Loss: 0.0009, Val Loss: 0.0004, RMSE: 4.50 kcal/mol  
Epochs: 60%| | 18/30 [02:04<01:32, 7.69s/it]  
Epoch 18 - Train Loss: 0.0008, Val Loss: 0.0004, RMSE: 4.48 kcal/mol  
Epochs: 63%| | 19/30 [02:11<01:23, 7.56s/it]  
Epoch 19 - Train Loss: 0.0008, Val Loss: 0.0004, RMSE: 4.44 kcal/mol

Epochs: 67%| | 20/30 [02:19<01:15, 7.59s/it]  
Epoch 20 - Train Loss: 0.0007, Val Loss: 0.0004, RMSE: 4.38 kcal/mol  
Epochs: 70%| | 21/30 [02:27<01:08, 7.66s/it]  
Epoch 21 - Train Loss: 0.0008, Val Loss: 0.0004, RMSE: 4.36 kcal/mol  
Epochs: 73%| | 22/30 [02:35<01:02, 7.78s/it]  
Epoch 22 - Train Loss: 0.0006, Val Loss: 0.0004, RMSE: 4.33 kcal/mol  
Epochs: 77%| | 23/30 [02:42<00:52, 7.54s/it]  
Epoch 23 - Train Loss: 0.0008, Val Loss: 0.0004, RMSE: 4.37 kcal/mol  
Epochs: 80%| | 24/30 [02:50<00:46, 7.73s/it]  
Epoch 24 - Train Loss: 0.0007, Val Loss: 0.0004, RMSE: 4.43 kcal/mol  
Epochs: 83%| | 25/30 [02:57<00:38, 7.64s/it]  
Epoch 25 - Train Loss: 0.0007, Val Loss: 0.0005, RMSE: 5.07 kcal/mol  
Epochs: 87%| | 26/30 [03:04<00:29, 7.40s/it]  
Epoch 26 - Train Loss: 0.0007, Val Loss: 0.0004, RMSE: 4.38 kcal/mol  
Epochs: 90%| | 27/30 [03:11<00:21, 7.30s/it]  
Epoch 27 - Train Loss: 0.0006, Val Loss: 0.0004, RMSE: 4.19 kcal/mol  
Epochs: 93%| | 28/30 [03:19<00:14, 7.32s/it]  
Epoch 28 - Train Loss: 0.0005, Val Loss: 0.0004, RMSE: 4.29 kcal/mol  
Epochs: 97%| | 29/30 [03:26<00:07, 7.43s/it]  
Epoch 29 - Train Loss: 0.0005, Val Loss: 0.0004, RMSE: 4.20 kcal/mol  
Epochs: 100%| | 30/30 [03:34<00:00, 7.15s/it]  
Epoch 30 - Train Loss: 0.0006, Val Loss: 0.0004, RMSE: 4.33 kcal/mol  
Final RMSE for fold 3: 4.3349 kcal/mol

--- Fold 4 ---

Epochs: 3%| | 1/30 [00:11<05:43, 11.85s/it]  
Epoch 1 - Train Loss: 2.1076, Val Loss: 0.0444, RMSE: 46.70 kcal/mol  
Epochs: 7%| | 2/30 [00:19<04:18, 9.23s/it]  
Epoch 2 - Train Loss: 0.1429, Val Loss: 0.0214, RMSE: 32.43 kcal/mol  
Epochs: 10%| | 3/30 [00:25<03:31, 7.82s/it]  
Epoch 3 - Train Loss: 0.0663, Val Loss: 0.0096, RMSE: 21.68 kcal/mol  
Epochs: 13%| | 4/30 [00:32<03:12, 7.41s/it]

Epoch 4 - Train Loss: 0.0254, Val Loss: 0.0032, RMSE: 12.52 kcal/mol  
Epochs: 17%| | 5/30 [00:40<03:13, 7.74s/it]

Epoch 5 - Train Loss: 0.0115, Val Loss: 0.0021, RMSE: 10.01 kcal/mol  
Epochs: 20%| | 6/30 [00:49<03:13, 8.07s/it]

Epoch 6 - Train Loss: 0.0077, Val Loss: 0.0015, RMSE: 8.51 kcal/mol  
Epochs: 23%| | 7/30 [00:55<02:52, 7.48s/it]

Epoch 7 - Train Loss: 0.0057, Val Loss: 0.0011, RMSE: 7.41 kcal/mol  
Epochs: 27%| | 8/30 [01:03<02:47, 7.60s/it]

Epoch 8 - Train Loss: 0.0043, Val Loss: 0.0009, RMSE: 6.58 kcal/mol  
Epochs: 30%| | 9/30 [01:10<02:34, 7.38s/it]

Epoch 9 - Train Loss: 0.0033, Val Loss: 0.0007, RMSE: 5.98 kcal/mol  
Epochs: 33%| | 10/30 [01:17<02:28, 7.43s/it]

Epoch 10 - Train Loss: 0.0027, Val Loss: 0.0006, RMSE: 5.44 kcal/mol  
Epochs: 37%| | 11/30 [01:24<02:15, 7.14s/it]

Epoch 11 - Train Loss: 0.0022, Val Loss: 0.0005, RMSE: 5.09 kcal/mol  
Epochs: 40%| | 12/30 [01:30<02:04, 6.91s/it]

Epoch 12 - Train Loss: 0.0019, Val Loss: 0.0005, RMSE: 4.86 kcal/mol  
Epochs: 43%| | 13/30 [01:36<01:52, 6.61s/it]

Epoch 13 - Train Loss: 0.0017, Val Loss: 0.0005, RMSE: 4.71 kcal/mol  
Epochs: 47%| | 14/30 [01:42<01:43, 6.46s/it]

Epoch 14 - Train Loss: 0.0015, Val Loss: 0.0004, RMSE: 4.56 kcal/mol  
Epochs: 50%| | 15/30 [01:48<01:33, 6.26s/it]

Epoch 15 - Train Loss: 0.0014, Val Loss: 0.0004, RMSE: 4.37 kcal/mol  
Epochs: 53%| | 16/30 [01:54<01:25, 6.11s/it]

Epoch 16 - Train Loss: 0.0013, Val Loss: 0.0004, RMSE: 4.14 kcal/mol  
Epochs: 57%| | 17/30 [02:00<01:18, 6.03s/it]

Epoch 17 - Train Loss: 0.0011, Val Loss: 0.0003, RMSE: 3.91 kcal/mol  
Epochs: 60%| | 18/30 [02:06<01:15, 6.28s/it]

Epoch 18 - Train Loss: 0.0011, Val Loss: 0.0003, RMSE: 3.78 kcal/mol  
Epochs: 63%| | 19/30 [02:13<01:09, 6.33s/it]

Epoch 19 - Train Loss: 0.0010, Val Loss: 0.0003, RMSE: 3.70 kcal/mol  
Epochs: 67%| | 20/30 [02:20<01:04, 6.49s/it]

Epoch 20 - Train Loss: 0.0009, Val Loss: 0.0003, RMSE: 3.61 kcal/mol  
Epochs: 70%| | 21/30 [02:28<01:01, 6.88s/it]  
Epoch 21 - Train Loss: 0.0009, Val Loss: 0.0003, RMSE: 3.54 kcal/mol  
Epochs: 73%| | 22/30 [02:35<00:56, 7.02s/it]  
Epoch 22 - Train Loss: 0.0009, Val Loss: 0.0002, RMSE: 3.45 kcal/mol  
Epochs: 77%| | 23/30 [02:42<00:49, 7.05s/it]  
Epoch 23 - Train Loss: 0.0008, Val Loss: 0.0002, RMSE: 3.38 kcal/mol  
Epochs: 80%| | 24/30 [02:51<00:46, 7.68s/it]  
Epoch 24 - Train Loss: 0.0008, Val Loss: 0.0002, RMSE: 3.32 kcal/mol  
Epochs: 83%| | 25/30 [02:59<00:38, 7.79s/it]  
Epoch 25 - Train Loss: 0.0008, Val Loss: 0.0002, RMSE: 3.25 kcal/mol  
Epochs: 87%| | 26/30 [03:07<00:31, 7.92s/it]  
Epoch 26 - Train Loss: 0.0008, Val Loss: 0.0002, RMSE: 3.18 kcal/mol  
Epochs: 90%| | 27/30 [03:16<00:24, 8.23s/it]  
Epoch 27 - Train Loss: 0.0007, Val Loss: 0.0002, RMSE: 3.12 kcal/mol  
Epochs: 93%| | 28/30 [03:24<00:15, 7.98s/it]  
Epoch 28 - Train Loss: 0.0007, Val Loss: 0.0002, RMSE: 3.08 kcal/mol  
Epochs: 97%| | 29/30 [03:35<00:08, 8.98s/it]  
Epoch 29 - Train Loss: 0.0007, Val Loss: 0.0002, RMSE: 3.05 kcal/mol  
Epochs: 100%| | 30/30 [03:47<00:00, 7.60s/it]  
Epoch 30 - Train Loss: 0.0007, Val Loss: 0.0002, RMSE: 3.02 kcal/mol  
Final RMSE for fold 4: 3.0220 kcal/mol

--- Fold 5 ---

Epochs: 3%| | 1/30 [00:14<07:09, 14.82s/it]  
Epoch 1 - Train Loss: 2.3109, Val Loss: 0.0335, RMSE: 40.61 kcal/mol  
Epochs: 7%| | 2/30 [00:27<06:14, 13.37s/it]  
Epoch 2 - Train Loss: 0.1092, Val Loss: 0.0157, RMSE: 27.77 kcal/mol  
Epochs: 10%| | 3/30 [00:34<04:51, 10.81s/it]  
Epoch 3 - Train Loss: 0.0461, Val Loss: 0.0073, RMSE: 18.89 kcal/mol  
Epochs: 13%| | 4/30 [00:45<04:36, 10.63s/it]  
Epoch 4 - Train Loss: 0.0193, Val Loss: 0.0030, RMSE: 12.21 kcal/mol

Epochs: 17%| | 5/30 [00:54<04:12, 10.11s/it]  
Epoch 5 - Train Loss: 0.0096, Val Loss: 0.0019, RMSE: 9.53 kcal/mol  
Epochs: 20%| | 6/30 [01:12<05:09, 12.88s/it]  
Epoch 6 - Train Loss: 0.0064, Val Loss: 0.0013, RMSE: 8.12 kcal/mol  
Epochs: 23%| | 7/30 [01:25<04:53, 12.78s/it]  
Epoch 7 - Train Loss: 0.0049, Val Loss: 0.0011, RMSE: 7.30 kcal/mol  
Epochs: 27%| | 8/30 [01:33<04:08, 11.32s/it]  
Epoch 8 - Train Loss: 0.0040, Val Loss: 0.0009, RMSE: 6.77 kcal/mol  
Epochs: 30%| | 9/30 [01:40<03:29, 9.98s/it]  
Epoch 9 - Train Loss: 0.0033, Val Loss: 0.0008, RMSE: 6.35 kcal/mol  
Epochs: 33%| | 10/30 [01:47<03:01, 9.06s/it]  
Epoch 10 - Train Loss: 0.0029, Val Loss: 0.0007, RMSE: 5.97 kcal/mol  
Epochs: 37%| | 11/30 [01:54<02:41, 8.50s/it]  
Epoch 11 - Train Loss: 0.0025, Val Loss: 0.0006, RMSE: 5.60 kcal/mol  
Epochs: 40%| | 12/30 [02:01<02:23, 7.96s/it]  
Epoch 12 - Train Loss: 0.0023, Val Loss: 0.0006, RMSE: 5.29 kcal/mol  
Epochs: 43%| | 13/30 [02:08<02:08, 7.54s/it]  
Epoch 13 - Train Loss: 0.0021, Val Loss: 0.0005, RMSE: 5.00 kcal/mol  
Epochs: 47%| | 14/30 [02:19<02:17, 8.59s/it]  
Epoch 14 - Train Loss: 0.0019, Val Loss: 0.0005, RMSE: 4.79 kcal/mol  
Epochs: 50%| | 15/30 [02:27<02:06, 8.45s/it]  
Epoch 15 - Train Loss: 0.0017, Val Loss: 0.0004, RMSE: 4.61 kcal/mol  
Epochs: 53%| | 16/30 [02:33<01:50, 7.89s/it]  
Epoch 16 - Train Loss: 0.0016, Val Loss: 0.0004, RMSE: 4.47 kcal/mol  
Epochs: 57%| | 17/30 [02:39<01:35, 7.31s/it]  
Epoch 17 - Train Loss: 0.0015, Val Loss: 0.0004, RMSE: 4.33 kcal/mol  
Epochs: 60%| | 18/30 [02:45<01:22, 6.91s/it]  
Epoch 18 - Train Loss: 0.0014, Val Loss: 0.0004, RMSE: 4.24 kcal/mol  
Epochs: 63%| | 19/30 [02:51<01:13, 6.65s/it]  
Epoch 19 - Train Loss: 0.0013, Val Loss: 0.0003, RMSE: 4.10 kcal/mol  
Epochs: 67%| | 20/30 [02:57<01:04, 6.47s/it]  
Epoch 20 - Train Loss: 0.0012, Val Loss: 0.0003, RMSE: 4.03 kcal/mol



Epochs: 70%| | 21/30 [03:04<00:59, 6.62s/it]  
Epoch 21 - Train Loss: 0.0012, Val Loss: 0.0003, RMSE: 3.91 kcal/mol  
Epochs: 73%| | 22/30 [03:14<01:01, 7.66s/it]  
Epoch 22 - Train Loss: 0.0011, Val Loss: 0.0003, RMSE: 3.84 kcal/mol  
Epochs: 77%| | 23/30 [03:25<00:59, 8.57s/it]  
Epoch 23 - Train Loss: 0.0010, Val Loss: 0.0003, RMSE: 3.75 kcal/mol  
Epochs: 80%| | 24/30 [03:33<00:50, 8.50s/it]  
Epoch 24 - Train Loss: 0.0010, Val Loss: 0.0003, RMSE: 3.68 kcal/mol  
Epochs: 83%| | 25/30 [03:40<00:38, 7.80s/it]  
Epoch 25 - Train Loss: 0.0009, Val Loss: 0.0003, RMSE: 3.60 kcal/mol  
Epochs: 87%| | 26/30 [03:46<00:29, 7.32s/it]  
Epoch 26 - Train Loss: 0.0009, Val Loss: 0.0003, RMSE: 3.54 kcal/mol  
Epochs: 90%| | 27/30 [03:53<00:21, 7.29s/it]  
Epoch 27 - Train Loss: 0.0009, Val Loss: 0.0002, RMSE: 3.47 kcal/mol  
Epochs: 93%| | 28/30 [04:00<00:14, 7.21s/it]  
Epoch 28 - Train Loss: 0.0008, Val Loss: 0.0002, RMSE: 3.43 kcal/mol  
Epochs: 97%| | 29/30 [04:09<00:07, 7.59s/it]  
Epoch 29 - Train Loss: 0.0008, Val Loss: 0.0002, RMSE: 3.39 kcal/mol  
Epochs: 100%| | 30/30 [04:16<00:00, 8.53s/it]  
Epoch 30 - Train Loss: 0.0007, Val Loss: 0.0002, RMSE: 3.36 kcal/mol  
Final RMSE for fold 5: 3.3601 kcal/mol

Average RMSE over 5 folds: 3.4312 ± 0.4773 kcal/mol

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