```python
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import os
import gc
from tqdm.notebook import tqdm

import torch
import torch.nn as nn
import torch.nn.functional as F
from torch.utils.data import Dataset, DataLoader
from torch.amp import autocast
from sklearn.manifold import TSNE
from sklearn.decomposition import PCA

import os
for dirname, _, filenames in os.walk('/kaggle/input'):
    for filename in filenames:
        print(os.path.join(dirname, filename))
```

```
/kaggle/input/secondary-protein-structure-prediction/
synthetic_data.csv
/kaggle/input/secondary-protein-structure-prediction/real_predictions.
csv
/kaggle/input/secondary-protein-structure-prediction/combined_data.csv
```

```python
def setup_gpu():
    if torch.cuda.is_available():
        print(f"GPU available: {torch.cuda.get_device_name(0)}")
        print(f"Number of GPUs: {torch.cuda.device_count()}")

        device = torch.device("cuda")

        torch.backends.cudnn.benchmark = True
        torch.backends.cudnn.deterministic = False

        torch.cuda.empty_cache()

        if torch.cuda.device_count() > 1:
            print(f"Using {torch.cuda.device_count()} GPUs")
    else:
        device = torch.device("cpu")
        print("No GPU available, using CPU")

    return device

device = setup_gpu()
```

```
GPU available: Tesla T4
Number of GPUs: 2
Using 2 GPUs
```

```python
class ProteinSecondaryStructureDataset(Dataset):
    def __init__(self, data_path, transform=None):
        self.data_path = data_path
        self.transform = transform
        self.data_files = self._get_data_files()

    def _get_data_files(self):
        files = [os.path.join(self.data_path, f) for f in
os.listdir(self.data_path)
                if f.endswith('.npy') or f.endswith('.npz')]
        return files

    def __len__(self):
        return len(self.data_files)

    def __getitem__(self, idx):
        structure = np.load(self.data_files[idx])

        if self.transform:
            structure = self.transform(structure)

        return torch.tensor(structure, dtype=torch.float32)

def create_data_loaders(data_path, batch_size=128, num_workers=4,
pin_memory=True):
    dataset = ProteinSecondaryStructureDataset(data_path)

    data_loader = DataLoader(
        dataset,
        batch_size=batch_size,
        shuffle=True,
        num_workers=num_workers,
        pin_memory=pin_memory,
        persistent_workers=(num_workers > 0),
        prefetch_factor=2 if num_workers > 0 else None,
    )

    return data_loader

def create_synthetic_dataset(output_dir, num_samples=1000,
input_dim=400):
    os.makedirs(output_dir, exist_ok=True)

    for i in range(num_samples):
        structure = np.random.rand(input_dim).astype(np.float32)
```

```
        np.save(os.path.join(output_dir, f"protein_{i}.npy"),
structure)

    print(f"Created {num_samples} synthetic protein structures in
{output_dir}")

class ProteinVAE(nn.Module):
    def __init__(self, input_dim, hidden_dim, latent_dim,
dropout_rate=0.1):
        super(ProteinVAE, self).__init__()

        self.encoder = nn.Sequential(
            nn.Linear(input_dim, hidden_dim),
            nn.BatchNorm1d(hidden_dim),
            nn.LeakyReLU(0.2),
            nn.Dropout(dropout_rate),
            nn.Linear(hidden_dim, hidden_dim),
            nn.BatchNorm1d(hidden_dim),
            nn.LeakyReLU(0.2),
            nn.Dropout(dropout_rate)
        )

        self.fc_mu = nn.Linear(hidden_dim, latent_dim)
        self.fc_var = nn.Linear(hidden_dim, latent_dim)

        self.decoder = nn.Sequential(
            nn.Linear(latent_dim, hidden_dim),
            nn.BatchNorm1d(hidden_dim),
            nn.LeakyReLU(0.2),
            nn.Dropout(dropout_rate),
            nn.Linear(hidden_dim, hidden_dim),
            nn.BatchNorm1d(hidden_dim),
            nn.LeakyReLU(0.2),
            nn.Dropout(dropout_rate),
            nn.Linear(hidden_dim, input_dim)
        )

    def encode(self, x):
        h = self.encoder(x)
        mu = self.fc_mu(h)
        log_var = self.fc_var(h)
        return mu, log_var

    def reparameterize(self, mu, log_var):
        std = torch.exp(0.5 * log_var)
        eps = torch.randn_like(std)
        z = mu + eps * std
        return z

    def decode(self, z):
```

```
        return self.decoder(z)

    def forward(self, x):
        mu, log_var = self.encode(x)
        z = self.reparameterize(mu, log_var)
        x_reconstructed = self.decode(z)
        return x_reconstructed, mu, log_var

def vae_loss_function(recon_x, x, mu, log_var, beta=1.0):
    BCE = F.binary_cross_entropy_with_logits(recon_x, x,
reduction='sum')

    KLD = -0.5 * torch.sum(1 + log_var - mu.pow(2) - log_var.exp())

    return BCE + beta * KLD

class EarlyStopping:
    def __init__(self, patience=7, min_delta=0,
save_path='best_model.pt'):
        self.patience = patience
        self.min_delta = min_delta
        self.counter = 0
        self.best_loss = None
        self.early_stop = False
        self.save_path = save_path

    def __call__(self, val_loss, model):
        if self.best_loss is None:
            self.best_loss = val_loss
            self.save_checkpoint(model)
        elif val_loss > self.best_loss - self.min_delta:
            self.counter += 1
            if self.counter >= self.patience:
                self.early_stop = True
        else:
            self.best_loss = val_loss
            self.save_checkpoint(model)
            self.counter = 0

    def save_checkpoint(self, model):
        torch.save(model.state_dict(), self.save_path)
        print(f'Model saved to {self.save_path}')

def train_model(model, train_loader, val_loader, device, epochs=100,
lr=1e-3,
                beta=1.0, weight_decay=1e-5, use_amp=True):
    optimizer = torch.optim.AdamW(
        model.parameters(),
        lr=lr,
        weight_decay=weight_decay
```

```
    )

    scheduler = torch.optim.lr_scheduler.CosineAnnealingLR(
        optimizer, T_max=epochs, eta_min=lr/10
    )

    early_stopping = EarlyStopping(patience=10,
save_path='best_vae_model.pt')

    scaler = GradScaler() if use_amp else None

    train_losses = []
    val_losses = []

    for epoch in range(epochs):
        model.train()
        train_loss = 0

        progress_bar = tqdm(train_loader, desc=f"Epoch
{epoch+1}/{epochs}")

        for batch_idx, data in enumerate(progress_bar):
            data = data.to(device, non_blocking=True)
            optimizer.zero_grad()

            if use_amp:
                with autocast(device_type='cuda'):
                    recon_batch, mu, log_var = model(data)
                    loss = vae_loss_function(recon_batch, data, mu,
log_var, beta=beta)

                scaler.scale(loss).backward()
                scaler.step(optimizer)
                scaler.update()
            else:
                recon_batch, mu, log_var = model(data)
                loss = vae_loss_function(recon_batch, data, mu,
log_var, beta=beta)
                loss.backward()
                optimizer.step()

            train_loss += loss.item()

            progress_bar.set_postfix({'loss': loss.item()})

            del data, recon_batch, mu, log_var, loss

        scheduler.step()
```

```
        avg_train_loss = train_loss / len(train_loader.dataset)
        train_losses.append(avg_train_loss)

        model.eval()
        val_loss = 0

        with torch.no_grad():
            for data in val_loader:
                data = data.to(device, non_blocking=True)

                if use_amp:
                    with autocast(device_type='cuda'):
                        recon_batch, mu, log_var = model(data)
                        loss = vae_loss_function(recon_batch, data,
mu, log_var, beta=beta)
                else:
                    recon_batch, mu, log_var = model(data)
                    loss = vae_loss_function(recon_batch, data, mu,
log_var, beta=beta)

                val_loss += loss.item()

                del data, recon_batch, mu, log_var, loss

        avg_val_loss = val_loss / len(val_loader.dataset)
        val_losses.append(avg_val_loss)

        early_stopping(avg_val_loss, model)
        if early_stopping.early_stop:
            print(f"Early stopping at epoch {epoch+1}")
            break

        print(f"Epoch {epoch+1}: Train Loss: {avg_train_loss:.4f}, Val
Loss: {avg_val_loss:.4f}")

        torch.cuda.empty_cache()
        gc.collect()

    model.load_state_dict(torch.load('best_vae_model.pt'))

    return model, train_losses, val_losses

@torch.no_grad()
def evaluate_model(model, test_loader, device, use_amp=True):
    model.eval()
    test_loss = 0
    reconstruction_error = 0
    kl_divergence = 0

    all_mu = []
```

```
    all_log_var = []

    with torch.no_grad():
        for data in tqdm(test_loader, desc="Evaluating"):
            data = data.to(device, non_blocking=True)

            if use_amp:
                with autocast(device_type='cuda'):
                    recon_batch, mu, log_var = model(data)
                    loss = vae_loss_function(recon_batch, data, mu,
log_var)
            else:
                recon_batch, mu, log_var = model(data)
                loss = vae_loss_function(recon_batch, data, mu,
log_var)

            test_loss += loss.item()

            recon_error =
F.binary_cross_entropy_with_logits(recon_batch, data,
reduction='sum').item()
            reconstruction_error += recon_error

            kld = -0.5 * torch.sum(1 + log_var - mu.pow(2) -
log_var.exp()).item()
            kl_divergence += kld

            all_mu.append(mu.cpu().numpy())
            all_log_var.append(log_var.cpu().numpy())

            del data, recon_batch, mu, log_var
            torch.cuda.empty_cache()

    test_loss /= len(test_loader.dataset)
    reconstruction_error /= len(test_loader.dataset)
    kl_divergence /= len(test_loader.dataset)

    all_mu = np.concatenate(all_mu, axis=0)
    all_log_var = np.concatenate(all_log_var, axis=0)

    mu_mean = np.mean(all_mu, axis=0)
    mu_std = np.std(all_mu, axis=0)
    var_mean = np.mean(np.exp(all_log_var), axis=0)

    metrics = {
        'test_loss': test_loss,
        'reconstruction_error': reconstruction_error,
        'kl_divergence': kl_divergence,
        'mu_mean': mu_mean,
```

```python
            'mu_std': mu_std,
            'var_mean': var_mean
        }

        return metrics, all_mu, all_log_var

class ProteinVAEInferenceEngine:

    def __init__(self, model, device, use_amp=True):
        self.model = model
        self.device = device
        self.use_amp = use_amp
        self.model.eval()

        self.is_data_parallel = hasattr(self.model, 'module')

        self.actual_model = self.model.module if self.is_data_parallel
else self.model

    @torch.no_grad()
    def encode(self, structure):
        if isinstance(structure, np.ndarray):
            structure = torch.tensor(structure, dtype=torch.float32)

        if len(structure.shape) == 1:
            structure = structure.unsqueeze(0)

        structure = structure.to(self.device)

        if self.use_amp:
            with autocast(device_type='cuda'):
                mu, log_var = self.actual_model.encode(structure)
                z = self.actual_model.reparameterize(mu, log_var)
        else:
            mu, log_var = self.actual_model.encode(structure)
            z = self.actual_model.reparameterize(mu, log_var)

        return z.cpu().numpy(), mu.cpu().numpy(),
log_var.cpu().numpy()

    @torch.no_grad()
    def decode(self, z):
        if isinstance(z, np.ndarray):
            z = torch.tensor(z, dtype=torch.float32)

        z = z.to(self.device)

        if self.use_amp:
            with autocast(device_type='cuda'):
                logits = self.actual_model.decode(z)
```

```
                decoded = torch.sigmoid(logits)
        else:
            logits = self.actual_model.decode(z)
            decoded = torch.sigmoid(logits)

        return decoded.cpu().numpy()

    @torch.no_grad()
    def reconstruct(self, structure):
        if isinstance(structure, np.ndarray):
            structure = torch.tensor(structure, dtype=torch.float32)

        if len(structure.shape) == 1:
            structure = structure.unsqueeze(0)

        structure = structure.to(self.device)

        if self.use_amp:
            with autocast(device_type='cuda'):
                logits, _, _ = self.model(structure)
                recon = torch.sigmoid(logits)
        else:
            logits, _, _ = self.model(structure)
            recon = torch.sigmoid(logits)

        return recon.cpu().numpy()

    def interpolate(self, structure1, structure2, steps=10):
        z1, _, _ = self.encode(structure1)
        z2, _, _ = self.encode(structure2)

        interpolations = []
        for alpha in np.linspace(0, 1, steps):
            z_interp = z1 * (1 - alpha) + z2 * alpha
            decoded = self.decode(z_interp)
            interpolations.append(decoded)

        return interpolations

    @torch.no_grad()
    def generate_novel_structures(self, n_samples=10,
latent_dim=None):
        if latent_dim is None:
            for name, param in self.actual_model.named_parameters():
                if 'fc_mu.weight' in name:
                    latent_dim = param.shape[0]
                    break

        if latent_dim is None:
```

```
            raise ValueError("Could not infer latent dimension, please
specify manually")

        z_samples = torch.randn(n_samples, latent_dim).to(self.device)

        if self.use_amp:
            with autocast(device_type='cuda'):
                logits = self.actual_model.decode(z_samples)
                novel_structures = torch.sigmoid(logits)
        else:
            logits = self.actual_model.decode(z_samples)
            novel_structures = torch.sigmoid(logits)

        return novel_structures.cpu().numpy()

    def latent_arithmetic(self, structure_a, structure_b,
structure_c):
        z_a, _, _ = self.encode(structure_a)
        z_b, _, _ = self.encode(structure_b)
        z_c, _, _ = self.encode(structure_c)

        z_result = z_a - z_b + z_c

        result_structure = self.decode(z_result)

        return result_structure

    def find_nearest_neighbors(self, query_structure,
reference_structures, k=5):
        query_z, _, _ = self.encode(query_structure)

        reference_z = []
        for structure in tqdm(reference_structures, desc="Encoding
reference structures"):
            z, _, _ = self.encode(structure)
            reference_z.append(z)

        reference_z = np.concatenate(reference_z, axis=0)

        distances = np.linalg.norm(reference_z - query_z, axis=1)

        nearest_indices = np.argsort(distances)[:k]

        return nearest_indices, distances[nearest_indices]

def plot_reconstructions(original, reconstructed, n_samples=5):
    n_samples = min(n_samples, len(original))

    fig, axes = plt.subplots(n_samples, 2, figsize=(12, 3*n_samples))
```

```
    for i in range(n_samples):
        orig_shape = int(np.sqrt(original[i].shape[0]))
        recon_shape = int(np.sqrt(reconstructed[i].shape[0]))

        axes[i, 0].imshow(original[i].reshape(orig_shape, -1),
cmap='viridis')
        axes[i, 0].set_title(f"Original {i+1}")
        axes[i, 0].axis('off')

        axes[i, 1].imshow(reconstructed[i].reshape(recon_shape, -1),
cmap='viridis')
        axes[i, 1].set_title(f"Reconstructed {i+1}")
        axes[i, 1].axis('off')

    plt.tight_layout()
    plt.savefig('reconstructions.png', dpi=300, bbox_inches='tight')
    plt.show()

def plot_latent_traversal(inference_engine, base_z, dim_idx,
range_vals=(-3, 3), steps=10):
    traversal_values = np.linspace(range_vals[0], range_vals[1],
steps)

    reconstructions = []
    for val in traversal_values:
        z_modified = base_z.copy()
        z_modified[0, dim_idx] = val

        reconstruction = inference_engine.decode(z_modified)
        reconstructions.append(reconstruction[0])

    fig, axes = plt.subplots(1, steps, figsize=(steps*2, 3))

    for i, (val, recon) in enumerate(zip(traversal_values,
reconstructions)):
        recon_shape = int(np.sqrt(recon.shape[0]))

        axes[i].imshow(recon.reshape(recon_shape, -1), cmap='viridis')
        axes[i].set_title(f"z_{dim_idx}={val:.1f}")
        axes[i].axis('off')

    plt.suptitle(f"Latent Dimension {dim_idx} Traversal")
    plt.tight_layout()
    plt.savefig(f'latent_traversal_dim_{dim_idx}.png', dpi=300,
bbox_inches='tight')
    plt.show()

def plot_interpolation(structures, steps):
    fig, axes = plt.subplots(1, steps, figsize=(steps*2, 3))
```

```
    for i, structure in enumerate(structures):
        struct_shape = int(np.sqrt(structure.shape[0]))

        axes[i].imshow(structure.reshape(struct_shape, -1),
cmap='viridis')
        axes[i].set_title(f"Step {i+1}")
        axes[i].axis('off')

    plt.suptitle("Interpolation in Latent Space")
    plt.tight_layout()
    plt.savefig('interpolation.png', dpi=300, bbox_inches='tight')
    plt.show()

def plot_latent_heatmap(all_mu, all_log_var):
    mu_mean = np.mean(all_mu, axis=0)
    mu_std = np.std(all_mu, axis=0)
    var_mean = np.exp(np.mean(all_log_var, axis=0))

    fig, axes = plt.subplots(3, 1, figsize=(12, 15))

    sns.barplot(x=np.arange(len(mu_mean)), y=mu_mean, ax=axes[0])
    axes[0].set_title('Mean of Latent Means (μ)')
    axes[0].set_xlabel('Latent Dimension')
    axes[0].set_ylabel('Mean Value')

    sns.barplot(x=np.arange(len(mu_std)), y=mu_std, ax=axes[1])
    axes[1].set_title('Standard Deviation of Latent Means (μ)')
    axes[1].set_xlabel('Latent Dimension')
    axes[1].set_ylabel('Std Value')

    sns.barplot(x=np.arange(len(var_mean)), y=var_mean, ax=axes[2])
    axes[2].set_title('Mean of Latent Variances (σ²)')
    axes[2].set_xlabel('Latent Dimension')
    axes[2].set_ylabel('Variance Value')

    plt.tight_layout()
    plt.savefig('latent_statistics.png', dpi=300, bbox_inches='tight')
    plt.show()

def plot_correlation_matrix(all_mu):
    corr_matrix = np.corrcoef(all_mu.T)

    plt.figure(figsize=(10, 8))
    sns.heatmap(corr_matrix, annot=True, cmap='coolwarm', vmin=-1,
vmax=1,
                fmt='.2f', linewidths=0.5)
    plt.title('Correlation Matrix of Latent Dimensions')
    plt.tight_layout()
```

```
    plt.savefig('latent_correlation.png', dpi=300,
bbox_inches='tight')
    plt.show()

    return corr_matrix

def plot_generated_structures(structures, n_samples=10):
    n_samples = min(n_samples, len(structures))

    fig, axes = plt.subplots(2, n_samples//2 + n_samples%2,
figsize=(n_samples*2, 6))
    axes = axes.flatten()

    for i in range(n_samples):
        struct_shape = int(np.sqrt(structures[i].shape[0]))

        axes[i].imshow(structures[i].reshape(struct_shape, -1),
cmap='viridis')
        axes[i].set_title(f"Generated {i+1}")
        axes[i].axis('off')

    plt.suptitle("Generated Protein Structures")
    plt.tight_layout()
    plt.savefig('generated_structures.png', dpi=300,
bbox_inches='tight')
    plt.show()

def plot_latent_space(all_mu, labels=None, method='tsne',
perplexity=30, n_components=2):
    if method.lower() == 'tsne':
        reducer = TSNE(n_components=n_components, random_state=42,
                      perplexity=perplexity, n_jobs=-1)
        print("Applying t-SNE dimensionality reduction...")
    elif method.lower() == 'umap':
        try:
            import umap
            reducer = umap.UMAP(n_components=n_components,
random_state=42)
            print("Applying UMAP dimensionality reduction...")
        except ImportError:
            print("UMAP not installed. Using PCA instead.")
            reducer = PCA(n_components=n_components)
            method = 'pca'
    else:
        reducer = PCA(n_components=n_components)
        print("Applying PCA dimensionality reduction...")

    reduced_data = reducer.fit_transform(all_mu)
```

```
    plt.figure(figsize=(12, 10))

    if labels is not None:
        scatter = plt.scatter(reduced_data[:, 0], reduced_data[:, 1],
c=labels,
                              cmap='viridis', alpha=0.7, s=10)
        plt.colorbar(scatter, label='Structure Class')
    else:
        plt.scatter(reduced_data[:, 0], reduced_data[:, 1], alpha=0.7,
s=10)

    plt.title(f'Latent Space Visualization using {method.upper()}')
    plt.xlabel('Component 1')
    plt.ylabel('Component 2')
    plt.tight_layout()
    plt.savefig(f'latent_space_{method.lower()}.png', dpi=300,
bbox_inches='tight')
    plt.show()

    return reduced_data


input_dim = 400
hidden_dim = 256
latent_dim = 32
batch_size = 128

data_path = '/kaggle/working/protein_data'
os.makedirs(data_path, exist_ok=True)
os.makedirs(os.path.join(data_path, 'train'), exist_ok=True)
os.makedirs(os.path.join(data_path, 'val'), exist_ok=True)
os.makedirs(os.path.join(data_path, 'test'), exist_ok=True)

create_synthetic_dataset(os.path.join(data_path, 'train'),
num_samples=1000, input_dim=input_dim)
create_synthetic_dataset(os.path.join(data_path, 'val'),
num_samples=200, input_dim=input_dim)
create_synthetic_dataset(os.path.join(data_path, 'test'),
num_samples=200, input_dim=input_dim)

train_loader = create_data_loaders(os.path.join(data_path, 'train'),
batch_size=batch_size)
val_loader = create_data_loaders(os.path.join(data_path, 'val'),
batch_size=batch_size)
test_loader = create_data_loaders(os.path.join(data_path, 'test'),
batch_size=batch_size)

model = get_model(input_dim, hidden_dim, latent_dim)

print("Starting training...")
```

```
trained_model, train_losses, val_losses = train_model(
    model,
    train_loader,
    val_loader,
    device,
    epochs=10,
    lr=3e-4,
    use_amp=True
)

plt.figure(figsize=(10, 6))
plt.plot(train_losses, label='Training Loss')
plt.plot(val_losses, label='Validation Loss')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.title('VAE Training and Validation Loss')
plt.legend()
plt.grid(True, alpha=0.3)
plt.savefig('loss_curves.png', dpi=300, bbox_inches='tight')
plt.show()

inference_engine = ProteinVAEInferenceEngine(trained_model, device,
use_amp=True)

print("Evaluating model...")
metrics, all_mu, all_log_var = evaluate_model(trained_model,
test_loader, device, use_amp=True)

print("\nEvaluation Metrics:")
for key, value in metrics.items():
    if isinstance(value, (int, float)):
        print(f"{key}: {value:.4f}")
    else:
        print(f"{key}: shape {np.array(value).shape}")

disentanglement_score, corr_matrix =
calculate_disentanglement_score(all_mu)
print(f"Disentanglement score: {disentanglement_score:.4f}")

print("Visualizing latent space...")
reduced_data_2d = plot_latent_space(all_mu, method='tsne')
plot_latent_space(all_mu, method='pca')

plot_latent_heatmap(all_mu, all_log_var)

plot_correlation_matrix(all_mu)

for test_batch in test_loader:
    original_data = test_batch.cpu().numpy()
    break
```

```
reconstructed_data = inference_engine.reconstruct(test_batch)

plot_reconstructions(original_data, reconstructed_data, n_samples=5)

print("Generating novel structures...")
novel_structures =
inference_engine.generate_novel_structures(n_samples=10,
latent_dim=latent_dim)
plot_generated_structures(novel_structures)

base_z, _, _ = inference_engine.encode(test_batch[0])

for dim in range(min(5, latent_dim)):
    plot_latent_traversal(inference_engine, base_z, dim, range_vals=(-
3, 3), steps=10)

print("Generating interpolation...")
interpolated = inference_engine.interpolate(test_batch[0],
test_batch[1], steps=10)
plot_interpolation(interpolated, steps=10)

torch.save({
    'model_state_dict': trained_model.state_dict(),
    'metrics': metrics,
    'latent_means': all_mu,
    'latent_log_vars': all_log_var
}, 'vae_results.pt')

print("Evaluation and visualization complete!")
```

```
Created 1000 synthetic protein structures in
/kaggle/working/protein_data/train
Created 200 synthetic protein structures in
/kaggle/working/protein_data/val
Created 200 synthetic protein structures in
/kaggle/working/protein_data/test
Starting training...
```

```
<ipython-input-57-639bcf3eaaf6>:18: FutureWarning:
`torch.cuda.amp.GradScaler(args...)` is deprecated. Please use
`torch.amp.GradScaler('cuda', args...)` instead.
  scaler = GradScaler() if use_amp else None
```

{"model_id":"ae3476f6141648fa93bdff4dff7c121d","version_major":2,"version_minor":0}

```
Model saved to best_vae_model.pt
Epoch 1: Train Loss: 291.7712, Val Loss: 278.6492
```

{"model_id":"6d84aebb78fc4fe1b2c6302ab8610399","version_major":2,"version_minor":0}

```
Epoch 2: Train Loss: 289.1974, Val Loss: 279.3876
```

{"model_id":"cf736091be554de5aa5219277e414674","version_major":2,"version_minor":0}

```
Epoch 3: Train Loss: 286.4207, Val Loss: 280.2085
```

{"model_id":"3f2d96d6156745c6963e40cc39639fa7","version_major":2,"version_minor":0}

```
Epoch 4: Train Loss: 284.9486, Val Loss: 280.7572
```

{"model_id":"cf05ea2315d042aeaf09bf0915e9219f","version_major":2,"version_minor":0}

```
Epoch 5: Train Loss: 284.1833, Val Loss: 281.1189
```

{"model_id":"fd10c4a195814be38e435fb9171fdbef","version_major":2,"version_minor":0}

```
Epoch 6: Train Loss: 283.6947, Val Loss: 281.1869
```

{"model_id":"51bbf8c719a640068d03752bbe437e4f","version_major":2,"version_minor":0}

```
Epoch 7: Train Loss: 283.2390, Val Loss: 281.1482
```

{"model_id":"047276c833dc423782a9ede3de6709b9","version_major":2,"version_minor":0}

```
Epoch 8: Train Loss: 282.9936, Val Loss: 281.0704
```

{"model_id":"f780e46d0c21471bbdb0ad60d3f1a163","version_major":2,"version_minor":0}

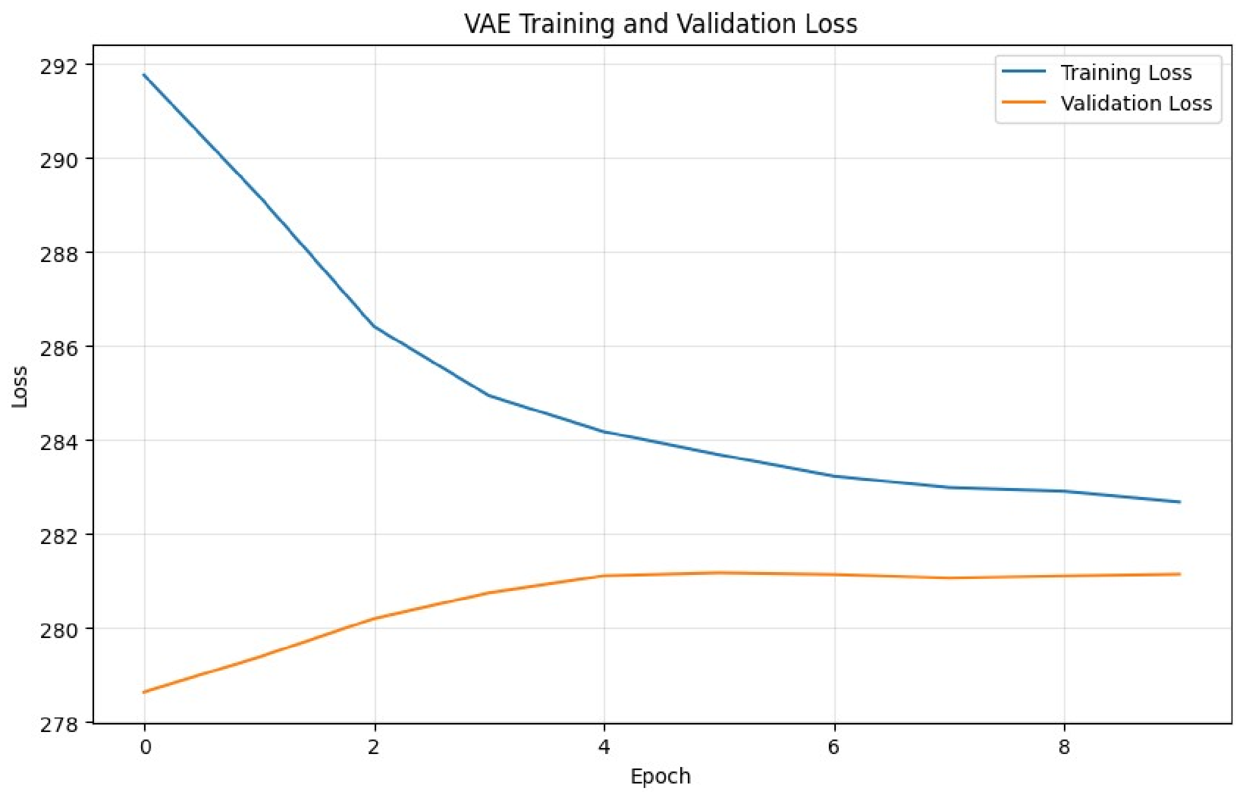
```
Epoch 9: Train Loss: 282.9159, Val Loss: 281.1162
```

{"model_id":"039969a87990456cbc25fec2fea41fbf","version_major":2,"version_minor":0}

```
Epoch 10: Train Loss: 282.6922, Val Loss: 281.1554
```

```
<ipython-input-57-639bcf3eaaf6>:102: FutureWarning: You are using
`torch.load` with `weights_only=False` (the current default value),
which uses the default pickle module implicitly. It is possible to
construct malicious pickle data which will execute arbitrary code
during unpickling (See
https://github.com/pytorch/pytorch/blob/main/SECURITY.md#untrusted-
models for more details). In a future release, the default value for
`weights_only` will be flipped to `True`. This limits the functions
```

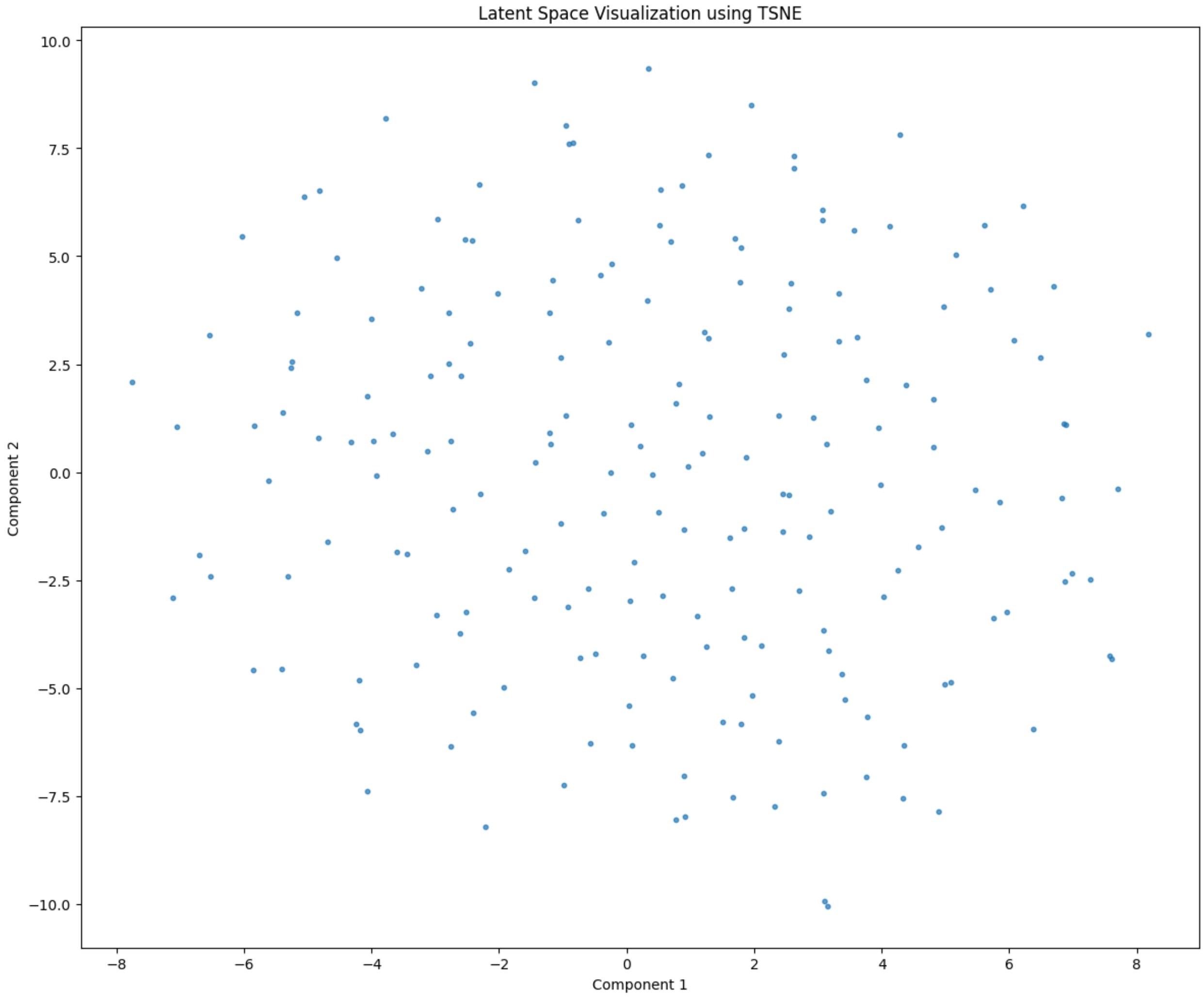
```
that could be executed during unpickling. Arbitrary objects will no
longer be allowed to be loaded via this mode unless they are
explicitly allowlisted by the user via
`torch.serialization.add_safe_globals`. We recommend you start setting
`weights_only=True` for any use case where you don't have full control
of the loaded file. Please open an issue on GitHub for any issues
related to this experimental feature.
  model.load_state_dict(torch.load('best_vae_model.pt'))
```



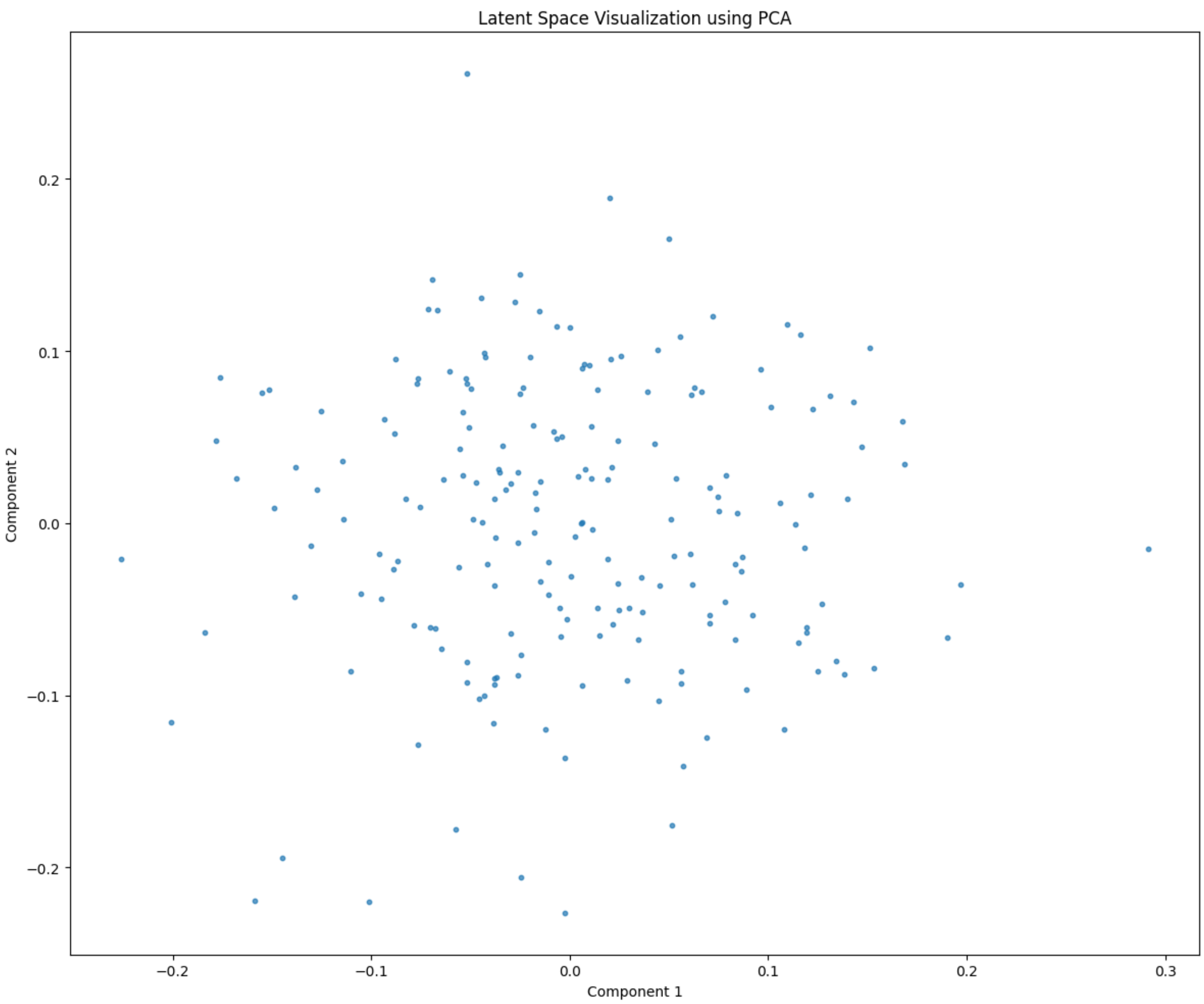

```
Evaluating model...
```

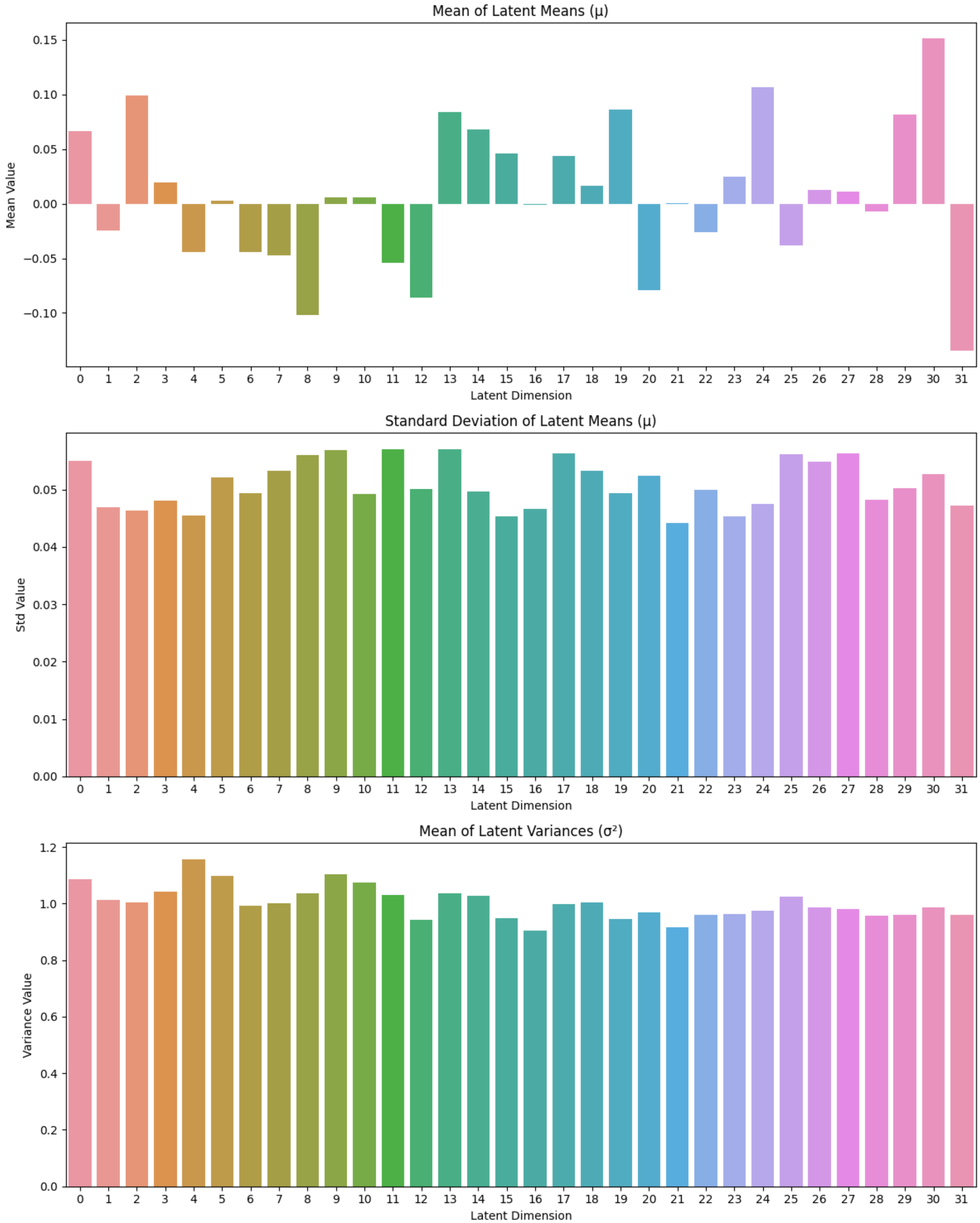
{"model_id":"8bdf1adba3de4a728192ba4fc69df26b","version_major":2,"version_minor":0}

```
Evaluation Metrics:
test_loss: 278.5146
reconstruction_error: 278.3618
kl_divergence: 0.1527
mu_mean: shape (32,)
mu_std: shape (32,)
var_mean: shape (32,)
Disentanglement score: 0.9024
Visualizing latent space...
Applying t-SNE dimensionality reduction...
```

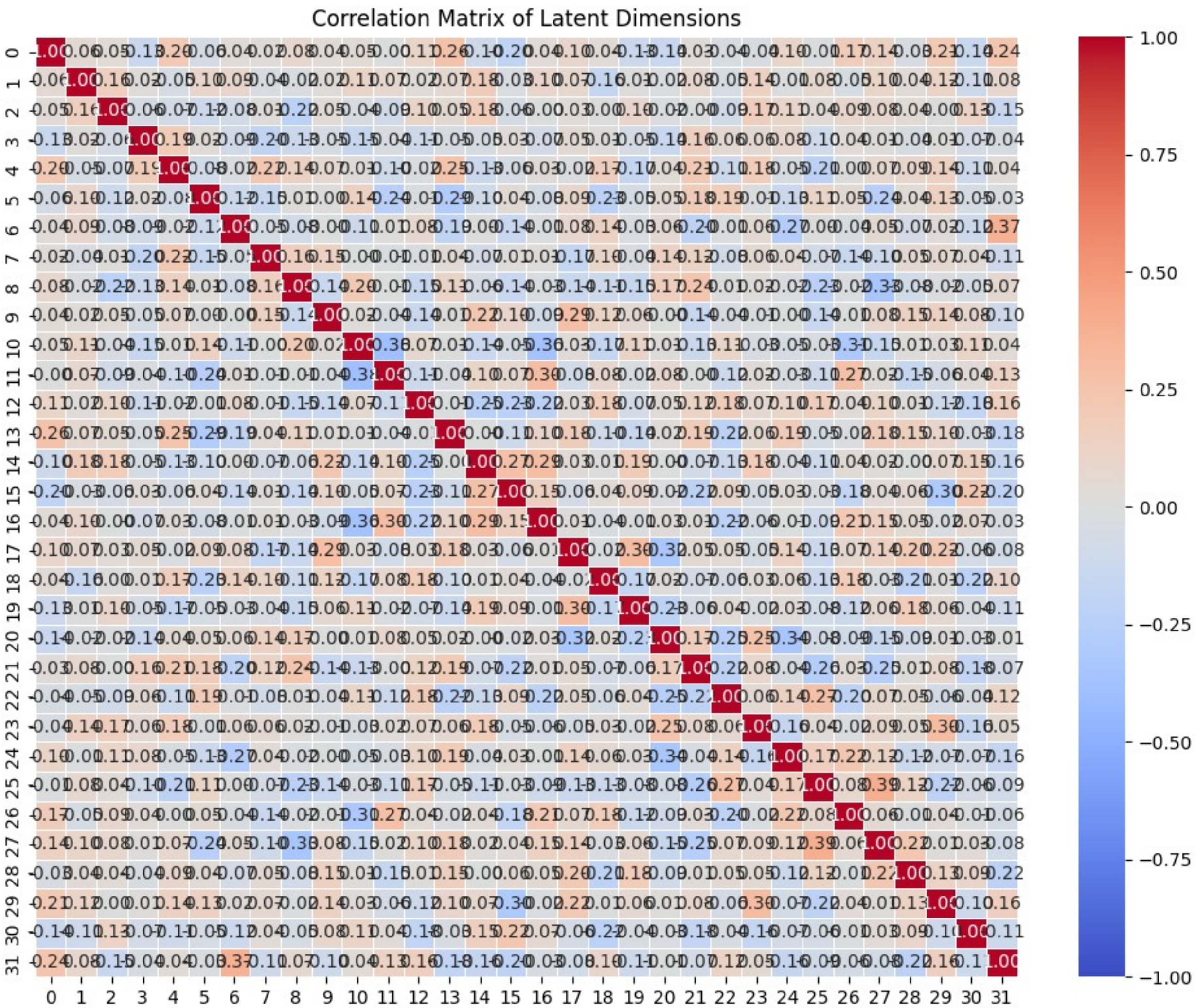


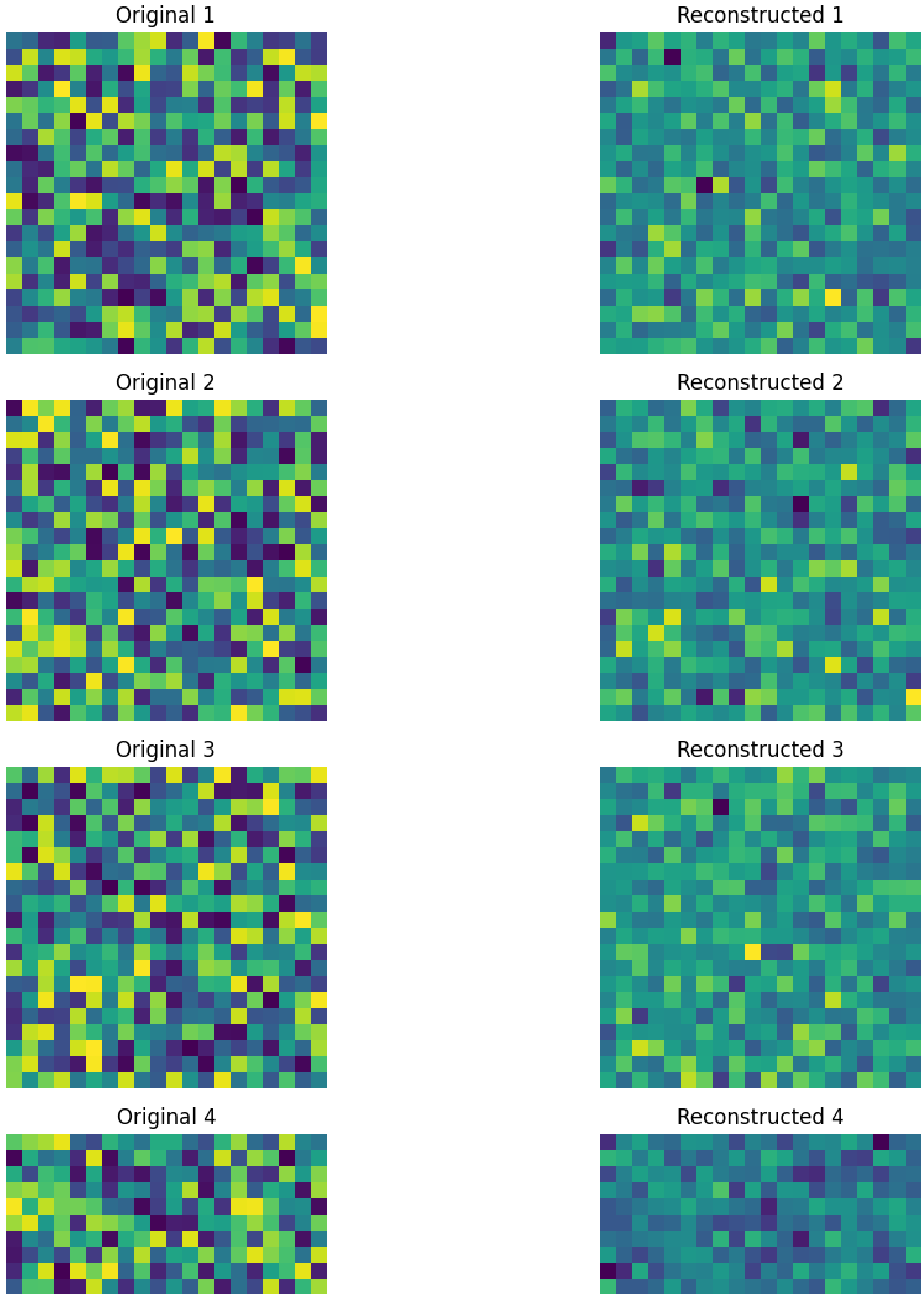

```
Applying PCA dimensionality reduction...
```


Latent Space Visualization using PCA
0.2
0.1
0.0
−0.1
−0.2
Component 2
−0.2
−0.1
0.0
0.1
0.2
0.3
Component 1

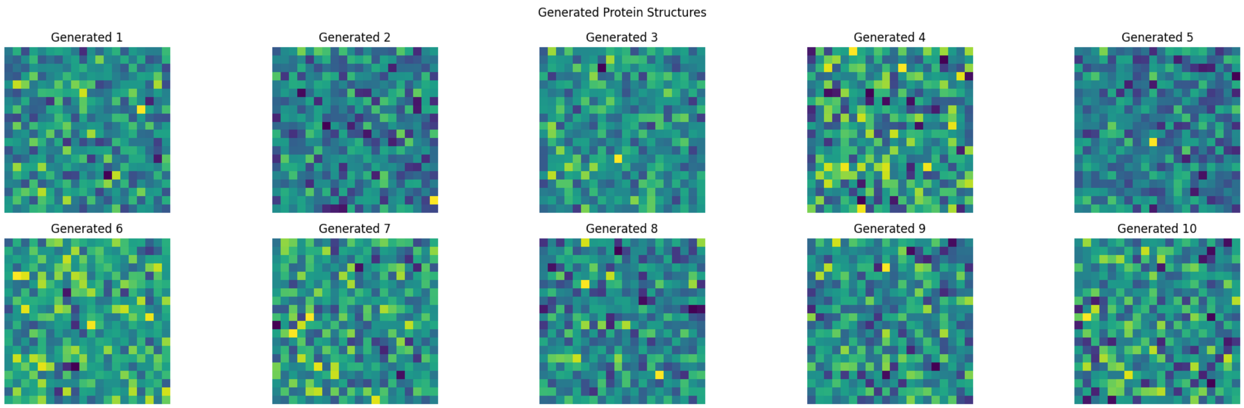


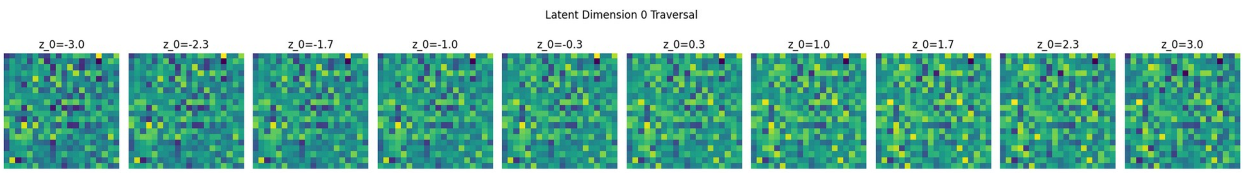
Mean of Latent Means (μ)
Mean Value
0.15
0.10
0.05
0.00
−0.05
−0.10
Latent Dimension
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31
Standard Deviation of Latent Means (μ)
Std Value
0.05
0.04
0.03
0.02
0.01
0.00
Latent Dimension
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31
Mean of Latent Variances (σ²)
Variance Value
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Latent Dimension
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31

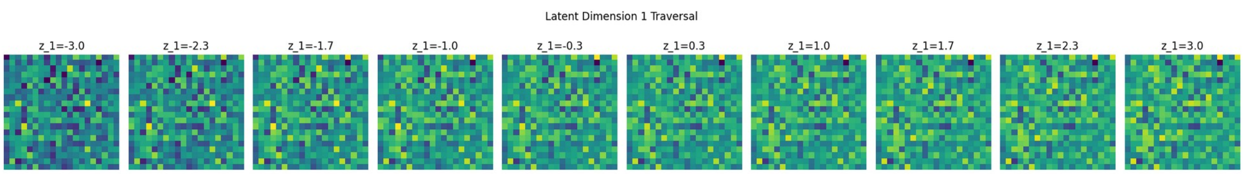

Correlation Matrix of Latent Dimensions
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00

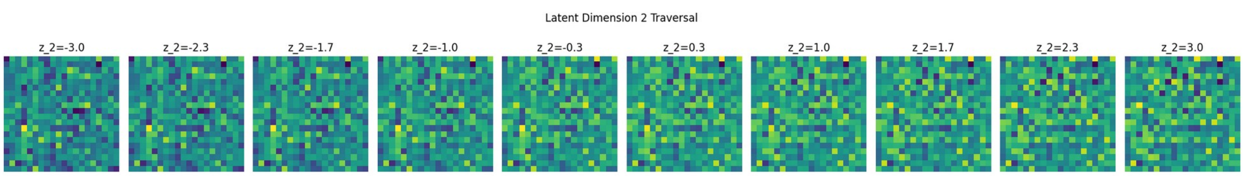

Original 1
Reconstructed 1
Original 2
Reconstructed 2
Original 3
Reconstructed 3
Original 4
Reconstructed 4

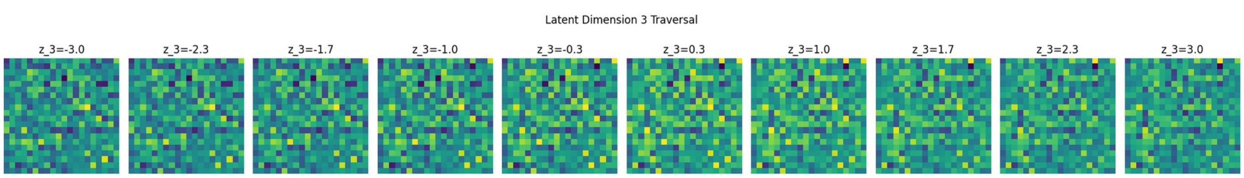
```
Generating novel structures...
```

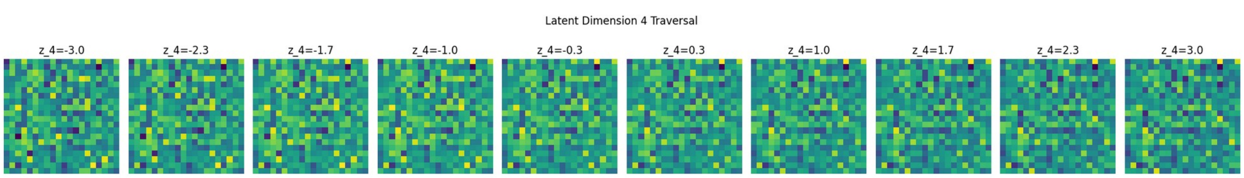













```
Generating interpolation...
```

```
Evaluation and visualization complete!
```