Task 1: Masking Reconstruction

Ligand SMILES

Ligand Encoder

Protein

Extract Interact-Ligands

K   K

M ...   T

Residue Sequence

Protein Mask

Structure-aware Sequence

Protein Encoder

Add & Norm
Feed Forward
Nx
Add & Norm
Multi-Head Attention
Positional Encoding
Input Embedding

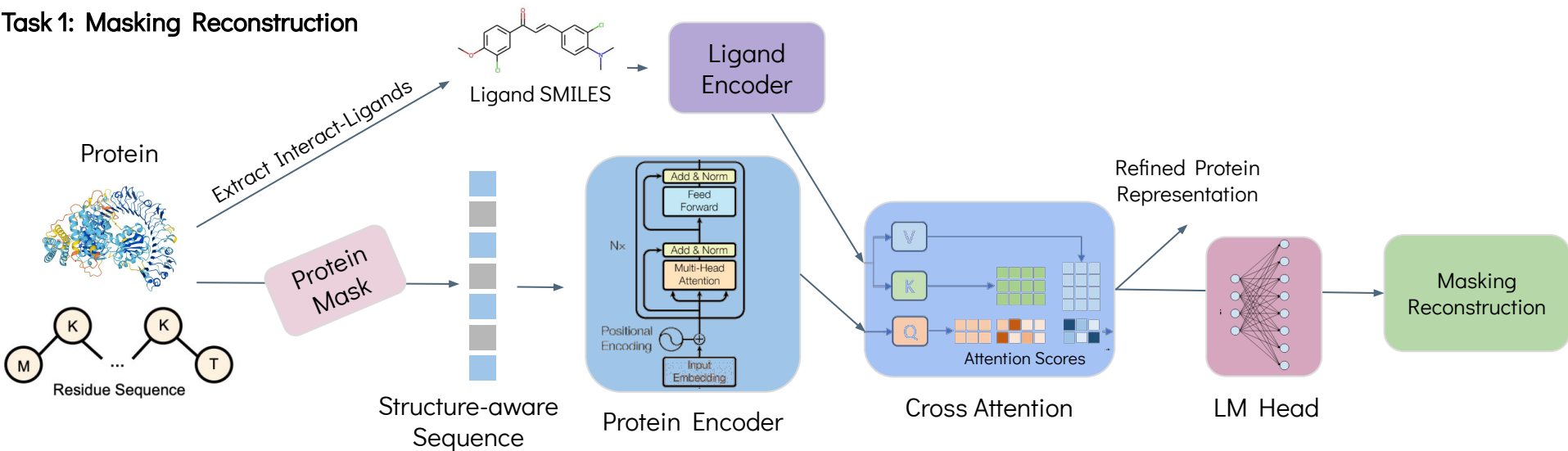Cross Attention

V
K
Q

Attention Scores

Refined Protein Representation

LM Head

Masking Reconstruction

Task 2: Predicting Interact-Ligands

Protein

K   K

M ...   T

Residue Sequence

Structure-aware Sequence

Protein Encoder

Add & Norm
Feed Forward
Nx
Add & Norm
Multi-Head Attention
Positional Encoding
Input Embedding

Ligand Generator

Add & Norm
Feed Forward
Nx
Add & Norm
Multi-Head Attention
Positional Encoding
Input Embedding

Cosine Similarity (With the Real Ligand)

Ligand Decoder

Softmax
Linear
Decod
Add & Norm
MLPs
Add & Norm
Multi-head Attention
Add & Norm
Masked Multi-head Attention
Positional encoding
Embeddings

Ligand SMILES