# Can KBQA Models Predict Their Reasoning Paths? Isomorphism Prediction Task as a Proxy

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## Abstract

Despite achieving correct answers, we find that existing Knowledge Base Question Answering (KBQA) models struggle to follow the expected reasoning structures. We introduce the task of isomorphism prediction to enhance reasoning fidelity beyond answer generation, with a focus on generalization. We propose a contrastive knowledge co-distillation framework that unifies textual and graphical KBQA paradigms, improving overall isomorphism prediction and model generalization. Furthermore, incorporating isomorphism prediction as an auxiliary task could also improve KBQA performance.

## 1 Introduction and Related Work

The task of question answering over knowledge bases (KBQA) involves reasoning over structured sources of knowledge in the form of knowledge bases (KB) to answer natural language queries. Beyond improved answer accuracy, a key challenge in KBQA lies in understanding how the models perform and ensuring that they faithfully reconstruct the reasoning process. To that end, recent work has leveraged the idea of isomorphisms (Dutt et al., 2023) to characterize the complexity of KBQA questions. Isomorphisms act as a structural proxy for reasoning difficulty by grouping instances that exhibit similar reasoning patterns over the knowledge base. Prior work has explored using isomorphisms as a diagnostic test to investigate the generalization capabilities of KBQA systems. For example, Dutt et al. shows that leveraging gold isomorphisms as inference-time scaffolds improves zero-shot generalization without retraining.

In this work, we introduce the task of **isomorphism prediction** to improve reasoning fidelity in KBQA. Our task formulation is motivated by the observation, that when optimized for answer prediction, KBQA systems are able to generate spurious logical forms that do not conform to the underlying reasoning path but can lead to partial correct answers (Table 3). Furthermore, we observe that predicting the correct isomorphism category is challenging even for large language models (LLMs) (Table 6), highlighting the fact that the task requires models to capture structural dependencies beyond surface-level answer generation. Rather than solely using isomorphisms as a diagnostic tool, we frame them as a learning objective to encourage models to explicitly predict their underlying reasoning structures.

An advantage of this formulation is that it is applicable to both major KBQA paradigms: (i) semantic parsing-based approaches, which translate natural language queries into logical forms (e.g., S-expressions or SPARQL) for execution over the KB (Xie et al., 2022; Ye et al., 2021; Li et al., 2024), and (ii) information retrieval-based approaches, where models directly interact with the knowledge graph to retrieve answers (Das et al., 2022; Dutt et al., 2022; He et al., 2021). Building on this, we also propose a contrastive knowledge co-distillation framework that unifies these two paradigms to enhance isomorphism prediction.

Our experiments show that multitask learning with isomorphism prediction improves both KBQA and isomorphism prediction performance. Additionally, the proposed knowledge co-distillation framework bridges the strengths of both KBQA paradigms and enables better generalization.

## 2 Preliminaries

### 2.1 Isomorphism Prediction

We introduce isomorphism prediction to characterize reasoning paths following the definitions in Dutt et al. (2023). Each subgraph $G_i$ represents the logical structure required to answer a question $Q_i$, where nodes correspond to entities and edges represent relations. Two subgraphs $G_i$ and $G_j$ are considered isomorphic if there exists a bijective

mapping $\psi : V_i \to V_j$ between their node sets and preserves structural adjacency:

$$(m, n) \in E_i \Leftrightarrow (\psi(m), \psi(n)) \in E_j$$

By assigning each subgraph to an isomorphism category $C_i$, we abstract away entity-specific details and focus purely on the structural reasoning pattern used to derive answers. We present the definitions and examples of each isomorphism type in Table 5.

Models are trained using a multi-class classification objective. We assess isomorphism prediction performance with macro F1-scores.

### 2.2 KBQA Tasks

**Text Model: S-expression Generation** Following Xie et al. (2022), the input to the text model consists of the question $Q_i$ and the linearized representation of the subgraph (upper-left in Figure 1). The model generates an S-expression that retrieves the predicted answers when executed on the KB.

**Graph Model: Node Classification** The graph model operates directly on the subgraph $G_i$. It assigns probabilities to all nodes in the subgraph, indicating their likelihood of being answers. Training is optimized with binary cross-entropy.

**KBQA Evaluation Mechanism** We evaluate the aforementioned KBQA tasks with Hits@$K$, where $K$ is the number of gold answers for a given question. This measures the proportion of correct answers in the top-$K$ predictions.

For the text model, since S-expression generation does not produce ranked outputs, we use beam search to generate $N_{beam}$ S-expression candidates, execute them through the KB, rank the executed answers by frequency, and compute Hits@$K$ likewise. Refer to Section A.2 for detailed equations.

## 3 Contrastive Knowledge Co-Distillation for Isomorphism Prediction

Our Contrastive Knowledge Co-Distillation framework (Figure 1) consists of two key objectives: isomorphism prediction augmentation and contrastive representation alignment.

### 3.1 Isomorphism Prediction Augmentation

We employ two parallel encoding pathways. The textual encoder produces a pooled embedding $h_t$ by processing the question along with a linearized subgraph. The graph encoder, implemented as a GNN, directly operates on the structured subgraph and generates a pooled graph-level representation $h_g$. These representations are concatenated as $h_{concat} = [h_t; , h_g]$ and passed through a classifier optimized via cross-entropy loss:

$$\mathcal{L}_{\text{iso}} = -\sum_i \log P(C_i \mid h_{concat}) \quad (1)$$

### 3.2 Contrastive Knowledge Co-Distillation

Unlike traditional one-way knowledge distillation, Contrastive Co-Distillation (Yao et al., 2024; Nourbakhsh et al., 2024) (CoD) fosters bidirectional knowledge transfer between text and graph models by contrastive representation learning and stop gradient operation.

As Tian et al. (2022) suggests, contrastive representation learning captures structural information from the teacher's representation space:

$$l_{\text{cl}}(t, s) = -\log \frac{e^{sim(t,s)/\tau}}{\sum_q \mathbb{1}_{[q \neq t]}\, e^{sim(t,q)/\tau}} \quad (2)$$

, where $t$ and $s$ are teacher and student representations, $q$ indicates other representations from the training data, $sim(.,.)$ is cosine similarity, $\tau$ is temperature.

Based on this, we first define MLP projection heads to map text and graph representations into a shared space: $z_t = \text{MLP}_t(h_t)$ and $z_g = \text{MLP}_t(h_g)$, respectively. The CoD loss is computed as:

$$\mathcal{L}_{\text{CoD}} = \frac{1}{2}\sum_i [l_{\text{cl}}(z_i^{\text{text}}, \hat{z}_i^{\text{graph}}) + l_{\text{cl}}(\hat{z}_i^{\text{text}}, z_i^{graph})] \quad (3)$$

, where $\hat{.}$ is the stop gradient operator (Chen and He, 2021) to set the input variable to a constant.

Putting these together, our final objective jointly performs mutual distillation and model optimization end-to-end through a single loss:

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{iso}} + \mathcal{L}_{\text{CoD}} \quad (4)$$

## 4 Experiments

### 4.1 Dataset

We employ the WebQuestionsSP (WebQSP) dataset (Yih et al., 2016), a popular benchmark in English for KBQA. Specifically, we use the dataset of Xie et al. (2022) where each question is accompanied with (i) a corresponding subgraph of the Freebase knowledge base (Bollacker et al., 2008) where the answer resides, and (ii) a corresponding logical form in the form of S-expressions or

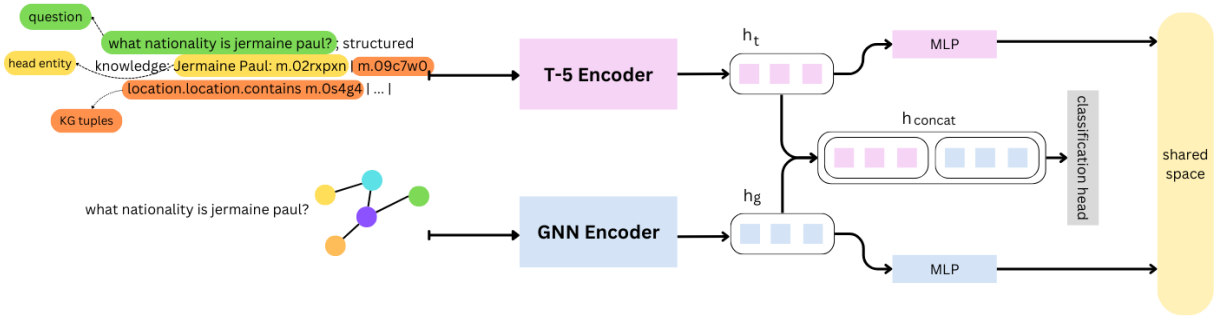


Figure 1: Our contrastive knowledge co-distillation framework. The T5 encoder processes a linearized knowledge subgraph representation, while the GNN directly operates on the KG. Their representations are concatenated for isomorphism classification and projected into a shared space for contrastive co-distillation.

SPARQL-query. Such a design enables us to evaluate the performance of KBQA systems from either a semantic parsing or information retrieval paradigm. Additionally, to investigate different levels of KBQA generalization, we use the approach of Jiang and Usbeck (2022) to obtain a dev or test split with equal proportion of i.i.d., compositional, and zero-shot examples. We present the statistics of our dataset in Table 1.

| Code | Desc. | i.i.d. | Comp | Z.S. | Total |
|---|---|---|---|---|---|
| T-0 | | 50.3 | 0.0 | 49.7 | 54.5 |
| T-1 | | 37.3 | 44.3 | 18.4 | 23.5 |
| T-2 | | 17.1 | 47.1 | 35.7 | 5.2 |
| T-3 | | 83.3 | 6.7 | 10.0 | 2.2 |
| T-4 | | 12.8 | 81.5 | 5.6 | 14.5 |
| ALL | | 40.8 | 24.9 | 34.3 | 100.0 |

Table 1: Distribution of isomorphisms over the generalization splits (i.i.d., compositional (Comp), zero-shot (Z.S.)) of WebQSP.

### 4.2 Models

Our text model is based on T5 (Raffel et al., 2023), while our graph model is built using Relational Graph Convolutional Network (RGCN) layers (Schlichtkrull et al., 2017). To incorporate question context, we first encode the question using T5 and concatenate the resulting embedding with each node before passing through the GNN.

### 4.3 Experiments

We establish T5 and GNN baselines, each trained separately for isomorphism prediction and their respective KBQA tasks defined in Section 2.2. We evaluate our approach under two settings: 1) CoD framework for isomorphism prediction; 2) Multi-task KBQA using isomorphism prediction as an auxiliary task. We report in Section 5 the average performance over three seeds.

Moreover, we show that isomorphism prediction is challenging through two diagnostic experiments.

Firstly, we evaluate several widely-used LLMs on the isomorphism prediction task using few-shot prompting. As shown in Table 6, the models struggle to reliably predict isomorphisms.

Further, we analyze whether optimizing for S-expression generation inherently preserves isomorphism structures. Although isomorphism categories can be deterministically derived from S-expressions, models like T5 are trained to optimize answer accuracy rather than faithfully reconstructing reasoning paths. As a result, they may reach correct answers through spurious reasoning rather than the intended structural pattern. Indeed, isomorphism prediction performance drops by 16% overall when inferred post-hoc from generated S-expressions compared with being explicitly learned in our T5 baseline (Table 3). This highlights the importance of directly modeling isomorphisms beyond relying on answer-driven supervision alone.

## 5 Results and Analysis

**Isomorphism Prediction with CoD** Overall, CoD outperforms both baselines (ALL in Table 2). We further stratify questions along generalization level and isomorphism category.

For generalization, GNN excels in i.i.d. cases but suffers in generalization, while T5 struggles the most in compositional settings. Although CoD performs lower in the i.i.d. setting, it significantly improves generalization, especially in compositional cases. This suggests that our contrastive knowledge co-distillation enables better adaptation rather than

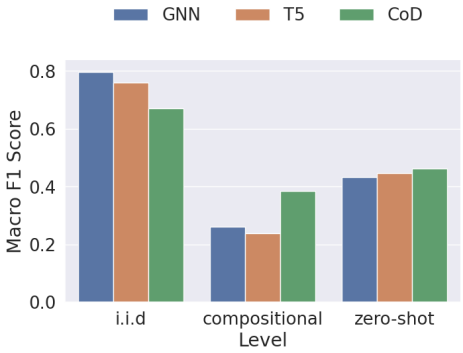


Figure 2: Macro-F1 performance of the models/settings for different generalization levels in WebQSP.

| Code | Desc. | T5 | GNN | CoD |
|---|---|---|---|---|
| T-0 | | **89.1** | 88.8 | 85.9 |
| T-1 | | 60.8 | 58.8 | **68.3** |
| T-2 | | 38.9 | **44.1** | 43.5 |
| T-3 | | 45.7 | 41.1 | **59.7** |
| T-4 | | 50.3 | **59.4** | 51.8 |
| ALL | | 57.0 | 58.4 | **61.9** |

Table 2: Macro-F1 of different settings (T5, GNN, and CoD) over isomorphism categories in WebQSP. ALL refers to the entire dataset. Best performance in bold, second-best underlined.

memorizing dataset biases.

Across isomorphism types, all models perform well in T-0 category (single-hop retrieval). As reasoning complexity increases, different model strengths become more evident. T5 performs well in linear chains (T-0, T-1) but struggles with more complex structures, while GNN is better with graph-structured constraints (T-2, T-4) but limited with sequential dependencies (T-3). Notably, CoD significantly improves on T-1 and T-3 and shows moderate gains in T-2 and T-4, which indicates that the unification brings together the complimentarities of the two models.

**Multitask with KBQA and Isomorphism Prediction** Table 4 shows that incorporating isomorphism prediction improves both KBQA and isomorphism prediction tasks compared to single-task baselines. Our preliminary result shows that isomorphism prediction provides additional structural supervision, which may help models better capture reasoning patterns beyond answer retrieval.

| Code | Desc. | T5 (Sexp) | T5 (Iso Pred) |
|---|---|---|---|
| T-0 | | 82.0 | **89.1** |
| T-1 | | 50.3 | **60.8** |
| T-2 | | 37.3 | **38.9** |
| T-3 | | 35.9 | **45.7** |
| T-4 | | 40.1 | **50.3** |
| ALL | | 40.9 | **57.0** |

Table 3: F1 performance of T5 on isomorphism prediction when inferred from generated S-expressions versus explicitly predicted as a supervised task.

| **Model** | **Task** | **KBQA** | **Iso Pred** |
|---|---|---|---|
| T5 | KBQA only | 50.7 | - |
| | Iso Pred only | - | 59.0 |
| | Multitask | **52.2** | **61.7** |
| GNN | KBQA only | 54.6 | - |
| | Iso Pred only | - | 59.4 |
| | Multitask | **55.3** | **64.0** |

Table 4: Comparison of the respective task baselines and the multitask setting using isomorphism prediction as an auxiliary task.

## 6 Conclusion

We introduce isomorphism prediction task to enhance reasoning fidelity in KBQA. Our contrastive knowledge co-distillation framework improves isomorphism prediction and generalization, particularly in compositional and zero-shot settings. Additionally, isomorphism prediction as an auxiliary task improves KBQA performance, suggesting structural reasoning signals could aid answer generation. Future work can explore broader model architectures and datasets.

## 7 Limitations

**Model Scope** We focus on T5 and GNN-based models; future work could extend to larger LLMs and alternative graph reasoning frameworks.

**Dataset Diversity** Our experiments use WebQSP. Future work could extend evaluations to benchmarks with more diverse KG schemas.

**Explicit Isomorphism Learning** Future work could explore unsupervised learning to infer reasoning structures without predefined labels.

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# A Appendix

## A.1 Isomorphism Examples

See Table 5.

## A.2 Hits@K Computations

Let $A_i$ be the gold answer set for a given question. The graph model ranks all nodes in the subgraph by predicted probabilities. Given a ranked list $\hat{A}_i$, for some $\varepsilon > 0$, Hits@$K_{\text{graph}}$ is computed as:

$$Hits@K_{\text{graph}} = \frac{|TopK(\hat{A}_i) \cap A_i|}{K + \varepsilon} \quad (5)$$

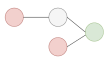
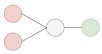
| Iso-Type | Illustration | Definition | Example Question | S-expression |
|---|---|---|---|---|
| T-0 |  | Direct 1-hop connection from constraint to answer | What is the name of money in Brazil? | (JOIN (R location.country.currency_used) m.015fr) |
| T-1 |  | 2-hop linear path | Where does the Queen of Denmark live? | (JOIN (R people.place_lived.location) (JOIN (R people.person.places_lived) m.0g2kv)) |
| T-2 |  | V-pattern with two constraints meeting at a shared node | What was Elie Wiesel's father's name? | (AND (JOIN people.person.gender m.05zppz) (JOIN (R people.person.parents) m.02vsp)) |
| T-3 |  | A chain pattern connecting constraints serially | Where did Joe Namath attend college? | (AND (JOIN common.topic.notable_types m.01y2hnl) (JOIN (R education.education.institution) (JOIN (R people.person.education) m.01p_3k))) |
| T-4 |  | Y-pattern with merging constraints | Who does Zach Galifianakis play in The Hangover? | (JOIN (R film.performance.character) (AND (JOIN film.performance.film m.0n3xxpd) (JOIN (R film.actor.film) m.02_0d2))) |

Table 5: Isomorphism types with their corresponding definitions, example questions, and S-expressions.

Unlike the graph model, the text model does not inherently rank its predictions. To approximate a ranking mechanism, we employ beam search to generate $N_{\text{beam}}$ candidate S-expressions $S_{i,j}, j = 1, ..., N_{\text{beam}}$. We then execute these S-expressions through KB to obtain a predicted answer set $P_i$, and aggregate $P_{i,j}$ by their frequency across all beams. Using this ranked set, for some $\varepsilon > 0$, Hits@$K_{\text{text}}$ is computed as:

$$Hits@K_{\text{text}} = \frac{|TopK(Rank(\cup^{N_{\text{beam}}} P_i)) \cap A_i|}{K + \varepsilon} \tag{6}$$

where $Rank(\cup^{N_{\text{beam}}} P_i)$ refers to the aggregated ranking of answer candidates obtained from executing $S_i$ through KB.

### A.3 Few-shot LLM on Isomorphism Prediction

We evaluate a couple of widely-used LLMs on the isomorphism prediction task with few-shot prompting, including GPT-3.5-turbo and GPT-4o-mini. As shown in Table 6, these models struggle to reliable predict isomorphisms even with multiple examples per type of isomorphism. We try $k$-shot prompting with $k = 1, 3$, where we include $k$ examples of each isomorphism type (T-0 to T-4), selected randomly from the training split. The exact prompts used can be found in Appendix A.4.

We experiment with not only the number of few-shot examples provided to the model, but also the technique used to serialize the knowledge graph tuples into a text format as well as the level of detail in the prompt about descriptions of particular isomorphisms. For serializing the knowledge graph tuples of the form (entity$_1$, rel, entity$_2$) we try:

1. **Basic serialization:** where we simply concatenate the knowledge graph tuples using whitespace, for example "entity$_1$ rel entity$_2$".

2. **Descriptive serialization:** where we concatenate each individual tuple with slightly more description, for example "entity$_1$ is connected to entity$_2$ via relation rel".

We try two levels of isomorphism description detail in our prompt. In the first setting, Prompt 1 (Appendix A.4.1), we provide a brief textual description of each of the isomorphisms' structural characteristics. Whereas in Prompt 2 (Appendix A.4.2), we do not provide any description whatsoever of individual isomorphism categories. The LLMs' final answers are extracted using a regex expression to match the last occurrence of the pattern "T-X", which indicates the model's isomorphism prediction. These predictions are then evaluated using a standard macro F-1 score. These scores, across all experiments, are shown in Table 6. We find that even with few-shot examples, and across all our prompting methods described above, the best performance achieved is a mean macro F-1 of 0.15 by the gpt-3.5-turbo model when given 3 examples per isomorphism class, basic serialized tuples and brief descriptions of isomorphisms' structure.

### A.4 Few-shot LLM Prompt

Below are the two versions of prompts we experimented with. Prompt 1 contains brief structural descriptions of each isomorphism category, whereas

| Model Configuration | Macro F1 |
|---|---|
| **GPT-3.5-turbo** | |
| k=1 (base) | 0.09220 |
| k=1 (descriptive tuples) | 0.14062 |
| k=1 (descriptive tuples, no iso. desc. in prompt) | 0.14118 |
| k=3 (base) | **0.15474** |
| **GPT-4o-mini** | |
| k=1 (base) | 0.10530 |
| k=3 (base) | 0.10273 |
| k=3 (descriptive tuples) | 0.14423 |
| k=3 (descriptive tuples, no iso. desc. in prompt) | 0.11832 |
| k=5 (base) | 0.07076 |
| k=5 (descriptive tuples) | 0.12022 |
| k=5 (descriptive tuples, no iso. desc. in prompt) | 0.09122 |

Table 6: Isomorphism prediction performance of GPT-3.5-turbo and GPT-4o-mini using few-shot prompting. The base configuration refers to when we serialize in a basic manner and provide brief isomorphism descriptions in the prompt.

Prompt 2 simply instructs the model to identify the isomorphism based on the examples provided.

#### A.4.1 Prompt 1: Structural Descriptions

**System prompt:** "You are a helpful assistant that identifies isomorphism patterns in knowledge graphs."

**User prompt:** "Given a question, its entities, and knowledge graph tuples, determine the isomorphism pattern that shows how constraints connect to reach the answer node. In this classification: T-0 means a direct 1-hop connection from constraint to answer, T-1 is a 2-hop linear path, T-2 is a V-pattern with two constraints meeting at a shared node, T-3 is a chain pattern connecting constraints serially, T-4 is a Y-pattern with merging constraints, and T-5+ involve more complex multi-hop patterns. Analyze the structure by tracing the paths from constraints to the answer, counting hops and noting how paths merge or branch. Respond with "Isomorphism: T-X" where X is the pattern number (0-4), output only the final answer. Find some examples below:

{ Question: ...
Entities: (example serialized entities)
Serialized tuples from knowledge graph: (example serialized knowledge graph tuples)
Isomorphism: T-X } (k examples for each type of isomorphism)

###
Question: (target question)
Entities: (target serialized entities)
Serialized tuples from knowledge graph: (target serialized knowledge graph tuples)
Isomorphism:"

#### A.4.2 Prompt 2: Non-descriptive instructions

**System prompt:** "You are a helpful assistant that identifies isomorphism patterns in knowledge graphs."

**User prompt:** "Given a question, its entities, and knowledge graph tuples, determine the isomorphism pattern that shows how constraints connect to reach the answer node. Analyze the structure by tracing the paths from constraints to the answer, counting hops and noting how paths merge or branch. Respond with "Isomorphism: T-X" where X is the pattern number (0-4), output only the final answer. Find some examples below:

{ Question: ...
Entities: (example serialized entities)
Serialized tuples from knowledge graph: (example serialized knowledge graph tuples)
Isomorphism: T-X } (k examples for each type of isomorphism)

###
Question: (target question)
Entities: (target serialized entities)
Serialized tuples from knowledge graph: (target serialized knowledge graph tuples)
Isomorphism:"

### A.5 Hyperparameter Settings

On average, our total experiments take around 15 GPU hours.

#### A.5.1 Experiments on Isomorphism Prediction with CoD

We use the following hyperparameters to obtain results in Table 2.

| Model | Batch | Dropout | Others |
|---|---|---|---|
| T5 | 8 | 0.2 | - |
| GNN | 10 | 0.2 | - |
| CoD | 6 | 0.3 | Weight Decay: 1e-3<br>Shared Space Dim: 2048 |
| Input Max Length: 512, Patience: 5, LR: 5e-5 | | | |

Table 7: Hyperparameters used for experiments in Table 2. Results are averaged over three seeds.

### A.5.2 Experiments on Multitask with KBQA and Isomorphism Prediction

We use the following hyperparameters to obtain results in Table 4.

| Model | Batch | Dropout | Others |
|---|---|---|---|
| T5 Baseline | 10 | - | Generation Max Len: 128 |
| GNN Baseline | 6 | 0.2 | - |
| T5 Multitask | 10 | 0.3 | Weight Decay: 1e-3<br>Generation Max Len: 128 |
| GNN Multitask | 4 | 0.2 | - |
| Input Max Length: 512, Patience: 5, LR: 5e-5 | | | |

Table 8: Hyperparameters used for KBQA and multitask experiments in Table 4. Results are averaged over three seeds.

## A.6 System Specifications

See Table 9.

| Component | Specification |
|---|---|
| GPU | NVIDIA A100 80GB PCIe |
| CPU | AMD EPYC 7763 (256 vCPUs) |
| RAM | 1TB |
| CUDA Version | 12.6 |
| GPU Memory | 80GB |

Table 9: Hardware specifications of the computational resources used for experiments.

## A.7 Potential Risks and Considerations

Our work builds on WebQSP and Freebase, which may inherit biases from their original data collection. While our focus is on structural reasoning rather than entity-specific biases, these biases could still affect model behavior. Additionally, although we do not train large models from scratch, prompting LLMs, fine-tuning T-5, and training GNN still lead to computational costs, contributing to the environmental footprint.