

KBQA-R1: Reinforcing Large Language Models for Knowledge Base Question Answering

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Abstract—Knowledge Base Question Answering (KBQA) challenges models to bridge the gap between natural language and strict knowledge graph schemas by generating executable logical forms. While Large Language Models (LLMs) have advanced this field, current approaches often struggle with a dichotomy of failure: they either generate hallucinated queries without verifying schema existence or exhibit rigid, template-based reasoning that mimics synthesized traces without true comprehension of the environment. To address these limitations, we present KBQA-R1, a framework that shifts the paradigm from text imitation to interaction optimization via Reinforcement Learning. Treating KBQA as a multi-turn decision process, our model learns to navigate the knowledge base using a list of actions, leveraging Group Relative Policy Optimization (GRPO) to refine its strategies based on concrete execution feedback rather than static supervision. Furthermore, we introduce Referenced Rejection Sampling (RRS), a data synthesis method that resolves cold-start challenges by strictly aligning reasoning traces with ground-truth action sequences. Extensive experiments on WebQSP, GrailQA, and GraphQuestions demonstrate that KBQA-R1 achieves state-of-the-art performance, effectively grounding LLM reasoning in verifiable execution.

Index Terms—Knowledge Base Question Answering, Large Language Models, Reinforcement Learning, ReAct

I. INTRODUCTION

Knowledge Base Question Answering (KBQA) aims to answer natural language questions by retrieving facts from large-scale Knowledge Bases (KBs) such as Freebase and Wikidata. Unlike Retrieval-Augmented Generation (RAG), which augments Large Language Models (LLMs) with unstructured text snippets, KBQA requires the model to generate executable logical forms (e.g., SPARQL or S-Expressions) that precisely navigate the KB’s schema. This task is particularly challenging: the model must not only comprehend natural language semantics but also master the strict relational schema and query syntax to perform multi-hop reasoning without error.

Despite significant progress in applying LLMs to KBQA, existing methodologies can be categorized into three paradigms, each with distinct limitations. The first category comprises End-to-end Approaches (e.g., KB-BINDER [1], KB-Coder [2], ChatKBQA [3]), which generate entire logical forms in a single pass. While computationally efficient, these

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methods operate without intermediate KB interaction, making them unable to verify the existence of schema elements during generation. This often leads to *schema hallucinations*—syntactically valid but semantically incorrect queries that reference non-existent relations or entities. The second category, Prompting-based Step-by-Step Approaches [4], [5], leverages powerful commercial model APIs with few-shot in-context learning to decompose complex queries into sequential reasoning steps. While these methods benefit from the strong reasoning capabilities of large-scale models, they lack task-specific training, resulting in suboptimal performance on domain-specific schema navigation and complex multi-hop queries. The third category, Supervised Agent Approaches [6], mitigates the above issues by fine-tuning models on reasoning traces synthesized from templates or heuristics. However, this paradigm risks *superficial reasoning*: since the training data is inherently formulaic, the model’s “thoughts” often reduce to **template-driven action announcements** (e.g., “At this step, we should find the relation...”) rather than genuine analysis of environmental feedback. The model declares *what* action to take without explaining *why*—it neither interprets the KB observations nor justifies its choices based on the question semantics. Such rigid patterns, while achieving local consistency, fail to generalize when novel schema structures or unexpected query patterns arise.

To address these limitations, we present **KBQA-R1**, an action-centric reinforcement learning framework that shifts the paradigm from text imitation to *interaction optimization*. Instead of generating raw query code, KBQA-R1 operates within a well-defined action space, treating KBQA as a multi-turn Markov Decision Process (MDP). At each step, the model selects an action (e.g., `Find_Relation`, `Merge`), observes concrete feedback from the KB execution engine, and dynamically adjusts its reasoning trajectory. Crucially, because the policy is optimized via **Group Relative Policy Optimization (GRPO)** [7] with outcome-based rewards rather than imitation loss, the model is incentivized to develop *adaptive reasoning*—genuinely analyzing observations and justifying action choices—rather than memorizing fixed reasoning templates. This closed-loop interaction grounds decisions in verifiable outcomes and enables the model to discover effective reasoning strategies through environmental exploration.

To bootstrap this process and address the “cold start” problem inherent in RL, we propose **Referenced Rejection Sampling (RRS)** for SFT (Supervised Fine-Tuning) data synthesis. Compared to standard rejection sampling, which draws trajectories from raw prompts and accepts only those that

accidentally reach the correct answer, KBQA is a particularly challenging setting: the model must generate syntactically valid S-Expressions, choose schema-consistent relations, and navigate multi-hop paths in a large KB. In this regime, the zero-shot success rate of unconstrained LLM sampling is very low, so naive rejection sampling would produce very few usable trajectories even with a large sampling budget. RRS alleviates this by conditioning generation on a *reference sequence of ground-truth actions* extracted from the gold S-Expression, and asking the model to reconstruct a coherent reasoning trace around these actions. This simple constraint dramatically increases the acceptance rate while still forcing the model to explain *why* each reference action leads toward the answer. As a result, the synthesized SFT data contains trajectories whose “thought” process is tightly aligned with verifiable execution steps, helping KBQA-R1 learn robust, KB-grounded reasoning rather than relying on brittle, hallucinated logic.

Our main contributions are summarized as follows:

- We propose **KBQA-R1**, a multi-turn reinforcement learning framework that grounds LLM reasoning in verifiable KB actions, enabling closed-loop interaction with the knowledge base.
- We introduce **Referenced Rejection Sampling (RRS)**, a novel data synthesis strategy that aligns reasoning traces with ground-truth action sequences, effectively preventing hallucinated logic.
- We conduct extensive experiments on WebQSP, GrailQA, and GraphQuestions, demonstrating that KBQA-R1 achieves state-of-the-art performance, significantly outperforming both end-to-end and agent-based baselines.

II. RELATED WORK

Knowledge Base Question Answering (KBQA). Before the rise of LLMs, KBQA studies are commonly categorized into information-retrieval-based (IR-based) methods [8]–[12] and semantic-parsing-based (SP-based) methods [13]–[16]. With LLMs, three paradigms have emerged: (i) *end-to-end approaches* that directly generate logical forms via in-context learning or fine-tuning [1]–[3], [17]; (ii) *step-by-step (agentic) approaches* that interleave reasoning with graph exploration and tool use [4], [5], [18]–[22]; and (iii) *search-augmented approaches* that leverage tree search algorithms such as Monte Carlo Tree Search (MCTS) for systematic exploration [6].

While MCTS-based methods like KBQA-o1 [6] achieve strong performance through heuristic exploration, they exhibit two key limitations. **First, they incur significant computational overhead from multiple rollouts per query and require separate policy and reward models during inference. Second, their reasoning traces are often template-driven** (e.g., “At this step, we should find the relation...”) rather than genuinely analytical—the model announces *what* action to take without explaining *why* based on observations. In contrast, we train a single policy via RL with outcome-based rewards, encouraging the model to develop *adaptive reasoning* that analyzes environmental feedback and justifies action choices, while eliminating test-time search overhead.

LLMs, tool use, and agentic reasoning. Chain-of-Thought (CoT) prompting improves reasoning by eliciting intermediate steps [23]; ReAct [24] interleaves “think” and “act” to ground reasoning in environment feedback; and heuristic search has been applied to agent traces (e.g., MCTS-style selection in [25] and tree-structured deliberation in [26]). Recent graph-augmented approaches such as Plan-on-Graph [21] incorporate self-correcting mechanisms with dynamic memory for adaptive planning on knowledge graphs. While these methods expand the search space or stabilize multi-step reasoning, free-form thoughts can overfit prompt templates and do not guarantee executability. We keep the interleaved think-act design but require typed, schema-aware actions with validators and an executor, turning traces into verifiable computations rather than narrative justifications.

Retrieval-augmented generation and search-as-a-tool. Classical RAG pipelines retrieve text snippets and feed them to the model for generation [27]. Recent work moves toward search-as-a-tool, prompting or training LLMs to issue search calls and iterate [24], [28]–[31]. GraphRAG approaches [32], [33] further integrate graph retrieval with LLM reasoning, enabling tighter coupling between structured knowledge and text-based evidence. These approaches reduce hallucination but depend heavily on retrieval quality and, in supervised variants, on labeled trajectories. Our setting differs fundamentally by treating a *knowledge graph* as the environment: actions are typed and executable against the KB schema, observations are structure-grounded entity sets rather than text passages, and step-wise executability can be validated programmatically rather than inferred from unstructured documents.

III. PRELIMINARIES

Knowledge Base and Executor. We consider a knowledge base (KB) as a directed multi-relational graph $\mathcal{K} = (\mathcal{E}, \mathcal{R}, \mathcal{F})$, where \mathcal{E} is the set of entities, \mathcal{R} is the set of relations, and \mathcal{F} is the set of factual triples. Each triple $f \in \mathcal{F}$ has the form (h, r, t) with head entity $h \in \mathcal{E}$, relation $r \in \mathcal{R}$, and tail entity $t \in \mathcal{E}$. An executor \mathcal{E} (e.g., a SPARQL endpoint) takes a structured query over \mathcal{K} and returns an answer set, which serves as the environment feedback in our framework.

KBQA Task. Given a natural language question q , the KB \mathcal{K} , and a set of topic entities $E_q \subseteq \mathcal{E}$ mentioned in q , the goal of Knowledge Base Question Answering (KBQA) is to produce an answer set $\mathcal{A}_q \subseteq \mathcal{E}$ that correctly responds to the question. Following prior work [6], we assume that entity mentions in q are already linked to the KB and the corresponding topic entities E_q are given as input. In classic semantic-parsing based KBQA, this task is realized by generating a logical form (e.g., SPARQL or S-Expression) in one shot and executing it against the KB. In contrast, our framework rephrases the task as learning a multi-step interaction policy.

Agentic KBQA as Sequential Decision Making. In our framework, we view the large language model as a stochastic policy π_θ that interacts with the KB environment via a compact, validated action space. At each step t , the agent observes a context c_t summarizing the dialogue history, including prior reasoning (<think> blocks), actions (<action> blocks),

and tool feedback (<information> blocks). Conditioned on c_t and the original question q , the policy samples an action a_t :

$$a_t \sim \pi_\theta(\cdot | q, c_t).$$

The action a_t is grounded into an S-Expression fragment and executed by the executor \mathcal{E} over \mathcal{K} , yielding an observation o_t (e.g., retrieved entities or diagnostic messages). The triple (c_t, a_t, o_t) is appended to the trajectory, and the context is updated accordingly. This interactive loop continues until the agent outputs a final answer \hat{A}_q or a maximum number of steps T is reached. We denote a complete trajectory by $\tau = \{(c_1, a_1, o_1), \dots, (c_T, a_T, o_T)\}$.

Policy Optimization Objective. Our goal is to learn a policy that produces trajectories leading to correct answers. The action a_t is grounded into an S-Expression fragment [15], [34] and executed by the executor over \mathcal{K} . Let $R(\tau)$ denote the cumulative reward of a trajectory. From the reinforcement learning perspective, we optimize the expected return:

$$J(\theta) = \mathbb{E}_{\tau \sim \pi_\theta} \left[\sum_{t=1}^T r_t \right], \quad r_t = r_{\text{outcome}} + r_{\text{format}}, \quad (1)$$

where r_{outcome} reflects answer correctness and r_{format} rewards valid S-Expression structure. Unlike methods [6] that require test-time search (e.g., MCTS), our approach trains a single policy end-to-end that directly generates high-quality trajectories at inference time without additional search overhead.

IV. METHOD: THE KBQA-R1 FRAMEWORK

A. Prompt and System Workflow

Our system is a multi-turn agent system inspired by the ReAct paradigm [24]. At each turn, the LLM emits one or more actions to interact with the KB environment, and the environment returns the corresponding observations. After multiple turns of KB exploration, the model outputs the final answer.

1) *Prompting Template for Action-Based Reasoning:* Table I shows the prompting template used to elicit action-based reasoning from the LLM. The template structures the model’s output into three parts in an iterative fashion: first, a reasoning process (<think>...</think>), similar to Chain-of-Thought prompting [23], then a Knowledge Graph exploration action (<action>...</action>), e.g., `Find_relation`, `Merge`), and finally the answer (<answer>...</answer>). Crucially, we only impose structural constraints on the output format, not on the reasoning content. This design choice ensures that the model learns to reason *adaptively* through RL, rather than mimicking template-driven patterns as in prior work [6].

2) *Action Space:* Prior semantic parsing approaches to KBQA [3], [13], [15] typically require the model to emit a full, nested S-expression in a single pass. This design is notoriously brittle: a single token-level error (e.g., a typo in a relation name or a mismatched parenthesis) can render the entire program unexecutable and cause the query to fail.

Following the recent KBQA-o1 framework [6], we instead adopt a compact, discrete action space that decomposes logical-form construction into a sequence of simple,

verifiable steps. Concretely, each action corresponds to an atomic operation over the evolving logical expression, such as extending from an entity along a relation (`Find_relation`), intersecting two partial expressions (`Merge`), or applying aggregation and comparison operators (`Order`, `Compare`, `Count`, `Time_constraint`). As summarized in Table II, every action is defined by (i) its arguments, (ii) a target functional update on the current expression (e.g., `JOIN`, `AND`, `ARG`, `CMP`, `TC`, `COUNT`), and (iii) the corresponding S-expression template.

Operationally, the agent does not generate the complete program at once. Instead, starting from candidate entities detected in the question, it emits one or more actions at each turn, observes the execution results against the KB, and then decides the next action based on this feedback. This interleaved generation–execution process, inherited from related iterative retrieval methods [28], [35], improves robustness in two ways: the environment can validate and correct individual actions (e.g., via schema-aware relation retrieval), and errors are localized to specific steps rather than invalidating the entire program.

Actions are converted into an S-Expression list, then translated into SPARQL queries [36] executed against the KB. The resulting observations are appended to the dialogue state visible to the model. This workflow mitigates the fragility of string-based S-expression program generation and lowers the error rate in actions produced by the LLM.

3) *Relation Retrieval and Confidence Gating:* LLM-proposed relations can be noisy or ambiguous due to the well-known hallucination problem [37]. To mitigate this, we introduce the **Relation Retrieval and Confidence Gating** (RRCG) module. The RRCG module acts as a validation layer, verifying the agent’s proposed textual relation before execution.

Let r_{agent} be the original textual relation proposed by the agent for the current entity e_c . Let $R(e_c)$ be the set of all neighboring schema relations of e_c in the knowledge base. The core of the RRCG module is a similarity function $\text{Sim}(\cdot, \cdot)$, implemented using dense retrieval techniques [38], [39], which scores r_{agent} against every schema relation $r_s \in R(e_c)$. We define $s_{\max} = \max_{r_s \in R(e_c)} \text{Sim}(r_{\text{agent}}, r_s)$ as the highest similarity score, with $r_s^* = \arg \max_{r_s \in R(e_c)} \text{Sim}(r_{\text{agent}}, r_s)$ being the best-matching schema relation.

Based on s_{\max} and predefined thresholds τ_{high} and τ_{low} (where $\tau_{\text{high}} > \tau_{\text{low}}$), the action is categorized into one of three confidence tiers:

- **Auto-Validation (High Confidence):** If $s_{\max} \geq \tau_{\text{high}}$, it indicates a reliable match between r_{agent} and r_s^* . The action is **auto-validated**. The system executes the action using r_s^* as the replacement for r_{agent} .
- **Tentative Acceptance (Medium Confidence):** If $\tau_{\text{low}} \leq s_{\max} < \tau_{\text{high}}$, r_s^* is considered a plausible but uncertain match. The action is **tentatively accepted**. To signal this ambiguity, the returned observation is annotated with *uncertainty cues*, such as the top- k candidate set $C_k = \{(r_s, \text{Sim}(r_{\text{agent}}, r_s))\}_{\text{top-}k}$, encouraging the agent to verify or issue corrective feedback in subsequent turns.

You are an expert assistant for querying the Freebase knowledge base using structured reasoning actions.

Answer the given question about Freebase knowledge base.

You MUST conduct reasoning inside `<think>...</think>` before emitting actions.

After reasoning, provide structured actions inside `<action>...</action>`.

The system will return query results between `<information>...</information>`.

When ready, return the final answer inside `<answer>...</answer>` using MIDs or literal values. For multiple answers, separate by spaces.

Available Actions : {Candidate Actions List}

Begin from the candidate entities detected in the question.

Candidate Entities: [{CANDIDATE_ENTITIES}]

Question: {QUESTION}.

TABLE I: Action-based reasoning prompt template for KBQA-R1. Placeholders {Candidate Actions List}, {CANDIDATE_ENTITIES}, and {QUESTION} are dynamically populated per instance.

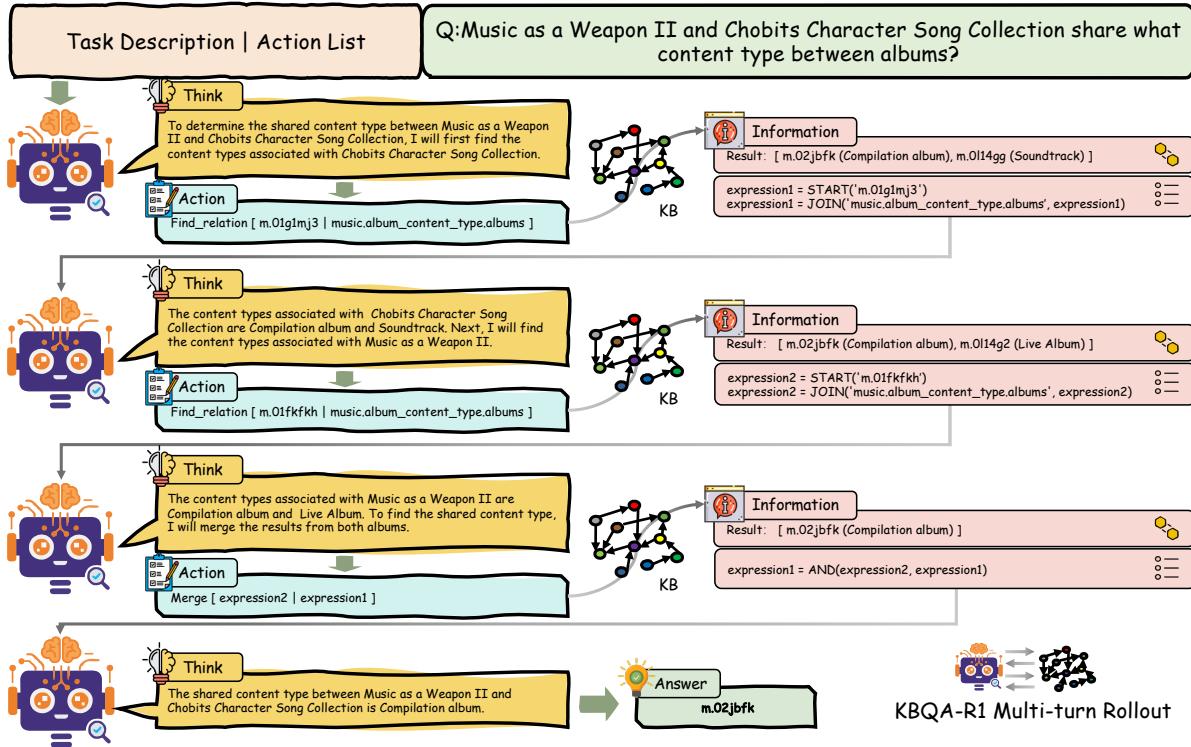


Fig. 1: Overview of the KBQA-R1 multi-turn reasoning framework. Given a natural language question, the LLM-based agent iteratively executes a *Think-Action-Information* loop: it first reasons about the current state, selects an atomic action (e.g., `Find_relation`, `Merge`), and receives grounded feedback from the knowledge base. The Relation Retrieval and Confidence Gating (RRCG) module validates each proposed relation against the KB schema, ensuring action validity. This process continues until the agent produces the final S-Expression and answer.

- Rejection (Low Confidence):** If $s_{\max} < \tau_{\text{low}}$, r_{agent} cannot be mapped to any reliable schema relation, as even the best-matching r_s^* is unreliable. The action is **marked as invalid**. The observation returned is a diagnostic message, such as the complete list of neighboring relations and their scores $L = \{(r_s, \text{Sim}(r_{\text{agent}}, r_s)) | r_s \in R(e_c)\}$. This steers the policy away from this low-confidence branch and prompts it to make a new selection.

B. Rejection Sampling and Supervised Fine-Tuning Warm-Start

To effectively warm-start the policy before RL and resolve the “cold start” problem, we propose Referenced Rejection

Sampling (RRS), a data synthesis strategy that grounds the model’s reasoning in verifiable execution steps. In practice, we run RRS with a stronger instruction-following backbone (Qwen-2.5-72B-Instruct) to obtain high-quality trajectories, and then distill these trajectories into our Llama-3.1-8B-Instruct policy via supervised fine-tuning. RRS conditions the generation process on a sequence of ground-truth actions derived from the gold logical form, and tasks the model with reconstructing the corresponding reasoning trace.

The key insight behind RRS is that successful KBQA trajectories must align with executable action sequences. Standard rejection sampling [40] from raw prompts suffers from very

Action	Arguments	Target Function	Equivalent Logical Form
Find_relation	entity relation	expression = JOIN('relation', START(entity))	(JOIN relation entity)
Merge	expression1 expression	expression = AND(expression1, expression)	(AND (expression1) (expression))
Order	MAX/MIN expression relation	expression = ARG('mode', expression, 'relation')	(mode (expression) relation)
Compare	le/lt/ge/gt relation number	expression = CMP('mode', 'relation', number, expression)	(mode relation number (expression))
Time_constraint	relation time	expression = TC(expression, 'relation', 'time')	(TC (expression) relation time)
Count	expression	expression = COUNT(expression)	(COUNT (expression))

TABLE II: Action space of KBQA-R1.

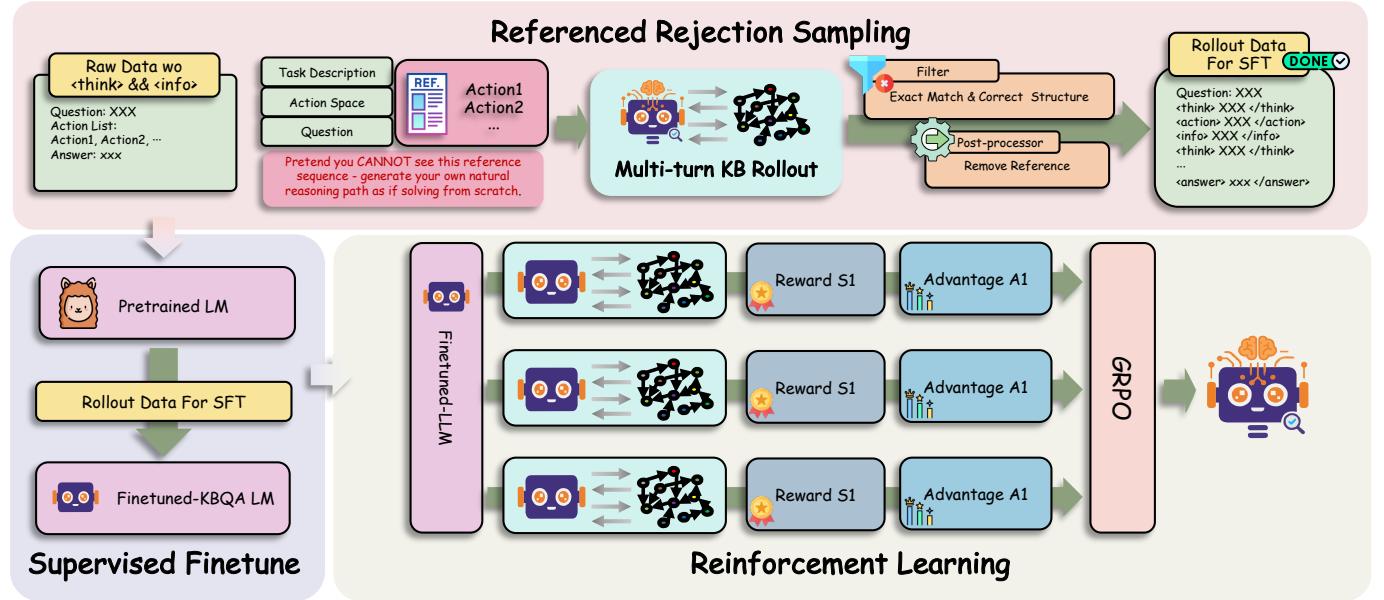


Fig. 2: The two-stage training pipeline of KBQA-R1. **Stage 1 (Referenced Rejection Sampling):** Raw training data is augmented with reference action sequences derived from gold S-Expressions. The LLM generates reasoning trajectories conditioned on these references, which are then filtered by execution correctness and post-processed to remove reference hints, yielding high-quality SFT data. **Stage 2 (Reinforcement Learning):** The SFT-initialized policy performs multi-turn KB rollouts, receiving outcome-based rewards. Group Relative Policy Optimization (GRPO) computes per-group advantages and updates the policy to maximize expected rewards while maintaining proximity to the reference distribution.

low acceptance rates due to the task complexity and the base LLM’s weak zero-shot ability on structured KB queries. Simply increasing sampling temperature or budget yields diminishing returns, as most generated trajectories contain hallucinated relations or malformed S-Expressions.

RRS addresses this by providing the model with a *reference action sequence*—extracted from the gold S-Expression—as implicit guidance during generation. This approach is inspired by rationalization techniques in STaR [41], where hints are provided when the model fails, but we extend it to agentic settings with environmental interaction. This constraint forces the model to: **① Ground reasoning in execution:** The model must justify *why* each reference action leads toward the correct answer, rather than fabricating post-hoc explanations. **② Learn action-observation correspondence:** By observing the actual KB feedback for each ground-truth action, the model internalizes the mapping between actions and their environmental consequences.

1) *RRS Pipeline:* Given a training example (q, \mathcal{A}, S^*) where q is the question, \mathcal{A} is the gold answer set, and S^* is the gold S-Expression, the RRS pipeline proceeds as follows:

Step 1: Action Extraction. Parse S^* to extract the ground-

truth action sequence $\mathbf{a}^* = (a_1^*, a_2^*, \dots, a_k^*)$, where each a_i^* corresponds to an atomic operation (e.g., Find_relation, Merge).

Step 2: Referenced Rollout. Execute a rollout where the model generates reasoning traces ($<\text{think}>$) conditioned on observing the reference actions. At each step t , the prompt includes the next ground-truth action a_t^* as a reference.

Step 3: Trajectory Filtering. Accept trajectories that (a) successfully reach the correct answer with $F1(\hat{\mathcal{A}}, \mathcal{A}) \geq \tau$, and (b) maintain correct structure format of the tags.

Step 4: Reference Stripping. Before adding accepted trajectories to the SFT dataset, we strip all reference hints from the prompts. This ensures the model learns to reason independently at inference time.

The resulting SFT dataset S_{RRS} contains high-quality trajectories where each reasoning step is grounded in verifiable KB interactions. This approach achieves significantly higher acceptance rates compared to raw rejection sampling while producing more robust reasoning patterns.

2) *SFT Training:* The SFT process fine-tunes the base LLM on S_{RRS} . Following best practices in instruction tuning [42], we compute the loss *only* on assistant-visible tokens (i.e.,

<think> reasoning and <action> blocks); tool messages (<information> segments) are masked from the loss and serve only as context. This selective masking ensures the model learns to generate actions and reasoning, not to memorize environmental feedback. The resulting SFT checkpoint initializes the policy for subsequent GRPO optimization.

C. Reinforcement Learning Optimization

The policy is further refined via Reinforcement Learning [43], optimizing a composite reward signal using our GRPO algorithm [7].

1) *Reward Formulation*: We define a composite reward R to guide the policy, composed of three main components: an outcome reward (r_{outcome}), a format reward (r_{format}). The primary component is the outcome reward (r_{outcome}), which measures the factual accuracy of the final answer. To make this signal robust against annotation variations, it is calculated as the $F1$ score between the predicted answers $\hat{\mathcal{A}}$ and all available gold answer variants \mathcal{A} for a given prompt. The second component is the format reward (r_{format}). This provides a bonus based on desirable structural properties, such as tag completeness and correct tag order. Crucially, this reward is applied *only when the outcome reward is positive* ($r_{\text{outcome}} > 0$), ensuring the agent is not rewarded for good syntax when the answer is completely wrong.

The total reward R for a trajectory is the weighted sum of these components, where $\mathbb{I}[\cdot]$ is the indicator function:

$$R = \lambda_{\text{outcome}} \cdot r_{\text{outcome}} + \lambda_{\text{format}} \cdot \mathbb{I}[r_{\text{outcome}} > 0] \cdot r_{\text{format}} \quad (2)$$

2) *Policy Optimization (GRPO)*: We optimize the policy π_θ using Grouped-Reward Policy Optimization (GRPO) [7], a PPO [44] variant that leverages a low-variance, per-prompt advantage estimation without requiring a learned value function. The overall objective maximizes the expected advantage, regularized by a KL-divergence term against a frozen reference policy π_{ref} to ensure training stability [42]:

$$\max_{\theta} \mathbb{E}_{s_t, a_t \sim \pi_\theta} [\hat{A}_t \log \pi_\theta(a_t | s_t)] - \beta \text{KL}(\pi_\theta(\cdot | s_t) \| \pi_{\text{ref}}(\cdot | s_t)) \quad (3)$$

where β controls the KL penalty strength.

The key feature of GRPO is its definition of the advantage function \hat{A}_t . For a given prompt x , we execute n rollouts with the current policy π_θ to generate n candidate trajectories $\{y_i\}_{i=1}^n$ and their corresponding scalar rewards $\{r_i\}_{i=1}^n$. Instead of using a learned value function (as in standard actor-critic methods [45]), GRPO computes the advantage by centering the rewards within this group, using the group's mean reward as a baseline:

$$\hat{A}_i = r_i - \frac{1}{n} \sum_{j=1}^n r_j \quad (4)$$

This per-prompt baseline significantly reduces reward variance, a technique that echoes the REINFORCE with baseline approach [46]. The final loss function integrates this advantage estimate, \hat{A}_i , with standard PPO mechanisms like value loss (if used) and clipping for robust optimization. Rollouts are efficiently executed using vLLM [47] with top-p/temperature sampling, and throughput is maximized via dynamic batching.

V. EXPERIMENTS

A. Experimental Setup

1) *Datasets*: We conduct experiments on three widely-used KBQA benchmarks, each designed to evaluate different aspects of model generalization and reasoning capabilities. All datasets are grounded on Freebase [48]. **GrailQA** [34] is a large-scale dataset specifically designed to evaluate KBQA models across three generalization levels: *i.i.d.*, *compositional*, and *zero-shot*. It contains 64,331 questions in total, with 44,337 training questions, 13,231 validation questions and 6,763 test questions. Following prior work [3], [6], we use the dev set for evaluation. The compositional and zero-shot settings are particularly challenging, requiring models to handle unseen combinations of entities and relations. **WebQSP** [49] is an enriched version of WebQuestions, providing semantic parses for 4,737 questions. The dataset is split into 3,098 training questions and 1,639 test questions. **GraphQuestions** [50] tests KBQA models on complex graph-structured reasoning. It contains 5,166 questions in total, with 2,508 for training and 2,658 for testing. The dataset challenges models to navigate multi-hop relationships.

2) *Baselines*: We compare KBQA-R1 with both Finetune and Prompt-based KBQA methods:

Finetune-based Methods. These methods are trained on the complete training datasets and serve as upper-bound references: **RnG-KBQA** [13] employs a retrieve-and-generate framework that first retrieves relevant knowledge from the KB and then generates executable logical forms. **DecAF** [51] uses multi-granular retrieval strategies to ensure robust KBQA performance by progressively refining retrieved knowledge. **TIARA** [14] is a semantic-parsing-based approach that maps questions to structured queries through iterative refinement. **KBQA-o1** [6] is a recent MCTS-based agentic KBQA method that employs heuristic search with policy and reward models.

For GraphQuestions, following KBQA-o1's setup, we also compare with **SPARQA** [52], **BERT+Ranking** [34], and **ArcaneQA** [15].

Prompt Based Methods. These methods operate under the same limited annotation constraint as KBQA-R1: **KB-BINDER** [1] leverages in-context learning with GPT-3.5-turbo to bind questions to KB entities and relations. **KB-Coder** [2] adopts a code-style in-context learning approach to generate logical forms with GPT-3.5-turbo. **ARG-KBQA** [53] uses augmented reasoning graphs with GPT-3.5-turbo for improved question answering.

3) *Evaluation Metrics*: We evaluate all methods using standard KBQA metrics: **Exact Match (EM)** measures the percentage of questions where the predicted answer set exactly matches the gold answer set. This is a strict metric that requires perfect precision and recall. **F1 Score** computes the harmonic mean of precision and recall at the entity level, providing a more lenient measure that accounts for partial correctness. For GrailQA, we report F1 scores across three generalization settings (*i.i.d.*, *compositional*, *zero-shot*) as well as overall performance. For WebQSP and GraphQuestions, we report the overall F1 score on their respective test sets. All metrics

TABLE III: Performance on the dev set of GrailQA. The **Bold** and underlined numbers indicate the best and second-best performance.

Method	LLM	I.I.D		Compositional		Zero-shot		Overall	
		EM	F1	EM	F1	EM	F1	EM	F1
<i>Prompting Methods</i>									
KB-BINDER [1]	Codex-davinci-002	40.0	43.3	33.9	36.6	40.1	44.0	38.7	42.2
KB-Coder [2]	GPT-3.5-turbo	40.6	45.5	34.5	38.6	42.2	47.3	40.1	44.9
ARG-KBQA [53]	GPT-3.5-turbo	46.6	51.5	36.4	41.8	46.6	52.1	43.8	48.5
<i>Fine-tune-based Methods</i>									
RnG-KBQA [13]	T5-large	86.7	89.0	61.7	68.9	68.8	74.7	69.5	76.9
DecAF [51]	T5-large	88.7	92.4	71.5	79.8	65.9	77.3	72.5	81.4
TIARA [14]	T5-large	88.4	91.2	66.4	74.8	73.3	80.7	75.3	81.9
KBQA-o1 [6]	Llama-3.1-8B	77.8 ± 0.5	85.5 ± 0.4	76.3 ± 0.6	77.6 ± 0.5	68.1 ± 0.8	76.1 ± 0.4	71.9 ± 0.3	78.5 ± 1.0
KBQA-R1	Llama-3.1-8B	90.0 ± 0.3	91.5 ± 0.2	78.0 ± 0.4	82.5 ± 0.3	83.6 ± 0.3	85.2 ± 0.3	83.9 ± 0.2	86.1 ± 0.3
<i>Improv. over KBQA-o1</i>		$+12.8\%$		$+7.0\%$		$+1.7\%$		$+6.3\%$	
		$+15.5\%$		$+15.5\%$		$+9.1\%$		$+12.0\%$	
		$+12.0\%$		$+7.6\%$					

TABLE IV: Results on the test set of WebQSP. The **Bold** and underlined numbers indicate the best and second-best performance.

Method	LLM	F1
<i>Prompting Methods</i>		
KB-BINDER [1]	Codex-davinci-002	52.6
KB-Coder [2]	GPT-3.5-turbo	55.7
ARG-KBQA [53]	GPT-3.5-turbo	58.8
Interactive-KBQA [20]	GPT-4-turbo	71.2
<i>Fine-tune-based Methods</i>		
RnG-KBQA [13]	T5-large	75.6
DecAF [51]	T5-large	76.7
TIARA [14]	T5-large	78.9
MCTS-KBQA [54]	Llama-3.1-8B	<u>76.0</u>
KBQA-o1 [6]	Llama-3.1-8B	57.8
KBQA-R1	Llama-3.1-8B	83.4 ± 0.3
<i>Improv. over KBQA-o1</i>		$+25.6\%$

are computed based on executed answers retrieved from the Freebase knowledge base back-end.

TABLE V: Results on the test set of GraphQ. The **Bold** and underlined numbers indicate the best and second-best performance.

Method	LLM	F1
<i>Prompting Methods</i>		
KB-BINDER [1]	Codex-davinci-002	27.1
KB-Coder [2]	GPT-3.5-turbo	31.1
<i>Fine-tune-based Methods</i>		
SPARQA [52]	BERT-base	21.5
BERT+Ranking [34]	BERT-base	25.0
ArcaneQA [15]	BERT-base	31.8
CoTKR [55]	Llama-3-8B	47.5
KBQA-o1 [6]	Llama-3.1-8B	48.7
KBQA-R1	Llama-3.1-8B	53.8 ± 0.7
<i>Improv. over KBQA-o1</i>		$+5.1\%$

4) **Training Setup: Model Architecture.** We use Llama-3.1-8B-Instruct as the default backbone. For fair comparison with KBQA-o1 [6], all experiments use the same base model architecture.

Two-Stage Training Pipeline. Following our RRS warm-start strategy (Section IV-B), training proceeds in two stages:

Stage 1 (SFT Warm-start): We first fine-tune the base model on Referenced Rejection Sampling trajectories, using a learning rate of 5×10^{-6} with cosine decay. Stage 2 (GRPO Training): Starting from the SFT checkpoint, we apply GRPO optimization with actor learning rate 1×10^{-6} and 30% linear warmup. GrailQA uses 1 training epochs due to its larger scale (44,337 training examples), while WebQSP and GraphQuestions use 8 epochs each. The training batch size is 256. Validation is performed every 10 training steps. We select the best model based on the highest F1 reward achieved on training set.

GRPO Configuration. We adopt the GRPO algorithm [7] with the following hyperparameters: (1) *Rollout sampling*: $n = 5$ responses per prompt with temperature $\tau = 1.0$ and top- $p = 0.99$; (2) *Clipping*: asymmetric clip ratios $\epsilon_{\text{low}} = 0.2$, $\epsilon_{\text{high}} = 0.28$ following DAPO [56]; (3) *KL regularization*: KL loss coefficient $\beta = 0.001$; (4) *Reward weights and gating*: we set $\lambda_{\text{outcome}} = 1.0$ and $\lambda_{\text{format}} = 0.1$, and use RRCG confidence thresholds $\tau_{\text{high}} = 0.95$ and $\tau_{\text{low}} = 0.3$ across all datasets; (5) *Batch configuration*: train batch size 256, PPO mini-batch size 128, with dynamic micro-batching enabled.

Infrastructure. Training is conducted on $8 \times$ NVIDIA A100-80GB GPUs with FSDP [57] for model sharding. The Freebase KB backend uses Virtuoso [58] with ODBC connection pooling (pool size 48, query timeout 600s).

B. Main Results Analysis

For GrailQA dataset (Table III), KBQA-R1 delivers consistent gains over the strongest fine-tuned baseline KBQA-o1 across all three generalization levels. In the i.i.d. split, KBQA-R1 improves EM by about +12% and F1 by roughly +6%. In the compositional split, which stresses recombinining seen schema elements, KBQA-R1 still achieves a solid margin of around +5% F1. **Most notably, in the zero-shot setting—where relations and compositions are unseen during training—KBQA-R1 boosts EM by more than +15% and F1 by about +9% over KBQA-o1.** Overall on GrailQA, these improvements translate into gains of roughly +8% F1 and +12% EM, highlighting that execution-grounded reinforcement learning significantly enhances out-of-distribution generalization rather than merely fitting the training distribution. On WebQSP (Ta-

TABLE VI: Component ablation study of KBQA-R1. We report Overall F1 (%) on three datasets. Each variant removes or modifies one component at a time to isolate its contribution.

Variant	WebQSP	GraphQ	GrailQA
Full KBQA-R1 (ours)	83.4	53.8	86.1
<i>Agent Architecture Ablations</i>			
w/o RRCG (no relation retrieval & gating)	64.1	37.7	67.1
w/o Multi-turn (single-turn action generation)	63.2	34.1	49.8
<i>Training Strategy Ablations</i>			
w/o RRS (standard rejection sampling)	78.9	49.2	78.3
w/o SFT warm-start (RL from scratch)	75.2	47.3	75.1
w/o GRPO (only SFT)	72.1	47.8	80.2
<i>Reward Design Ablations</i>			
w/o Format Reward ($r_{\text{format}} = 0$)	81.1	51.6	84.2

TABLE VII: Standard Rejection Sampling (RS) vs. Referenced RS (RRS) across three datasets. “RS F1 (pre-SFT)” is the average F1 of raw RS trajectories before fine-tuning. “Filtered SFT Samples” counts trajectories with $F1 > 0.9$ and $r_{\text{format}} = 0.1$ used for SFT. “SFT Init F1” reports dev-set F1 after SFT initialized from the corresponding RS data.

Dataset	Method	RS F1 (pre-SFT)	# Accepted / Total	Acceptance (%)	SFT Init F1
GrailQA	Standard RS	54.2	17248 / 43851	39.3	73.8
	Referenced RS (RRS)	70.2	29384 / 43851	67.0	80.2
WebQSP	Standard RS	49.1	1120 / 2929	38.3	65.8
	Referenced RS (RRS)	62.5	1505 / 2929	51.4	72.1
GraphQ	Standard RS	48.1	986 / 2332	42.3	41.1
	Referenced RS (RRS)	73.1	1562 / 2332	67.0	47.8

ble IV), KBQA-R1 attains 83.4% F1, outperforming the best prompting baseline by over 20 percentage points and exceeding fine-tuned systems such as TIARA and DecAF. Compared with the Llama-3.1-8B-based MCTS-KBQA, KBQA-R1 achieves about +7% absolute F1 improvement, suggesting that learned policies are more effective than MCTS search heuristics under the same backbone. On GraphQuestions (Table V), which emphasizes long multi-hop queries, KBQA-R1 yields around +5% absolute F1 gain over KBQA-o1 and consistently surpasses earlier graph-based methods such as CoTKR and ArcaneQA. These results indicate that KBQA-R1 effectively enhances reasoning capabilities across diverse KBQA challenges, including complex multi-hop queries.

C. Ablation Study

We conduct ablation studies to quantify the contribution of the key components introduced in Section IV, including Relation Retrieval and Confidence Gating (RRCG), the structured action space, the RRS warm-start, and GRPO-based RL optimization.

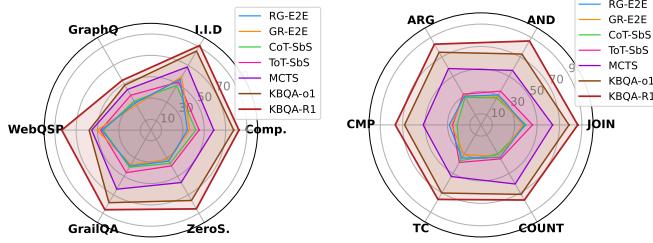
Agent Architecture Ablations. The most significant performance drops occur when removing core architectural components. (1) *w/o RRCG* results in an average F1 drop of about 18%, with GrailQA suffering the largest degradation (−19.0%). Without relation retrieval and confidence gating, the agent must rely solely on the LLM’s parametric knowledge to select relations, leading to frequent hallucinations on unseen schema elements. The impact is particularly severe on GraphQ (−16.1%), where complex multi-hop queries require precise relation grounding. (2) *w/o Multi-turn* causes the most dramatic decline (about −25% on average), confirming that iterative refinement through KB feedback is essential.

Single-turn generation forces the model to produce complete S-Expressions without intermediate validation, resulting in cascading errors. GrailQA shows the steepest drop (−36.3%), as its compositional and zero-shot questions inherently require exploratory reasoning that cannot be captured in a single generation step.

Training Strategy Ablations. Both training components contribute meaningfully to final performance. (1) *w/o RRS* (using standard rejection sampling instead of Referenced Rejection Sampling) reduces average F1 by about 5.6%. This validates our hypothesis that leveraging reference action list during warm-start trajectory generation produces higher-quality training signals. Standard rejection sampling often generates syntactically valid but semantically suboptimal trajectories that provide weaker supervision. (2) *w/o SFT warm-start* (training RL from scratch) incurs a larger penalty (about −8.6% on average). Without warm-start initialization, the RL agent begins with near-random behavior, requiring substantially more exploration to discover viable reasoning strategies.

Reward Design Ablations. Removing the format reward ($r_{\text{format}} = 0$) causes a moderate but consistent drop (about −2.1% on average). The format reward supplies dense intermediate feedback that steers the agent toward syntactically well-formed actions and encourages necessary thinking before acting, thereby complementing the sparse outcome reward. Without this signal, the agent can produce incorrect tag ordering or incomplete tags, which prevent the system from correctly extracting information. The relatively smaller impact compared to architectural ablations suggests that the outcome reward remains the primary driver of learning, with format rewards serving as a stabilizing auxiliary signal.

Referenced RS vs. Standard RS To better understand the



(a) F1 scores across datasets and generalization levels.
(b) F1 scores across logical operation types.

Fig. 3: Comprehensive performance comparison of KBQA-R1 with baseline methods using Llama-3.1-8B.

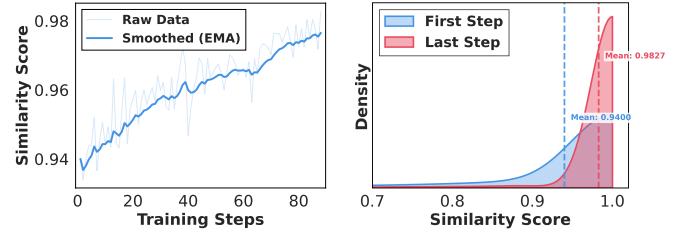
TABLE VIII: Average number of LLM forward calls per question on 200 sampled examples from each dataset.

Dataset	Method	Avg. LLM calls / sample ↓
WebQSP	KBQA-o1	28.8
	KBQA-R1	2.65
GrailQA	KBQA-o1	32.3
	KBQA-R1	3.08
GraphQ	KBQA-o1	78.0
	KBQA-R1	3.16

effect of Referenced Rejection Sampling (RRS) compared to standard Rejection Sampling (RS), we compare three aspects of the training pipeline on all three datasets: (1) the raw F1 score obtained directly from RS trajectories before any SFT, (2) the number of trajectories that pass both the outcome filter ($F1 > 0.9$) and the structure reward filter ($r_{\text{format}} = 0.1$) and are used for SFT, and (3) the initial test-set F1 after SFT trained on the corresponding RS data. As shown in Table VII, RRS consistently improves the quality and efficiency of trajectory collection across all datasets. The acceptance statistics reveal that RRS yields markedly more usable trajectories under the same filtering criteria, demonstrating that RRS is substantially more sample-efficient than standard RS. Finally, these higher-quality and denser trajectories translate into stronger SFT initialization. Starting RL from an RRS-initialized SFT checkpoint places the policy closer to a good solution, which complements the ablation result that removing RRS leads to a noticeable drop in final performance. Together, these observations justify RRS as a key component for obtaining stable and high-performing RL training in KBQA-R1.

D. LLM Call Efficiency.

To quantify the computational overhead between KBQA-o1 and KBQA-R1, we compare the number of LLM forward calls required by KBQA-R1 and the MCTS-based KBQA-o1 during inference. Table VIII reports average calls per question on 200 randomly sampled examples for each dataset. KBQA-o1 performs many LLM calls per query and additionally invokes separate policy and reward models, leading to substantially more LLM evaluations. In contrast, KBQA-R1 uses a single GRPO-trained policy without test-time search, reducing LLM calls by over 80% while achieving higher accuracy. In a 8-A100 GPU setup, KBQA-R1 processes about 155.6 questions per minute on GrailQA, compared to only 5.9 questions



(a) Relation similarity score evolution during training.

(b) Distribution shift of similarity scores: first step vs. last step.

Fig. 4: Relation similarity analysis of dataset WebQSP during RL.

per minute for KBQA-o1, demonstrating significant efficiency gains alongside performance improvements.

E. Compared with Llama-3.1-8B based Methods

Following the experimental setup of KBQA-o1 [6], we conduct a focused comparison among methods that share the same Llama-3.1-8B backbone and Freebase execution environment. The compared baselines can be grouped into three categories. (1) *End-to-end generation methods*: RG-E2E and GR-E2E are adapted from DecAF [51] and ChatKBQA [3], respectively. RG-E2E follows a retrieve-then-generate paradigm, while GR-E2E first generates a preliminary logical form and then refines it with KB retrieval. (2) *Step-by-step prompting methods*: CoT-SbS and ToT-SbS are implemented by instantiating the CoT-based QueryAgent [19] and the ToT-based ToG framework [4] on Llama-3.1-8B, prompting the model to alternate between intermediate thoughts and KB queries. (3) *MCTS-based agentic method*: MCTS corresponds to the MCTS-optimized variant in KBQA-o1 [6] without incremental Fine-tuning. Figure 3a visualizes F1 scores across six evaluation dimensions. KBQA-R1 achieves the largest coverage area, demonstrating superior overall performance across all settings, with the most pronounced gap in zero-shot dimensions. This validates our hypothesis that RL-based training fosters more robust reasoning capabilities than SFT. In contrast, end-to-end and step-by-step baselines cluster in the inner region, reflecting limited generalization. Figure 3b further breaks down performance by logical operation type. KBQA-R1 dominates across all categories, showing particularly significant advantages in complex operations. Conversely, baselines struggle with rare operations, underscoring their inability to generalize to infrequent query patterns.

F. Training Dynamics Analysis

Relation Similarity Score Evolution. Figure 4 provides a comprehensive analysis of how the agent’s relation selection capability evolves during RL training. Figure 4a tracks the top-1 relation similarity score throughout training, which measures how well the agent’s selected relations match the selected relations in the reference action list. Starting from approximately 0.94 at initialization (reflecting the warm-start SFT checkpoint), the similarity score steadily increases to approximately 0.98 by the end of training. This monotonic improvement demonstrates that GRPO effectively guides the

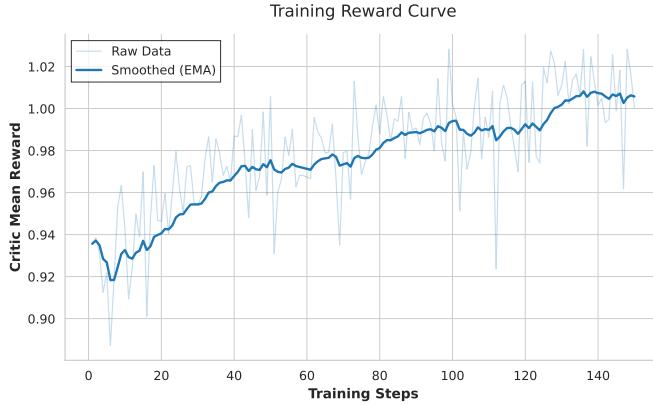


Fig. 5: Training reward of dataset GrailQA curve during RL.

agent toward more accurate relation selection. Figure 4b visualizes the distribution shift of similarity scores between the first and last training steps, providing complementary insights to the temporal evolution shown in Figure 4a. At the first step, the similarity distribution exhibits a broader spread with mean 0.9400, reflecting the uncertainty in relation selection inherited from the SFT warm-start. By the last step, the distribution becomes significantly more concentrated toward 1.0 with mean 0.9827, indicating that the agent has learned to consistently select highly relevant relations. The rightward shift and reduced variance demonstrate that RL training not only improves average performance but also reduces the frequency of low-confidence relation selections, leading to more reliable query generation.

Training Reward Dynamics. Figure 5 illustrates the evolution of the critic mean reward during GRPO training. The reward signal, which combines outcome reward (F1-based) and format reward, shows a clear upward trajectory from approximately 0.89 to 1.00. The reward briefly decreases during steps 0-5, reflecting the exploration phase where the agent deviates from the SFT-initialized policy to discover potentially better strategies. Between steps 5-60, the reward increases rapidly, indicating successful policy refinement through the GRPO objective. After step 140, the reward stabilizes around 1.00 with reduced variance. Given the maximum achievable reward of 1.10 (1.0 for outcome and 0.1 for structure), this suggests that the policy has converged to a near-optimal state.

VI. CONCLUSION

We presented KBQA-R1, a reinforcement learning framework for agentic knowledge base question answering. By integrating a structured action space, a relation retrieval and confidence gating module, and a novel Referenced Rejection Sampling warm-start strategy, KBQA-R1 effectively leverages execution feedback from the knowledge base to learn robust reasoning policies via the GRPO algorithm. Extensive experiments on three challenging KBQA benchmarks demonstrate that KBQA-R1 significantly outperforms state-of-the-art prompting and fine-tuning baselines, particularly in out-of-distribution generalization settings. Ablation studies confirm the importance of each component in achieving strong

performance. Our work establishes that outcome-based RL training enables genuine reasoning capabilities that transfer to unseen scenarios, moving beyond the surface-level pattern matching inherent in supervised fine-tuning.

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VII. BIOGRAPHY SECTION

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