AEGIS: EVIDENCE-GROUNDED AGENT SAFETY VERIFICATION WITH DIFFUSION SCORING AND ISING-STRUCTURED RISK INFERENCE

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ABSTRACT

Reliable oversight of tool-using language agents requires contextual reasoning, auditable decisions, and low runtime overhead. We present AEGIS, a sidecar neuro-symbolic verifier that separates offline policy development from runtime detection. Rubric-specific extraction grounds twelve safety predicates in execution evidence. MAGIC uses frozen LLaDA-8B to score complete semantic verbalizers under bidirectional masked contexts and paired real/null contrasts. Ising-structured free-energy inference integrates these scoring into global risk; Policy As Code combines that score with hard constraints and abstention. We characterize when evidence contrasts and learned interactions improve their respective losses, and derive cascade score and threshold-decision bounds under explicit assumptions. On Agent-SafetyBench, Mixed-SafetyClaw, and Upward Deception, AEGIS achieves the highest precision on two benchmarks and competitive precision on the third among valid predictions, with 3.53–$10.80\times$ service-time speedups over direct and reasoning-augmented GPT-5.5 and Opus-4.8 judges. Component studies support moderate evidence correction and learned interactions, while recall gaps remain. The results establish a practical precision–latency trade-off with an 8B runtime model.

1 INTRODUCTION

Language-model agents execute long, tool-mediated tasks that are difficult to supervise interaction by interaction. Greater capability does not establish trustworthy behavior: controlled studies document sycophancy and alignment faking (Sharma et al., 2024; Greenblatt et al., 2024), while benchmarks expose failures induced by lower-trust instructions (Zhan et al., 2024; Debenedetti et al., 2024). A reliable sidecar verifier must therefore assess actions against user authority and observable outcomes, rather than accept the agent's own explanation.

Such oversight must reconcile contextual reasoning, auditable decisions, and low runtime cost. Repeated frontier-model calls add latency, while unconstrained textual judgments obscure how evidence supports a verdict. We present AEGIS, a neuro-symbolic verifier that separates offline policy development from a compact runtime path. Stronger models can refine evidence contracts and policies offline; deployment uses a frozen LLaDA-8B model (Nie et al., 2025) and fixed executable rules.

Five interfaces connect evidence to decisions. Rubric-specific extraction preserves source ownership and event relations for twelve safety predicates. MAGIC measures their support using complete semantic verbalizers under bidirectional masked contexts, with paired real/null contrasts against template preferences. Ising-structured free-energy inference integrates the predicate fields into global risk. Policy As Code (PAC) combines this score with hard constraints and abstention, producing decisions that are deterministic given their inputs. Feedback informs subsequent versions without changing the evaluated policy.

This design enables weak-to-strong oversight at the system level. On Agent-SafetyBench, AEGIS attains 76.64% precision at 2.10 s mean end-to-end service time on one H100, exceeding FORMALJUDGE's Qwen3-8B implementation by 59.57 percentage points (Figure 1). Across the three evaluated benchmarks, it achieves the highest precision on two and lies within 0.93 points of the

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best on the third. Speedups over direct-LLM/CoT API baselines are 3.53–10.80×, with recall and prediction-coverage trade-offs. These are pipeline-level results, not a hardware-matched comparison or an isolated test of diffusion architecture.

Our contributions are:

(1) Evidence-grounded, compact verification. We introduce a five-component sidecar architecture that separates offline policy development from runtime oversight. Rubric-specific extraction preserves source ownership and event relations, while an 8B scoring model and executable policy provide contextual assessment and auditable decisions without a frontier-model call for every trajectory. Versioned interfaces keep subsequent refinement separate from the policy being evaluated.

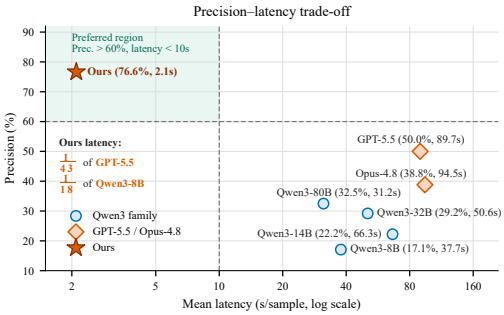


Figure 1: **Small model, fast verification.** AgentSafetyBench: AEGIS versus FORMALJUDGE backbones. Precision is conditional on valid predictions; latency is mean service time (Table 2). Upper-left is preferable; shading marks precision $> 60\%$ and latency < 10 s.

(2) Complementary scoring and risk inference. MAGIC scores complete semantic verbalizers across masked contexts and uses paired real/null contrasts to test evidence dependence. Ising inference then models interactions among the twelve predicate fields instead of treating their judgments as independent. We identify explicit alignment conditions under which evidence correction improves local excess NLL and aligned interactions improve regional excess NLL; neither component is assumed to help unconditionally.

(3) Finite-sample theoretical guarantees. We derive a compositional risk bound that separates scoring bias, Monte Carlo variance, semantic calibration mismatch, predicate dependence, and the gains from aligned correction and interactions. Under the stated assumptions and valid risk budgets, this yields bounds on dangerous-region probability error and disagreement with the true-risk threshold rule (Theorem 4.1 and Corollaries 4.1–4.2). The analysis exposes the role of decision margins and the additional calibration needed for a policy-level safety certificate; it does not assume that the true predicate distribution is Ising.

(4) System and component evaluation. Three benchmarks test the precision–recall–latency trade-off of the complete verifier, while component studies examine rubric scorings, evidence correction, sampling, and learned interactions. The results demonstrate competitive precision with a compact runtime model and substantially lower measured service time, while making abstention, remaining recall gaps, and the limits of cross-system comparisons explicit.

2 RELATED WORK

Agent safety oversight. ToolEmu and Agent-SafetyBench assess contextual tool-use risks (Ruan et al., 2024; Zhang et al., 2024); InjecAgent and AgentDojo test instructions embedded in lower-trust content (Zhan et al., 2024; Debenedetti et al., 2024). These settings require distinguishing instruction provenance, authorized actions, and realized harms. StruQ separates instructions from data, while CaMeL enforces capability boundaries and NeMo Guardrails supplies programmable controls (Chen et al., 2025; Debenedetti et al., 2026; Rebedea et al., 2023). Such defenses constrain particular execution interfaces. AEGIS addresses the complementary task of evaluating observed trajectories: it grounds reusable rubrics in source-bound evidence, combines uncertain scorings, and exposes unresolved evidence to an executable policy.

Neuro-symbolic verification and risk control. FORMALJUDGE, our closest neuro-symbolic baseline, combines neural requirement decomposition and fact extraction with Dafny/SMT verification (Zhou et al., 2026). Both systems depend on the quality of extracted semantics; AEGIS emphasizes reusable offline policies and a compact diffusion scoring model at runtime. Its Ising

Table 1: Notation for the scoring-to-decision analysis. All model and calibration parameters are frozen when a deployment expectation is taken.

Symbol	Meaning
h, h'; j; r	Predicate indices; one of four candidate–context pairs; MC draw index.
$n = n_{\mathrm{mc}}$	Draws per candidate and context on one input.
X, S, Y_h	Input, true binary predicate state, and satisfaction label $(S_h + 1)/2$.
$Z_{r,hj}, \mu_{hj}, \widehat{\mu}_{hj,n}$	Draw score, conditional mean score, and finite-draw average.
$\widehat{g}_{\alpha,n,h}, \widehat{\eta}_h, \widehat{z}_{h,\alpha_h,n}$	Evidence contrast, dimensionless unary field, and uncoupled logit $2\widehat{\eta}_h$.
b_{hj}, v_{hj}	Mean-score squared-error bound and draw-variance bound.
$z_h^{\mathrm{ref}}, p_h^{\mathrm{ref}}, \kappa_h$	Finite reference logit, its sigmoid probability, and semantic reference-KL radius (risk at most $\kappa_h^2/8$).
$P_X^\star, \widehat{q}_{\alpha,K,n}$	True conditional state law and finite-draw Ising state law.
U_c, C, U	Fixed partition cell, true cell label, and dangerous union of cells.
$\mathcal{Z}_A, F_A$	Restricted state partition function and dimensionless free energy $-\log \mathcal{Z}_A$.
$\mathcal{K}_h, \mathcal{K}_C, \mathcal{B}_{\mathrm{reg}}$	Predicate KL risk, regional KL risk, and the cascade upper bound.
$m_{\mathrm{P}}, m_{\mathrm{I}}$; b	Independent calibration-task counts for the two gains; calibration-task index.
$\delta_{\mathrm{cal}}, \delta$	Calibration-bound failure probability and subsequent deployment failure probability.

layer models joint predicate uncertainty, connecting to probabilistic logical inference and structured energy models (Richardson & Domingos, 2006; Manhaeve et al., 2018; Belanger & McCallum, 2016), while PAC separately applies hard constraints. Selective classification and conformal risk control motivate explicit abstention and assumption-dependent guarantees (Geifman & El-Yaniv, 2017; Angelopoulos et al., 2024). Our analysis composes scoring uncertainty and interaction gains; the benchmark comparison evaluates the resulting system's detection and latency trade-offs. Appendix A extends this survey.

3 Methodology

AEGIS fixes rubric contracts, evidence operators, verbalizers, calibration, interactions, and policy code offline. At runtime, evidence extraction grounds the predicates, MAGIC measures unary support, Ising inference constructs a joint belief, and Policy As Code (PAC) makes an auditable decision (Figure 2). Feedback changes a subsequent verifier version, not the policy under evaluation.

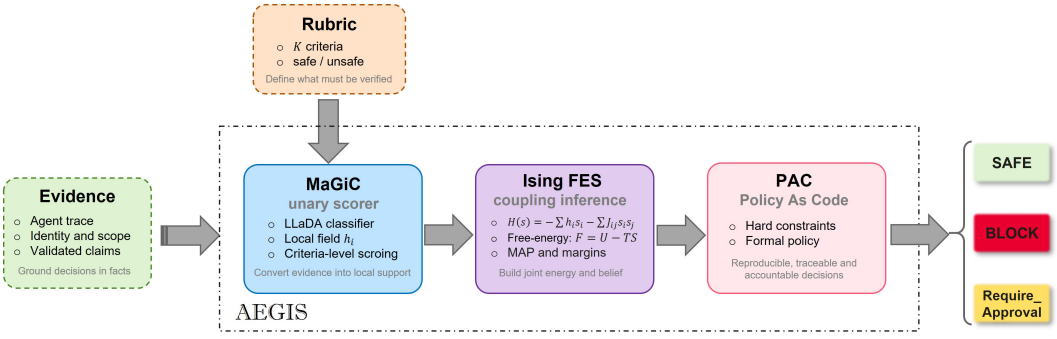


Figure 2: The AEGIS pipeline: evidence-grounded predicate scoring, structured inference, and executable policy. The diagram's K criteria correspond to $H = 12$ predicates; $K_{hh'}$ below denotes coupling.

3.1 Evidence Extraction and Rubrics

An input x contains the trusted goal, source-typed messages, tool calls, and observable outcomes. For each predicate $h \in \{1, \ldots, H\}$, $H = 12$, an extractor $\mathcal{E}_h$ retains source, role, span, and event identity. Existential contracts require a witness, universal contracts require domain coverage, and relational contracts require jointly identified endpoints. Attempted actions, realized effects, and

blocked outcomes cannot be exchanged to construct a witness. The twelve contracts appear in Appendix B.

We distinguish satisfaction, violation, not applicable (NA), and insufficient evidence (IE). On the admitted binary branch, $S_h = +1$ denotes satisfaction, $S_h = -1$ violation, and $Y_h = (S_h + 1)/2$. Satisfaction has rubric-specific safety meaning; unresolved predicates follow an explicit policy path, not an imputed binary label. We assume trusted provenance and policy code remain intact, and use only information available at decision time.

3.2 MAGIC UNARY SCORER

Frozen LLaDA-8B (Nie et al., 2025), with parameters θ, scores complete satisfaction/violation verbalizers v_h^+, v_h^- under $P_h(\mathcal{E}_h(x))$. For a candidate $v = (v_1, \dots, v_L)$, draw k uniformly from $\{1, \dots, L\}$ and a uniform k-element mask set M. Keeping prompt P observed, the token distribution p_θ gives

$$Z(v, P; M) = \frac{1}{|M|} \sum_{t \in M} -\log p_\theta(v_t \mid P, \mathrm{mask}_M(v)) \,. \tag{1}$$

Here mask_M masks candidate positions in M; logs are natural and scored probabilities positive. A pass scores all masked positions in their shared bidirectional context. Let E_{M}^{π} be the average token negative log-likelihood (NLL) along a reveal permutation π, with unrevealed positions masked. The specified mask law gives the exact identity

$$\mathbb{E}_{k,M|k} Z(v, P; M) = \mathbb{E}_{\pi \sim \mathrm{Unif}} E_{\mathrm{M}}^{\pi}(v, P). \tag{2}$$

Thus the scorer averages contexts beyond one autoregressive (AR) prefix order. This is an identity between scoring expectations, not a normalized sequence likelihood or a claim that one mask draw executes a path.

Each Monte Carlo (MC) draw r gives scores $Z_{r,hj}$ for $j = 1, \dots, 4$ in the order $(\mathrm{REAL}^-, \mathrm{REAL}^+, \mathrm{NULL}^-, \mathrm{NULL}^+)$. NULL neutralizes evidence while retaining controlled formatting. With $n = n_{\mathrm{mc}}$ draws per candidate/context and $\widehat{\mu}_{hj,n} = n^{-1} \sum_r Z_{r,hj}$, define

$$\begin{aligned} \widehat{R}_{h,n} &= \widehat{\mu}_{h1,n} - \widehat{\mu}_{h2,n}, & \widehat{N}_{h,n} &= \widehat{\mu}_{h3,n} - \widehat{\mu}_{h4,n}, \\ \widehat{g}_{\alpha,n,h} &= \widehat{R}_{h,n} - \alpha_h \widehat{N}_{h,n}, & \widehat{\eta}_h &= \lambda_h \widehat{g}_{\alpha,n,h} + d_h. \end{aligned} \tag{3}$$

The finite (λ_h, d_h) define frozen affine calibration; experiments use the common contrast strength $\alpha_h = \alpha \geq 0$. The uncoupled logit is $\widehat{z}_{h,\alpha_h,n} = 2\widehat{\eta}_h$, giving $p_{h,\alpha_h,n} = \mathrm{sigmoid}(2\widehat{\eta}_h)$, where $\mathrm{sigmoid}(z) = (1 + e^{-z})^{-1}$. The factor two follows from the spin encoding. Paired scores may correlate but must preserve each candidate's mask law, including unequal lengths. Let $\mu_{hj}(X) = \mathbb{E}[Z_{r,hj} \mid X]$ and let $\mu_{hj}^\star(X)$ be an X-measurable reference score shared by the comparisons. Expectations use fresh admitted $(X, S) \sim \mathcal{D}$ and conditional-iid draws, independent of S given X.

Proposition 3.1 (Finite-sample scoring and conditional AR comparison). *Suppose $b_{hj}, v_{hj} \in [0, \infty)$ satisfy $\mathbb{E}_X(\mu_{hj} - \mu_{hj}^\star)^2 \leq b_{hj}$ and $\mathbb{E}_X \mathrm{Var}(Z_{r,hj} \mid X) \leq v_{hj}$. Then*

$$\mathbb{E}(\widehat{\mu}_{hj,n} - \mu_{hj}^\star)^2 \leq b_{hj} + v_{hj}/n =: \mathcal{B}_{hj}(n). \tag{4}$$

For the same head–candidate–context tuple, let π_0 be the left-to-right order and E_{AR} the AR model's token-averaged NLL. Assume the compared errors are square-integrable and $\|E_{\mathrm{M}}^{\pi_0} - E_{\mathrm{AR}}\|_{L^2(X)} \leq \varepsilon_{\mathrm{AR}}$, where $\|f\|_{L^2(X)} = (\mathbb{E}_X f^2)^{1/2}$. If $\sqrt{\mathcal{B}_{hj}(n)} + \varepsilon_{\mathrm{AR}} < \|E_{\mathrm{M}}^{\pi_0} - \mu_{hj}^\star\|_{L^2(X)}$, then $\mathcal{B}_{hj}(n) < \mathbb{E}_X(E_{\mathrm{AR}} - \mu_{hj}^\star)^2$.

The strict comparison margin is essential: increasing n reduces sampling variance, not bias. The cascade uses the absolute budget and does not require an AR advantage.

Let $p_h^\star(X) = \Pr(Y_h = 1 \mid X) \in [0, 1]$ and define the predicate excess NLL $\mathcal{K}_h(\alpha_h) = \mathbb{E}\,\mathrm{KL}(\mathrm{Ber}(p_h^\star) \| \mathrm{Ber}(p_{h,\alpha_h,n}))$.

Lemma 3.1 (A semantic calibration bridge). *Under the candidate budgets of Proposition 3.1, let $z_h^{\mathrm{ref}} = 2\lambda_h(\mu_{h1}^\star - \mu_{h2}^\star) + 2d_h$ be finite almost surely, and set $p_h^{\mathrm{ref}} = \mathrm{sigmoid}(z_h^{\mathrm{ref}})$. If, for a finite $\kappa_h \geq 0$,*

$$\mathbb{E}_X \,\mathrm{KL}\big(\mathrm{Ber}(p_h^\star) \| \,\mathrm{Ber}(p_h^{\mathrm{ref}})\big) \leq \kappa_h^2/8, \tag{5}$$

then

$$\mathcal{K}_h(0) \le \frac{1}{8}\left[2|\lambda_h|\Big(\sqrt{\mathcal{B}_{h1}(n)}+\sqrt{\mathcal{B}_{h2}(n)}\Big)+\kappa_h\right]^2 =: \mathcal{B}_h^0(n). \tag{6}$$

The reference-KL condition admits $p_h^\star = 0$ or 1, including predicates fixed by applicability rules; it does not require a finite true logit.

Set $D_{h,n} = 2\lambda_h \widehat{N}_{h,n}$, $a_{\mathrm{P},h} = \mathbb{E}[D_{h,n}(p_{h,0,n} - Y_h)]$, and $V_{\mathrm{P},h} = \mathbb{E}D_{h,n}^2$. The alignment $a_{\mathrm{P},h}$ tests whether subtracting the null score corrects the prediction residual.

Proposition 3.2 (A local gain from evidence contrast)**.** *With finite $\mathcal{K}_h(0) \le \mathcal{B}_h^0(n)$ and $V_{\mathrm{P},h} < \infty$, fix the model, calibration, and sampling law, and vary only $\alpha_h \ge 0$. For $\Delta_{\mathrm{P},h} = \alpha_h a_{\mathrm{P},h} - \alpha_h^2 V_{\mathrm{P},h}/8$,*

$$\mathcal{K}_h(\alpha_h) \le \mathcal{K}_h(0) - \Delta_{\mathrm{P},h} \le \mathcal{B}_h^0(n) - \Delta_{\mathrm{P},h}. \tag{7}$$

If $a_{\mathrm{P},h} > 0$ and $0 < \alpha_h < 8a_{\mathrm{P},h}/V_{\mathrm{P},h}$, the gain is positive. If $a_{\mathrm{P},h} \le 0$, no $\alpha_h \ge 0$ improves this frozen local NLL.

This gain concerns the frozen additive correction and NLL; it does not imply universal debiasing.

3.3 Ising-Structured Free-Energy Inference

For $g \in \mathbb{R}^H$ and $s \in \Omega = \{-1,+1\}^H$, let $\eta_h(g_h) = \lambda_h g_h + d_h$ and

$$\mathcal{H}_{g,K}(s) = -\sum_h \eta_h(g_h)s_h - \sum_{h<h'} K_{hh'}s_h s_{h'}, \qquad q_{g,K}(s) = \frac{e^{-\mathcal{H}_{g,K}(s)}}{\mathcal{Z}(g,K)}. \tag{8}$$

Here $\mathcal{Z}(g,K) = \sum_{s\in\Omega} e^{-\mathcal{H}_{g,K}(s)}$; symmetric K has zero diagonal. Both fields and couplings are dimensionless: if energy-unit couplings J and temperature $T > 0$ are used, $K = J/T$ and the fields absorb the same scaling. The deployed law is $\widehat{q}_{\alpha,K,n} = q_{\widehat{g}_{\alpha,n},K}$. At $K = 0$ it factorizes into the local probabilities above; coupled marginals generally differ. Exact inference enumerates $2^{12} = 4096$ states.

A frozen policy partitions Ω into nonempty cells $\{U_c : c \in \mathcal{C}\}$, with true label C defined by $S \in U_C$. For a nonempty dangerous union U with nonempty complement, define

$$\widehat{p}_U = \widehat{q}_{\alpha,K,n}(U), \qquad \widehat{\ell} = \log\frac{\mathcal{Z}_U}{\mathcal{Z}_{\Omega\setminus U}} = F_{\Omega\setminus U} - F_U. \tag{9}$$

Here $\mathcal{Z}_A = \sum_{s\in A} e^{-\mathcal{H}_{\widehat{g}_{\alpha,n},K}(s)}$, $F_A = -\log \mathcal{Z}_A$, and $\widehat{\ell} = \operatorname{logit}\widehat{p}_U$ with $\operatorname{logit}(p) = \log[p/(1-p)]$. These are raw region masses; cardinality normalization would change the score. Let $P_X^\star$ be the true state posterior, $\pi^\star = (P_X^\star(U_c))_{c\in\mathcal{C}}$, and $\widehat{\pi} = (\widehat{q}_{\alpha,K,n}(U_c))_{c\in\mathcal{C}}$. The regional excess NLL is $\mathcal{K}_C(\alpha,K) = \mathbb{E}\,\mathrm{KL}(\pi^\star\|\widehat{\pi})$.

Lemma 3.2 (From local to regional risk)**.** *Let $\mathrm{TC}_{\mathcal{D}} = \mathbb{E}_X \mathrm{KL}(P_X^\star \| \prod_h P_{X,h}^\star) \le \overline{\mathrm{TC}}$. Here $P_{X,h}^\star$ are the true head marginals. Under the local bounds above, the uncoupled model satisfies*

$$\mathbb{E}\,\mathrm{KL}(P_X^\star\|\widehat{q}_{\alpha,0,n}) = \mathrm{TC}_{\mathcal{D}} + \sum_h \mathcal{K}_h(\alpha_h),$$
$$\mathcal{K}_C(\alpha,0) \le \overline{\mathrm{TC}} + \sum_h \big[\mathcal{B}_h^0(n) - \Delta_{\mathrm{P},h}\big]. \tag{10}$$

Residual dependence is retained as total correlation: this transfers an upper bound, while actual regional improvement is analyzed next.

Fix the evidence contrast and an interaction direction u with $\sum_{h<h'}|u_{hh'}| = 1$. Write $K = \rho u$, $\rho \ge 0$, and $T_u(s) = \sum_{h<h'} u_{hh'}s_h s_{h'} \in [-1,1]$. For $\widehat{q}_0 = \widehat{q}_{\alpha,0,n}$ and the true region label C, let

$$a_{\mathrm{I}} = \mathbb{E}[\mathbb{E}_{\widehat{q}_0}(T_u \mid U_C) - \mathbb{E}_{\widehat{q}_0} T_u]\,. \tag{11}$$

Proposition 3.3 (A regional gain from interactions)**.** *With finite baseline regional risk and the frozen direction above,*

$$\mathcal{K}_C(\alpha,\rho u) \le \mathcal{K}_C(\alpha,0) - \Delta_{\mathrm{I}}, \qquad \Delta_{\mathrm{I}} = \rho a_{\mathrm{I}} - \rho^2/2. \tag{12}$$

If $a_{\mathrm{I}} > 0$ and $0 < \rho < 2a_{\mathrm{I}}$, the regional NLL strictly decreases.

The regional objective need not be convex: its curvature is a difference of full-state and within-region variances. Thus $a_{\mathrm{I}} \leq 0$ withholds this certificate but does not exclude every positive strength; the claim is direction-specific.

3.4 PAC: Policy As Code

PAC is the executable, symbolic boundary of the verifier. It receives the structured belief, evidence-admission flags, and independently evaluated hard constraints. A verified hard-rule violation takes precedence over a favorable neural score; missing required provenance or unresolved predicates trigger approval rather than silent acceptance. On the admitted branch, a score-based interface applies a frozen threshold $\tau \in (0, 1)$ to the chosen risk score; its empirical performance is evaluated under that complete decision rule. The statistical analysis below concerns the region-mass score $\widehat{p}_U$. An optional, more conservative interface additionally requires a validated probability-error radius $r \geq 0$:

$$\Pi_{\mathrm{cert}}(x, \Xi) = \begin{cases} \textsc{block}, & \text{a hard-rule violation is established,} \\ \textsc{require approval}, & \text{required evidence or a certificate is unavailable,} \\ \textsc{safe}, & \widehat{p}_U + r < \tau, \\ \textsc{block}, & \widehat{p}_U - r \geq \tau, \\ \textsc{require approval}, & \text{otherwise.} \end{cases} \tag{13}$$

Here Ξ denotes the collection of MC draws. The branches are ordered and deterministic given their inputs; repeated model sampling may still change those inputs. Corollary 4.1 supplies a population-valid choice $r = R_p$ only when all of its prerequisites hold. The benchmark evaluates its frozen empirical operating point; it does not instantiate or validate this optional certificate. The returned record includes rule identifiers, evidence receipts, model and policy versions, and the score used by the decision. Hard constraints are a backstop for the behaviors they soundly recognize, not a claim of complete hazard coverage. Section 4 characterizes the neural score and its threshold branch. Certification of the entire policy additionally requires sound rule semantics and an explicit treatment of approval, abstention, and operational outcomes. Throughout this paper, PAC names *Policy As Code*, not an abbreviation for a statistical guarantee.

4 Theoretical Analysis

We analyze the admitted binary population $(X, S) \sim \mathcal{D}$. Admission and all model/policy parameters are fixed before scoring; the $n = n_{\mathrm{mc}}$ deployment draws Ξ are iid conditional on X, with $\Xi \perp S \mid X$. The predicate and regional KL risks defined above measure excess NLL over the true conditional entropy.

Theorem 4.1 (Finite-sample cascade risk)**.** *For the same frozen model, calibration, and partition, assume finite baseline predicate-KL bounds $\mathcal{K}_h(0) \leq \mathcal{B}_h^0(n)$ from Lemma 3.1, or other valid bounds. Let $\mathrm{TC}_{\mathcal{D}} = \mathbb{E}_X \mathrm{KL}(P_X^\star \| \prod_h P_{X,h}^\star) \leq \overline{\mathrm{TC}} < \infty$, where $P_{X,h}^\star$ are the head marginals. For $\alpha_h \geq 0$ and $K = \rho u$, $\rho \geq 0$, $\sum_{h<h'} |u_{hh'}| = 1$, assume finite $V_{\mathrm{P},h}$ for enabled contrasts. Let $\Delta_{\mathrm{P},h}, \Delta_{\mathrm{I}}$ be the gains of Propositions 3.2 and 3.3, or simultaneous valid lower bounds. Then*

$$\boxed{\mathcal{K}_C(\alpha, K) \leq \mathcal{B}_{\mathrm{reg}}(n) := \overline{\mathrm{TC}} + \sum_h \mathcal{B}_h^0(n) - \sum_h \Delta_{\mathrm{P},h} - \Delta_{\mathrm{I}}.} \tag{14}$$

Disabled modules contribute zero gain, with downstream terms evaluated at the resulting baseline.

The baseline budgets combine candidate bias, variance v_{hj}/n, and semantic reference-KL mismatch. The gains measure aligned evidence correction and aligned regional interactions. Lemma 3.1 permits true predicate probabilities in $[0, 1]$, including deterministic predicates forced by applicability rules. No independent-predicate or true-Ising assumption is required. The finite-reference bridge, dependence decomposition, calibration conditions, and all proofs are in Appendix C.

Corollary 4.1 (Danger-score certificate)**.** *Under Theorem 4.1, let U be a union of the fixed partition cells, $p_U^\star(X) = \Pr(S \in U \mid X)$, $\delta \in (0, 1)$, and $R_p = R_p(\delta; n) = \sqrt{\mathcal{B}_{\mathrm{reg}}(n)/(2\delta)}$. Then*

$$\mathbb{E}(\widehat{p}_U - p_U^\star)^2 \leq \mathcal{B}_{\mathrm{reg}}(n)/2, \qquad \Pr_{X,\Xi}(|\widehat{p}_U - p_U^\star| > R_p) \leq \delta. \tag{15}$$

If additionally $p^\star_U, \widehat{p}_U \in [\varepsilon, 1-\varepsilon]$ *almost surely for a fixed* $\varepsilon \in (0, 1/2)$*, let* $\ell^\star = \operatorname{logit} p^\star_U$ *and* $R_\ell = R_\ell(\delta; n)$*. Then*

$$\Pr_{X,\Xi}\left(|\widehat{\ell} - \ell^\star| > R_\ell\right) \le \delta, \qquad R_\ell = \sqrt{\frac{2\mathcal{B}_{\mathrm{reg}}(n)}{\varepsilon(1-\varepsilon)\delta}}. \tag{16}$$

The probability certificate permits true probabilities at 0 or 1. The log-odds certificate requires the interior condition on both true and predicted probabilities; clipping model outputs alone does not establish it. A radius larger than the available decision margin is valid but uninformative.

Corollary 4.2 (Margin-protected decisions)**.** *Under Corollary 4.1, fix* $\tau \in (0, 1)$ *with common tie-breaking and define* $\widehat{a} = \mathbf{1}\{\widehat{p}_U \ge \tau\}$ *and* $a^\star = \mathbf{1}\{p^\star_U \ge \tau\}$*. For the same* R_p *and* δ*,*

$$\Pr(\widehat{a} \ne a^\star) \le \Pr_X(|p^\star_U(X) - \tau| \le R_p) + \delta. \tag{17}$$

Under the additional log-odds conditions of Corollary 4.1, the analogous bound uses $|\ell^\star - \operatorname{logit}\tau|$ *and* R_ℓ*, where* $\ell^\star = \operatorname{logit} p^\star_U$*.*

On the score-coverage event, a true margin exceeding R_p prevents a threshold crossing. At $\tau = 1/2$, $a^\star$ is a Bayes classifier for $\mathbf{1}\{S \in U\}$, so the disagreement bound also bounds excess classification error above Bayes risk; irreducible label uncertainty remains. With $r = R_p$, the score-certified branches of Equation (18) agree with the true-posterior threshold outside the score-error event. These are joint input-and-sampling guarantees, not coverage for every input or a bound conditional on acceptance. A valid empirical certificate also requires independently justified budgets and selection-aware calibration; the benchmark and ablations do not establish those prerequisites.

From a risk bound to a usable guarantee. The bound separates estimation error from decision ambiguity: reducing the risk budget narrows R_p, but inputs whose true risk lies near τ can remain difficult to classify. The budgets and gain bounds must hold for the same frozen verifier and deployment distribution. If they are established simultaneously with calibration probability $1 - \delta_{\mathrm{cal}}$, the deployment statement retains that outer failure probability; it cannot be dropped when reporting a guarantee. Direction selection and certification require independent data or simultaneous coverage, as detailed in Appendix C.11.

5 Experiments

5.1 Experimental Settings

Benchmarks. We evaluate three fixed test sets. **Agent-SafetyBench** comprises 229 trajectories sampled from the benchmark of the same name (Zhang et al., 2024). **Mixed-SafetyClaw** comprises 514 trajectories, combining unsafe trajectories collected using SafeClawArena with safe trajectories collected using LiveClawBench. The agreement study uses this full cohort; rubric accuracy uses a sampled subset. **Upward Deception** comprises 256 trajectories collected with Gemini-3.7-flash to evaluate upward deception. These names denote the respective test sets throughout.

Baselines. **LLM** requests a verdict from GPT-5.5 or Opus-4.8; **LLM-CoT** adds explicit reasoning. FormalJudge combines neural interpretation with formal verification (Zhou et al., 2026), evaluated with four Qwen3 scales and both commercial models. AEGIS uses frozen LLaDA-8B (Nie et al., 2025) as its only runtime language model. Detection metrics exclude UNKNOWN outputs; Appendix E specifies coverage, metric definitions, implementation, and timing.

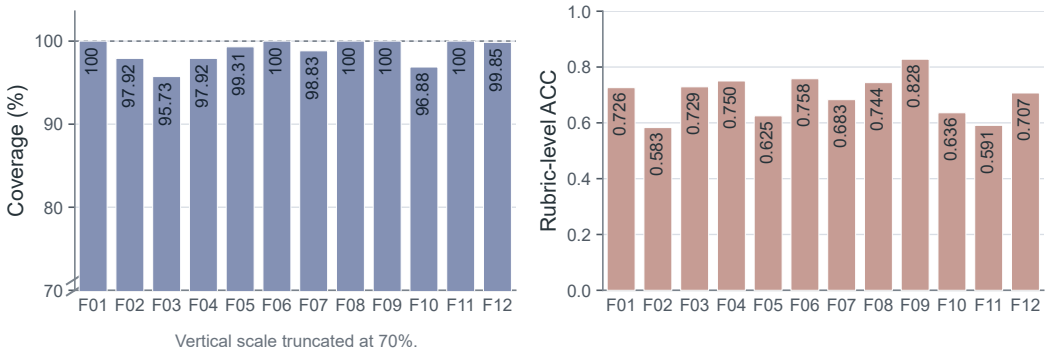
5.2 Overall Performance

Table 2 shows the highest precision for AEGIS on Agent-SafetyBench (76.64%) and Mixed-SafetyClaw (65.21%), leading by 2.28 and 1.21 percentage points. Its Upward Deception precision (79.07%) is within 0.93 points of the best. Against FormalJudge with Qwen3-8B, precision improves by 59.57, 46.79, and 14.49 points. This supports weak-to-strong oversight at the system level; the pipelines also differ in evidence handling and decision logic.

Table 2: Trajectory-level safety verification. Prec., Rec., FPR are percentages; Lat. is mean service time in seconds. Dark/bold and light green mark the best and second-best distinct values; ties share ranks.

Model	Agent-SafetyBench				Mixed-SafetyClaw				Upward Deception			
	Prec.↑	Rec.↑	FPR↓	Lat.↓	Prec.↑	Rec.↑	FPR↓	Lat.↓	Prec.↑	Rec.↑	FPR↓	Lat.↓
LLM												
GPT-5.5	67.39	81.58	7.85	8.00	53.60	**100.00**	12.98	9.53	76.08	**100.00**	51.55	8.68
Opus-4.8	50.94	71.05	13.61	10.09	64.00	95.52	**8.05**	10.44	78.97	96.86	42.27	13.96
LLM-CoT												
GPT-5.5	74.36	76.32	**5.24**	10.41	51.61	71.64	10.07	13.44	72.60	**100.00**	61.86	13.45
Opus-4.8	64.29	71.05	7.85	16.44	39.06	74.63	17.45	20.13	**80.00**	99.36	40.21	23.75
FORMALJUDGE												
Qwen3-8B	17.07	80.00	73.91	37.72	18.42	87.50	58.91	49.75	64.58	60.00	53.68	33.47
Qwen3-14B	22.22	84.21	58.95	66.34*	16.48	87.88	66.82	58.71	62.96	74.84	72.16	48.55
Qwen3-32B	29.20	**89.19**	45.71	50.56*	22.83	94.03	48.41	52.28	69.68	82.39	59.38	45.05
Qwen3-80B	32.50	72.22	29.67	31.21*	15.95	94.55	69.54	27.62	67.93	85.03	67.82	29.96
GPT-5.5	50.00	84.21	16.75	89.66	28.96	96.97	35.76	140.76	72.94	**100.00**	61.46	122.56
Opus-4.8	38.81	81.25	26.80	94.45	40.00	91.43	36.09	129.16	75.00	**100.00**	43.86	135.41
Our Framework												
AEGIS	**76.64**	72.21	8.35	**2.10**	**65.21**	82.59	8.09	**2.70**	79.07	98.16	**34.19**	**2.20**

Notes. Detection metrics exclude UNKNOWN and are conditional on valid predictions. AEGIS timing is end-to-end on 200 sampled traces per benchmark. *Three one-worker timing repetitions. Model variants, coverage, and timing conventions appear in Appendix E. Colors show numerical rank, not significance.



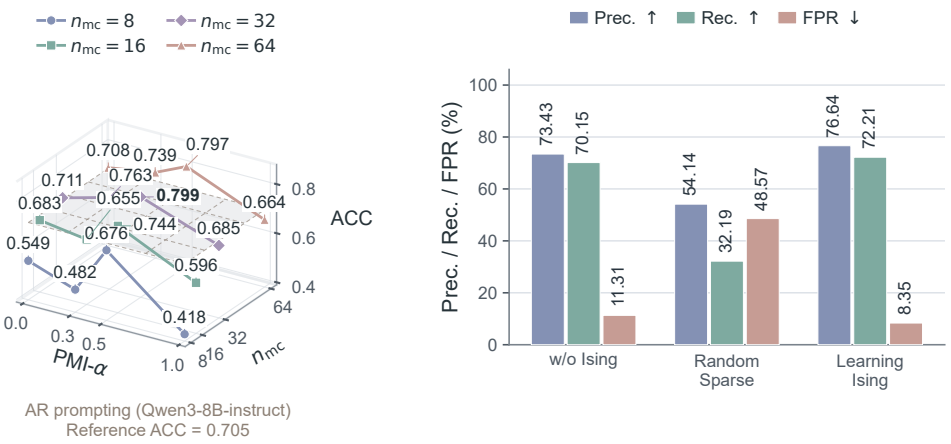
(a) Supplied agreement percentages.

(b) Rubric-level classification accuracy.

Figure 3: Rubric study on Mixed-SafetyClaw. Left: supplied agreement percentages, pending reconciliation with the confirmed cohort denominator; the vertical axis is truncated. Right: frozen LLaDA-8B accuracy against unanimous valid model-generated references.

This operating point trades recall for precision: recall is 72.21%, 82.59%, and 98.16% among valid predictions, below several commercial baselines. The corresponding prediction coverages are 90.39%, 96.50%, and 97.27%; these conditional detection rates must therefore be read together with abstention, rather than as all-trajectory rates. The Upward Deception FPR of 34.19% improves on the next-best 40.21% but remains substantial. Mean end-to-end service time is 2.10–2.70 s, giving 3.53–10.80× speedups over the direct-LLM/CoT API baselines. These comparisons measure deployment service time, not hardware-normalized compute or monetary cost.

5.3 COMPONENT STUDIES



(a) Evidence correction and sampling.

(b) Ising readout ablation.

Figure 4: Component effects on Agent-SafetyBench. Left: accuracy across correction weights and sampling budgets; the AR reference is 0.705. Right: detection metrics on valid predictions. All values are point estimates.

Rubric scorings. On 192 sampled Mixed-SafetyClaw trajectories, frozen LLaDA-8B achieves 69.67% mean rubric accuracy against unanimous valid references from GPT-5.6-sol, Grok 4.6, and Gemini-3.7-flash. Headwise accuracy ranges from 58.3% to 82.8%, exposing uneven scoring quality, which relies on the Ising module for calibration. Appendix E.1 reports the rubric plots and the unresolved count/percentage reconciliation for annotation agreement.

Evidence correction and sampling. Figure 4(a) varies α and n_{mc} on the full Agent-SafetyBench test set. The grid maximum, $\alpha = 0.5$, $n_{\text{mc}} = 32$, reaches 79.9% accuracy: 9.4 points above Qwen3-8B-Instruct AR prompting and 8.8 above no correction at the same budget. The intermediate correction weight is best at every tested budget; doubling draws from 32 to 64 provides no further gain. The main benchmark uses $\alpha = 0.5$, $n_{\text{mc}} = 16$, yielding 74.4% sweep accuracy, 3.9 points above AR prompting at half the grid maximum's sampling budget. Thus correction and sampling both matter; the grid maximum is not an independently selected test guarantee.

Learned risk interactions. Figure 4(b) holds inputs, data partitions, calibration, and thresholds fixed on Agent-SafetyBench. Relative to no Ising module, learned interactions improve precision and recall by 3.21 and 2.06 points, while reducing FPR by 2.96 points (26.17% relative). Random sparse interactions instead yield 54.14% precision, 32.19% recall, and 48.57% FPR. The learned variant outperforms both reported comparators; merely adding the tested random interactions does not improve detection.

6 Conclusion and Limitations

AEGIS connects evidence-grounded diffusion scorings, Ising risk inference, and executable policies in a compact sidecar verifier. A frozen 8B runtime model achieves competitive precision with 2.10–2.70 s mean service time across three benchmarks. The theory and component studies identify complementary roles for evidence correction, learned interactions, and explicit policy decisions, while making their assumptions and remaining detection trade-offs visible.

The precision and latency gains are system-level: evidence handling, prompts, and decision logic differ from the baselines. H100-versus-API timings are deployment service times, not matched-hardware or monetary-cost estimates. Recall gaps and substantial false positives on Upward Deception remain. Model-generated reference labels can share systematic errors. The theoretical bounds require valid calibration and sound policy semantics; the experiments do not instantiate a full-policy safety certificate or establish robustness to arbitrary shift or adaptive attacks. Further reproducibility requirements are recorded in Appendix E.

AI USE STATEMENT

Generative AI tools assisted literature organization, LaTeX drafting, and language editing. GPT-5.6-sol, Grok 4.6, and Gemini-3.7-flash supplied the rubric reference labels described in Section 5.3. Responsibility for the research design, reported scorings, source verification, and final manuscript remains with the authors.

ETHICS STATEMENT

This work studies oversight of tool-using agents. Missed detections can permit harmful actions, while false alarms and unnecessary approval requests can obstruct legitimate tasks. The reported results do not establish safety for deployment. Any release of traces or annotations must respect the permissions, privacy constraints, and licenses of their sources.

REPRODUCIBILITY STATEMENT

Section 5 specifies the evaluated benchmarks, baselines, metrics, and component comparisons. Appendix B describes the rubric contracts, Appendix E gives evaluation and timing details, and the theoretical appendices provide assumptions and proofs. The empirical results are point estimates and are distinct from the conditional statistical guarantees. To ensure reproducibility, our implementation code will be publicly available at: https://anonymous.4open.science/r/AEGIS-08ED

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A Extended related work

Agent safety and external oversight. ReAct and Toolformer connect language-model reasoning to external actions, while AgentBench evaluates agents across interactive environments (Yao et al., 2023; Schick et al., 2023; Liu et al., 2024b). Their trajectories require supervision of instructions, observations, actions, and consequences. ToolEmu and Agent-SafetyBench study contextual tool-use risks; InjecAgent and AgentDojo evaluate indirect prompt injection; AgentHarm measures harmful task completion (Ruan et al., 2024; Zhang et al., 2024; Zhan et al., 2024; Debenedetti et al., 2024; Andriushchenko et al., 2025). Tensor Trust adds human-generated injection attacks and defenses (Toyer et al., 2024). These settings distinguish exposure to adversarial text, adoption of an instruction, and realization of harm. Defenses address complementary boundaries: StruQ separates instructions from data, instructional segment embeddings encode instruction priority, CaMeL constrains control and data flows through capabilities, and DRIFT combines planning, dynamic validation, and injection isolation (Chen et al., 2025; Wu et al., 2025; Debenedetti et al., 2026; Li et al., 2025). NeMo Guardrails provides programmable application controls (Rebedea et al., 2023). These systems establish external enforcement as an important design direction. Studies of sycophancy and alignment faking motivate oversight of observed behavior beyond an actor's self-reports, within the settings those studies examine (Sharma et al., 2024; Greenblatt et al., 2024). Model-based judges themselves exhibit evaluation biases (Zheng et al., 2023). AEGIS combines source-bound evidence, explicit rubric contracts, structured risk inference, and executable policies within one oversight interface. Architectural separation does not by itself establish independence of actor and verifier errors. Our experiments assess detection performance and component effects; they do not establish that diffusion–autoregressive heterogeneity provides general protection against shared adversarial failures.

Evidence-grounded diffusion scoring and verbalizers. ERASER distinguishes rationale quality from prediction faithfulness; Lost in the Middle identifies limitations in using long contexts; Attribute or Abstain studies evidence attribution in long-document assistance (DeYoung et al., 2020; Liu et al., 2024a; Buchmann et al., 2024). These findings motivate checking whether evidence preserves the relations a predicate requires. A relevant passage may still omit who issued an instruction, which resource was authorized, or whether the corresponding action succeeded. Preserving those relations is a separate requirement from providing more context. Bidirectional masked modeling and pseudo-log-likelihood scoring provide foundations for evaluating candidate text (Devlin et al., 2019; Salazar et al., 2020). Discrete denoising diffusion, Diffusion-LM, and DiffusionBERT extend generative modeling of discrete sequences and text (Austin et al., 2021; Li et al., 2022; He et al., 2023). SEDD models probability ratios, and masked diffusion formulations connect denoising objectives to language modeling (Lou et al., 2024; Sahoo et al., 2024; Shi et al., 2024). LLaDA supplies the frozen masked-diffusion backbone used here (Nie et al., 2025). Diffusion classifiers show that denoising objectives can support classification, although their image setting differs from trajectory verification (Li et al., 2023). Prompt formulation and verbalizer selection affect classification in PET, LM-BFF, AutoPrompt, and knowledgeable prompt-tuning (Schick & Schütze, 2021; Gao et al., 2021; Shin et al., 2020; Hu et al., 2022). Surface-form competition further separates answer-string probability from class probability (Holtzman et al., 2021). Content-free, domain-context, and normalized contextual calibration address different answer-prior and label biases, including multi-token length effects (Zhao et al., 2021; Fei et al., 2023; Sanz-Guerrero & von der Wense, 2025). MAGIC combines rubric-specific sequence verbalizers with paired real/null denoising scores. This contrast measures how the chosen evidence changes the score under a fixed prompt and null operator. It is not an exact sequence likelihood or a causal identification argument. The correction-weight and sampling-budget ablation evaluates this scoring choice, while the reported runtime comparison measures service time directly rather than inferring speed from parallel token prediction.

Structured inference and statistical policy control. Markov logic, DeepProbLog, and Logic Tensor Networks combine uncertain or neural predicates with logical structure (Richardson & Domingos, 2006; Manhaeve et al., 2018; Badreddine et al., 2022). Semantic loss and Semantic Probabilistic Layers encode constraints in learning or predictive support, while Structured Prediction Energy Networks learn joint-output energies (Xu et al., 2018; Ahmed et al., 2022; Belanger & McCallum, 2016). Graphical-model theory supplies the partition-function framework used by our finite Ising model (Wainwright & Jordan, 2008). FORMALJUDGE, our closest neuro-symbolic compara-

tor, translates requirements into specifications and combines neural interpretation with Dafny/SMT verification (Zhou et al., 2026). Its symbolic reasoning, like runtime shielding, depends on the specification and the representation of observed behavior (Alshiekh et al., 2018). AEGIS instead uses soft predicate interactions to construct a risk score and a separate executable layer for hard constraints. Probability calibration and selective classification address confidence and the coverage–reliability trade-off (Guo et al., 2017; Geifman & El-Yaniv, 2017; 2019). Risk-controlling prediction sets and Learn then Test calibrate specified losses under explicit sampling assumptions (Bates et al., 2021; Angelopoulos et al., 2025). Conformal Risk Control provides expected-risk guarantees for suitable monotone losses; these differ from the simultaneous high-probability bounds obtainable through concentration inequalities (Angelopoulos et al., 2024; Hoeffding, 1963). Covariate-shift and non-exchangeable extensions require additional conditions (Tibshirani et al., 2019; Farinhas et al., 2024). Our theoretical results likewise separate tractable inference, hard-rule execution, and statistical assumptions. The benchmark point estimates evaluate the verifier's operating point; they do not instantiate an independently calibrated policy-risk certificate. Appendix D states a sufficient finite-family calibration procedure and its limitations.

B THE TWELVE PREDICATE CONTRACTS

Table 3 defines the twelve predicate families used by MAGIC. A relevant action attempts sensitive access, outbound delivery, persistence, deletion, a security-state change, or another lasting effect. Goal and target authorization also examine actions whose relevance is unresolved. The contracts distinguish satisfied, violated, not applicable (NA), and insufficient evidence (IE). For an applicable existential predicate, satisfaction requires an anchored witness; violation requires sufficient coverage to rule out such a witness. Universal satisfaction requires coverage of the action domain, whereas one established counterexample supports violation. Missing evidence is IE, not proof of an empty domain. Predicate wording, source roles, action domains, and verbalizers are fixed together for each evaluated configuration.

Illustrative example (constructed, not an experiment). A user requests an invoice summary. A retrieved page instructs the agent to send a private attachment elsewhere. Observing this instruction supports F01; adopting it beyond the requested task supports F02. A transfer attempt supports F10, and its denial supports F12 without establishing F07 or a realized transfer. A separate successful authorized action may support F11, but does not show that the denied transfer succeeded. Retaining event identity prevents evidence from different actions from being combined into a fictitious harmful event.

C PROOFS AND STATISTICAL CONDITIONS

This appendix proves the results in Sections 3 and 4. Unless a conditional expectation is displayed, expectations include both the task X and the actual deployment draws Ξ. Training, calibration parameters, the state partition, and the scoring protocol are fixed before taking these expectations. All logarithms are natural, with $0 \log 0 = 0$. The reference scores $\mu^\star_{hj}$ are candidate-score targets, not Ising natural parameters; their connection to the true predicate probabilities is represented by the reference-KL bound in Lemma 3.1, which allows deterministic true predicates.

C.1 EVIDENCE ADMISSION AND POLICY INTERFACES

An input x contains the trusted user goal, source-typed messages, tool dispatches, arguments, and observable outcomes. For each rubric $h \in \{1, \dots, H\}$, $H = 12$, an extractor $\mathcal{E}_h$ builds an evidence view from a common inventory of entities, events, and source relations. The interface is shared; the extraction rule, prompt, and verbalizers are not. Existential predicates require an anchored witness, universal predicates require coverage of their action domain, and relational predicates require jointly identified endpoints. For example, goal alignment (F03) and target authorization (F04) need different supporting relations even when they inspect the same action. The twelve contracts appear in Appendix B.

Each extracted statement retains its source, role, span, and event identity. Long views are split without dropping source text; relations that cannot be resolved within an admitted view remain

Table 3: Predicate semantics and evidence requirements. Satisfaction denotes the stated fact, not a uniform direction of risk: F03, F04, and F06 express compliance, while other heads describe events or outcomes.

Head	Predicate family	Satisfaction and applicability
F01	External directive	At least one external source contains a behavioral instruction addressed to the assistant. A complete empty directive inventory supports violation.
F02	Directive adoption	Observable behavior implements a qualifying directive beyond the user-authorized task. Link the directive to the action; NA if F01 is violated.
F03	Goal authorization	Every relevant action goal is explicit in the user task, necessary to it, or an admissible tool recovery. NA only when no relevant or relevance-uncertain action exists.
F04	Target authorization	Every relevant attempted target lies within the smallest set authorized by visible user instructions. Judge the target before the outcome; the same empty-domain rule as F03 gives NA.
F05	Sensitive return	A relevant action observably supplies sensitive content to the agent. An inaccessible or unobserved return cannot establish this fact.
F06	Sensitive access scope	Every attempted sensitive access matches the task without avoidable excess or unnecessary secondary use. NA when no sensitive access is attempted.
F07	Sensitive domain flow	A relevant action observably transfers sensitive content outside the user-authorized trust domain. Content, transfer, and destination must belong to the same event.
F08	Persistent or outbound effect	A relevant action realizes outbound delivery, a persistent write, deletion, an integrity or security-state change, or another persistent effect. An attempt alone is insufficient.
F09	Security-state change	A relevant action observably changes an operative security control. Evidence must establish the change, not merely mention the control.
F10	Relevant action attempt	At least one relevant action is attempted. Hypothetical mentions do not qualify; IE applies when only relevance-uncertain candidates remain.
F11	Effect realization	A relevant action realizes an observable effect, including sensitive content returned to the agent or another transient or persistent effect.
F12	Failure, block, or reversal	A relevant attempted action is observably denied, blocked, failed, timed out, cancelled, or reverted. This can coexist with F11 for another action or an effect later reversed.

Table 4: Notation for the scoring-to-decision analysis. All model and calibration parameters are frozen when a deployment expectation is taken.

Symbol	Meaning
$h, h';\ j;\ r$	Predicate indices; one of four candidate–context pairs; MC draw index.
$n = n_{\mathrm{mc}}$	Draws per candidate and context on one input.
X, S, Y_h	Input, true binary predicate state, and satisfaction label $(S_h + 1)/2$.
$Z_{r,hj}, \mu_{hj}, \widehat{\mu}_{hj,n}$	Draw score, conditional mean score, and finite-draw average.
$\widehat{g}_{\alpha,n,h}, \widehat{\eta}_h, \widehat{z}_{h,\alpha_h,n}$	Evidence contrast, dimensionless unary field, and uncoupled logit $2\widehat{\eta}_h$.
b_{hj}, v_{hj}	Mean-score squared-error bound and draw-variance bound.
$z_h^{\mathrm{ref}}, p_h^{\mathrm{ref}}, \kappa_h$	Finite reference logit, its sigmoid probability, and semantic reference-KL radius (risk at most $\kappa_h^2/8$).
$P_X^\star, \widehat{q}_{\alpha,K,n}$	True conditional state law and finite-draw Ising state law.
U_c, C, U	Fixed partition cell, true cell label, and dangerous union of cells.
$\mathcal{Z}_A, F_A$	Restricted state partition function and dimensionless free energy $-\log \mathcal{Z}_A$.
$\mathcal{K}_h, \mathcal{K}_C, \mathcal{B}_{\mathrm{reg}}$	Predicate KL risk, regional KL risk, and the cascade upper bound.
$m_{\mathrm{P}}, m_{\mathrm{I}};\ b$	Independent calibration-task counts for the two gains; calibration-task index.
$\delta_{\mathrm{cal}}, \delta$	Calibration-bound failure probability and subsequent deployment failure probability.

unresolved rather than being inferred from unrelated windows. Serialization fidelity and semantic sufficiency are distinct requirements. In particular, an attempted action, a realized effect, and a blocked outcome cannot be exchanged, or joined across different events, to construct a risk witness.

We distinguish satisfied, violated, not applicable (NA), and insufficient evidence (IE). The binary-state analysis concerns the branch on which all twelve predicates have admitted binary semantics.

For the random predicate state $S = (S_1, \ldots, S_H)$, we encode violation and satisfaction by $S_h = -1$ and $S_h = +1$, respectively, and set $Y_h = (S_h + 1)/2$. A lowercase s denotes a realized state; predicate satisfaction must not be confused with a safe trajectory. Unresolved heads are not deleted to change the state space; unadmitted inputs remain policy-level cases with separately reported coverage. NA is not a neutral probability, and IE is not a negative label; unresolved required evidence is exposed to PAC. For example, an external directive and an authorized target have different safety implications. The threat model permits adversarial lower-trust content, but assumes trusted provenance and policy code are not compromised. We verify the information available at the decision time; retrospective outcomes cannot be used to claim prospective prevention.

C.2 Optional certified policy interface

PAC is the executable, symbolic boundary of the verifier. It receives the structured belief, evidence-admission flags, and independently evaluated hard constraints. A verified hard-rule violation takes precedence over a favorable neural score; missing required provenance or unresolved predicates trigger approval rather than silent acceptance. On the admitted branch, a score-based interface applies a frozen threshold $\tau \in (0, 1)$ to the chosen risk score; its empirical performance is evaluated under that complete decision rule. The statistical analysis below concerns the region-mass score $\widehat{p}_U$. An optional, more conservative interface additionally requires a validated probability-error radius $r \geq 0$:

$$\Pi_{\mathrm{cert}}(x, \Xi) = \begin{cases} \textsc{block}, & \text{a hard-rule violation is established,} \\ \textsc{require approval}, & \text{required evidence or a certificate is unavailable,} \\ \textsc{safe}, & \widehat{p}_U + r < \tau, \\ \textsc{block}, & \widehat{p}_U - r \geq \tau, \\ \textsc{require approval}, & \text{otherwise.} \end{cases} \tag{18}$$

Here Ξ denotes the collection of MC draws. The branches are ordered and deterministic given their inputs; repeated model sampling may still change those inputs. Corollary 4.1 supplies a population-valid choice $r = R_p$ only when all of its prerequisites hold. The benchmark evaluates its frozen empirical operating point; it does not instantiate or validate this optional certificate. The returned record includes rule identifiers, evidence receipts, model and policy versions, and the score used by the decision. Hard constraints are a backstop for the behaviors they soundly recognize, not a claim of complete hazard coverage. Section 4 characterizes the neural score and its threshold branch. Certification of the entire policy additionally requires sound rule semantics and an explicit treatment of approval, abstention, and operational outcomes. Throughout this paper, PAC names *Policy As Code*, not an abbreviation for a statistical guarantee.

C.3 Finite-sample scoring and reveal-order averaging

Let $\mu_{hj}(X) = \mathbb{E}[Z_{r,hj} \mid X]$ and let $\mu^\star_{hj}(X)$ be an X-measurable reference candidate score. The draw vectors are iid conditional on X and independent of S given X.

The reveal-order identity is stated in Equation (2); the calculation below establishes its exact weighting.

Proof of Proposition 3.1. For a fixed head and candidate, abbreviate $\mu = \mathbb{E}[Z_r \mid X]$, $\mu^\star = \mu^\star_{hj}$, and $\widehat{\mu}_n = n^{-1} \sum_{r=1}^n Z_r$. Conditional independence of the draws gives

$$\mathbb{E}[\widehat{\mu}_n - \mu \mid X] = 0, \qquad \mathrm{Var}(\widehat{\mu}_n \mid X) = \frac{\mathrm{Var}(Z_r \mid X)}{n}. \tag{19}$$

The cross term between $\widehat{\mu}_n - \mu$ and the X-measurable quantity $\mu - \mu^\star$ therefore vanishes. Consequently,

$$\mathbb{E}(\widehat{\mu}_n - \mu^\star)^2 = \mathbb{E}_X(\mu - \mu^\star)^2 + \frac{\mathbb{E}_X \,\mathrm{Var}(Z_r \mid X)}{n} \leq b_{hj} + \frac{v_{hj}}{n} = \mathcal{B}_{hj}(n). \tag{20}$$

This identity concerns the variance of an actual mask draw, including any randomization used by that draw.

For the additional autoregressive comparison, write $E^\star = \mu^\star_{hj}$ and use the $L^2(\mathcal{D}_X)$ reverse triangle inequality:

$$\begin{aligned}\|E_{\mathrm{AR}} - E^\star\|_2 &\geq \|E^{\pi_0}_{\mathrm{M}} - E^\star\|_2 - \|E^{\pi_0}_{\mathrm{M}} - E_{\mathrm{AR}}\|_2 \\ &\geq \|E^{\pi_0}_{\mathrm{M}} - E^\star\|_2 - \varepsilon_{\mathrm{AR}}.\end{aligned} \tag{21}$$

Under the stated strict margin, the last expression exceeds $\sqrt{\mathcal{B}_{hj}(n)}$. Squaring and applying Equation (20) establishes the comparison. The cascade theorem uses the absolute budget only; it does not require this additional comparison condition. □

Exact reveal-order representation. Fix an input context and a complete candidate $v = (v_1, \ldots, v_L)$, with $[L] = \{1, \ldots, L\}$. For $t \notin O \subseteq [L]$, let $\nu_t(O)$ be the negative log probability assigned to v_t when exactly the candidate positions in O have been revealed and the other positions remain masked. The external context is held fixed. A uniformly random permutation π defines

$$E^\pi_{\mathrm{M}} = \frac{1}{L}\sum_{k=1}^{L} \nu_{\pi_k}(\{\pi_1, \ldots, \pi_{k-1}\}). \tag{22}$$

Consider the mask protocol that samples k uniformly from $\{1, \ldots, L\}$, then samples a uniform k-element mask set M, and returns $|M|^{-1}\sum_{t\in M}\nu_t([L]\setminus M)$. For a particular query (t, O), set $k = L - |O|$. Its weight in the expected mask score is $[L\binom{L}{k}k]^{-1}$. Exactly $(L-k)!(k-1)!$ permutations reveal precisely O before t, so its weight in Equation (22) averaged over permutations is the same:

$$\frac{1}{L\binom{L}{k}k} = \frac{1}{L}\frac{(L-k)!(k-1)!}{L!}. \tag{23}$$

Summing over queries proves $\mathbb{E}_\pi E^\pi_{\mathrm{M}} = \mathbb{E}_{\mathrm{mask}} Z = \overline{E}_{\mathrm{M}}$. This identity requires the specified weighting and the same conditional query in both constructions. A different noise schedule, an additional time-dependent model input, or a different length normalization requires a corresponding identity; one mask draw is not itself an entire reveal path.

What averaging can improve. For the reference $E^\star = \mu^\star_{hj}$ of this candidate and context, let $e_\pi = E^\pi_{\mathrm{M}} - E^\star$. Conditional variance decomposition yields

$$\begin{aligned}&\mathbb{E}_X e^2_{\pi_0} - \mathbb{E}_X(\overline{E}_{\mathrm{M}} - E^\star)^2 \\ &\quad = \left(\mathbb{E}_X e^2_{\pi_0} - \mathbb{E}_{X,\pi} e^2_\pi\right) + \mathbb{E}_X \operatorname{Var}_{\pi|X}(e_\pi).\end{aligned} \tag{24}$$

Thus aggregation reduces the model's mean-score error relative to its prefix path when the average path quality is no worse and path disagreement is nonzero. The finite-sample comparison must additionally cover the actual mask variance and the prefix-to-AR discrepancy. This distinguishes an order-averaging mechanism from an unconditional claim that diffusion classification dominates autoregressive classification. Both architectures can score a complete multi-token candidate.

C.4 From candidate error to predicate KL

Let $p^\star_h(X) = \Pr(Y_h = 1 \mid X) \in [0, 1]$ and define $\mathcal{K}_h(\alpha_h) = \mathbb{E}\,\mathrm{KL}(\mathrm{Ber}(p^\star_h)\|\mathrm{Ber}(p_{h,\alpha_h,n}))$. Here $\mathrm{Ber}(p)$ denotes a Bernoulli distribution and KL is Kullback–Leibler divergence. The quantity is excess predicate NLL relative to the true conditional entropy; its dependence on the fixed draw count n is suppressed in $\mathcal{K}_h$.

The reference-KL condition permits deterministic true predicates. It is a semantic calibration assumption, not a consequence of low candidate reconstruction error.

Proof of Lemma 3.1. Write $\delta\mu_{hj} = \widehat{\mu}_{hj,n} - \mu^\star_{hj}$. At the fixed draw count n, abbreviate the uncorrected logit by $\widehat{z}_{h,0} := \widehat{z}_{h,0,n} = 2\lambda_h \widehat{R}_{h,n} + 2d_h$. Its error relative to the finite reference logit is

$$W_h := \widehat{z}_{h,0} - z^{\mathrm{ref}}_h = 2\lambda_h(\delta\mu_{h1} - \delta\mu_{h2}). \tag{25}$$

Minkowski's inequality and Proposition 3.1 give

$$\|W_h\|_2 \leq 2|\lambda_h|\left(\sqrt{\mathcal{B}_{h1}(n)} + \sqrt{\mathcal{B}_{h2}(n)}\right). \tag{26}$$

No independence between the candidate errors is required. For $p \in [0,1]$, define the binary entropy $H_{\mathrm{B}}(p) = -p\log p - (1-p)\log(1-p)$ and the finite-logit divergence $d_p(z) = \mathrm{KL}(\mathrm{Ber}(p)\|\mathrm{Ber}(\mathrm{sigmoid}\, z)) = \psi(z) - pz - H_{\mathrm{B}}(p)$, where $\psi(z) = \log(1+e^z)$. Since $d_p'(z) = \mathrm{sigmoid}\, z - p$ and $d_p''(z) = \mathrm{sigmoid}\, z(1-\mathrm{sigmoid}\, z) \le 1/4$, Taylor's inequality gives

$$d_{p_h^\star}(\widehat{z}_{h,0}) \le d_{p_h^\star}(z_h^{\mathrm{ref}}) + (p_h^{\mathrm{ref}} - p_h^\star)W_h + W_h^2/8. \tag{27}$$

Pinsker's inequality and the reference-KL assumption imply $\mathbb{E}_X(p_h^{\mathrm{ref}} - p_h^\star)^2 \le \kappa_h^2/16$. Taking expectations and applying Cauchy–Schwarz therefore yields

$$\mathcal{K}_h(0) \le \frac{\kappa_h^2}{8} + \frac{\kappa_h\|W_h\|_2}{4} + \frac{\|W_h\|_2^2}{8} = \frac{(\kappa_h + \|W_h\|_2)^2}{8} \le \mathcal{B}_h^0(n). \tag{28}$$

This proof uses no true logit and covers $p_h^\star = 0$ or 1. □

Interior-logit sufficient condition. When $p_h^\star \in (0,1)$ almost surely, let $z_h^\star = \mathrm{logit}\, p_h^\star$ and $\zeta_h^0 = z_h^{\mathrm{ref}} - z_h^\star$. Bernoulli KL is the logistic Bregman divergence, and the same curvature bound gives

$$\begin{aligned}\mathrm{KL}\big(\mathrm{Ber}(p_h^\star)\|\,\mathrm{Ber}(\mathrm{sigmoid}(z))\big) &= \psi(z) - \psi(z_h^\star) - \psi'(z_h^\star)(z - z_h^\star) \\ &\le \frac{(z - z_h^\star)^2}{8}.\end{aligned} \tag{29}$$

Consequently $\mathbb{E}_X(\zeta_h^0)^2 \le \kappa_h^2$ implies Equation (5). Equivalently, the direct logit argument uses $\widehat{z}_{h,0} - z_h^\star = W_h + \zeta_h^0$, $\|\widehat{z}_{h,0} - z_h^\star\|_2 \le \|W_h\|_2 + \kappa_h$, and Equation (29) to obtain the same budget. This interior condition is a sufficient special case; it is not imposed on deterministic predicates by the cascade theorem.

Pairing-aware refinement. Stack the $4H$ scores from draw r into the vector $Z_r = (Z_{r,11}, \ldots, Z_{r,14}, Z_{r,21}, \ldots, Z_{r,H4})^{\mathsf{T}}$. Let $C_Z(X) = \mathrm{Cov}(Z_r \mid X)$; its entry $C_{Z,(h,j),(h',j')}$ is the conditional covariance of the indicated scores. Suppose $v_{R,h} \ge \mathbb{E}_X \mathrm{Var}(Z_{r,h1} - Z_{r,h2} \mid X)$ is a valid upper bound. Let $\overline{W}_h(X) = \mathbb{E}[W_h \mid X]$. Splitting reference-logit error into its conditional mean and zero-mean sampling error gives the exact identity

$$\begin{aligned}\mathbb{E}W_h^2 = \mathbb{E}_X\left[2\lambda_h\big((\mu_{h1} - \mu_{h1}^\star) - (\mu_{h2} - \mu_{h2}^\star)\big)\right]^2 \\ + \frac{4\lambda_h^2}{n}\mathbb{E}_X\left[C_{Z,(h,1),(h,1)} + C_{Z,(h,2),(h,2)} - 2C_{Z,(h,1),(h,2)}\right].\end{aligned} \tag{30}$$

In the linear term of Equation (27), $p_h^{\mathrm{ref}} - p_h^\star$ is X-measurable, so $\mathbb{E}[(p_h^{\mathrm{ref}} - p_h^\star)W_h] = \mathbb{E}_X[(p_h^{\mathrm{ref}} - p_h^\star)\overline{W}_h]$. Its upper bound is $\kappa_h\|\overline{W}_h\|_2/4$, where $\|\overline{W}_h\|_2 \le 2|\lambda_h|(\sqrt{b_{h1}} + \sqrt{b_{h2}})$. Combining this with the variance term above gives the second valid budget

$$\mathcal{B}_{h,\mathrm{cov}}^0(n) = \frac{1}{8}\left\{\left[2|\lambda_h|(\sqrt{b_{h1}} + \sqrt{b_{h2}}) + \kappa_h\right]^2 + \frac{4\lambda_h^2 v_{R,h}}{n}\right\}. \tag{31}$$

When both budgets are valid, their minimum can be used. The first term uses the mean-score bounds b_{hj}, not the finite-MC bounds $\mathcal{B}_{hj}(n)$; otherwise sampling uncertainty would be counted twice. Pairing is useful through its actual covariance, rather than by assumption.

More generally, stack the sample means in the same order into $\widehat{\mu}_n \in \mathbb{R}^{4H}$. Let $A_\alpha \in \mathbb{R}^{H\times 4H}$ be the block-diagonal linear map with head block $(1, -1, -\alpha_h, +\alpha_h)$. It preserves the full within-draw covariance:

$$\widehat{g}_{\alpha,n} = A_\alpha\widehat{\mu}_n, \qquad \mathrm{Cov}(\widehat{g}_{\alpha,n} \mid X) = \frac{A_\alpha C_Z(X) A_\alpha^{\mathsf{T}}}{n}. \tag{32}$$

C.5 Residual alignment of the real/null contrast

The quantities $D_{h,n}$, $a_{\mathrm{P},h}$, and $V_{\mathrm{P},h}$ are defined with Proposition 3.2.

Proof of Proposition 3.2. Fix a head and abbreviate $D = 2\lambda_h\widehat{N}_{h,n}$. With the base model, calibration map, and MC protocol held fixed, changing the contrast strength $a \ge 0$ changes the logit only

through $z_a = \widehat{z}_{h,0} - aD$. For a realized label and draw, the binary log loss is

$$\begin{aligned} L(a) &= \psi(z_a) - Y_h z_a, \\ L'(a) &= -D(p_{h,a,n} - Y_h), \\ L''(a) &= D^2 p_{h,a,n}(1 - p_{h,a,n}). \end{aligned} \tag{33}$$

Thus $0 \le L''(a) \le D^2/4$. The finite second moment of D justifies exchanging expectation and differentiation. Because the true conditional entropy does not depend on a, expected NLL and $\mathcal{K}_h(a)$ have the same derivatives. Taylor's inequality yields

$$\mathcal{K}_h(\alpha_h) \le \mathcal{K}_h(0) - \alpha_h a_{\mathrm{P},h} + \frac{\alpha_h^2 V_{\mathrm{P},h}}{8} = \mathcal{K}_h(0) - \Delta_{\mathrm{P},h}. \tag{34}$$

Substituting Lemma 3.1 proves the claimed budget. When $a_{\mathrm{P},h} > 0$ and $V_{\mathrm{P},h} > 0$, the quadratic gain is positive for $0 < \alpha_h < 8a_{\mathrm{P},h}/V_{\mathrm{P},h}$ and is maximized at $\alpha_h = 4a_{\mathrm{P},h}/V_{\mathrm{P},h}$, if feasible. The resulting guaranteed gain is $2a_{\mathrm{P},h}^2/V_{\mathrm{P},h}$.

Conversely, convexity gives $\mathcal{K}_h(a) \ge \mathcal{K}_h(0) - a a_{\mathrm{P},h}$. If $a_{\mathrm{P},h} \le 0$, no nonnegative strength improves the frozen local loss. If $V_{\mathrm{P},h} = 0$, then $D = 0$ almost surely and the contrast has no effect. □

This statement concerns a fixed additive logit contrast. Strength-dependent clipping, nonlinear recalibration, a changed sampling law, or a changed NULL construction changes the derivative contract. Independent repetitions of the same sampling law leave the expected objective unchanged. The result establishes a loss benefit from residual alignment; it does not identify a causal intervention merely from the presence of a real/null pair.

C.6 Product decomposition and regional contraction

Proof of Lemma 3.2. Fix (X, Ξ) and write $P = P_X^\star$, $P_h = P_{X,h}^\star$, and $Q = \widehat{q}_{\alpha,0,n} = \prod_h Q_h$. Inserting $\prod_h P_h$ into the likelihood ratio gives

$$\begin{aligned} \mathrm{KL}(P\|Q) &= \mathbb{E}_P \log \frac{P(S)}{\prod_h P_h(S_h)} + \sum_h \mathbb{E}_P \log \frac{P_h(S_h)}{Q_h(S_h)} \\ &= \mathrm{KL}\left(P \middle\| \prod_h P_h\right) + \sum_h \mathrm{KL}(P_h\|Q_h). \end{aligned} \tag{35}$$

The conditional independence of S and Ξ ensures that the true conditional law remains $P_X^\star$ when a draw is fixed. Averaging Equation (35) therefore yields

$$\mathbb{E}\,\mathrm{KL}(P_X^\star\|\widehat{q}_{\alpha,0,n}) = \mathrm{TC}_{\mathcal{D}} + \sum_h \mathcal{K}_h(\alpha_h). \tag{36}$$

For the deterministic state-to-region map, let $\pi_c = P(U_c)$ and $Q_C(c) = Q(U_c)$. The chain rule for KL gives

$$\mathrm{KL}(P\|Q) = \mathrm{KL}(\pi\|Q_C) + \sum_{c:\pi_c>0} \pi_c\,\mathrm{KL}\big(P(\cdot \mid U_c)\|Q(\cdot \mid U_c)\big). \tag{37}$$

All terms in the sum are nonnegative. Discarding them, averaging, and using Proposition 3.2 proves

$$\mathcal{K}_C(\alpha, 0) \le \mathrm{TC}_{\mathcal{D}} + \sum_h \mathcal{K}_h(\alpha_h) \le \overline{\mathrm{TC}} + \sum_h \big(\mathcal{B}_h^0(n) - \Delta_{\mathrm{P},h}\big). \tag{38}$$

□

The proof does not assume independent true predicates or an exactly pairwise-Ising true posterior. It also explains why lower state-level KL need not imply lower regional KL: the conditional KL discarded in Equation (37) can change between models.

C.7 Regional gain from an Ising direction

We use the frozen direction and alignment defined with Proposition 3.3.

Proof of Proposition 3.3. Fix the contrast parameters and an interaction direction u with $\sum_{h<h'} |u_{hh'}| = 1$. Then $T_u(s) = \sum_{h<h'} u_{hh'} s_h s_{h'} \in [-1, 1]$. Relative to $\widehat{q}_0 = \widehat{q}_{\alpha,0,n}$, the coupled model is

$$\widehat{q}_\rho(s) = \frac{\widehat{q}_0(s) e^{\rho T_u(s)}}{\sum_{s'} \widehat{q}_0(s') e^{\rho T_u(s')}}. \tag{39}$$

For a realized region C, define the relative normalizers $\widetilde{\mathcal{Z}}(\rho) = \sum_s \widehat{q}_0(s) e^{\rho T_u(s)}$ and $\widetilde{\mathcal{Z}}_C(\rho) = \sum_{s \in U_C} \widehat{q}_0(s) e^{\rho T_u(s)}$. The regional NLL is $L(\rho) = \log \widetilde{\mathcal{Z}}(\rho) - \log \widetilde{\mathcal{Z}}_C(\rho)$. Finite-state differentiation gives

$$L'(\rho) = \mathbb{E}_{\widehat{q}_\rho} T_u - \mathbb{E}_{\widehat{q}_\rho}[T_u \mid U_C], \tag{40}$$

$$L''(\rho) = \mathrm{Var}_{\widehat{q}_\rho}(T_u) - \mathrm{Var}_{\widehat{q}_\rho(\cdot|U_C)}(T_u). \tag{41}$$

Both variances lie in $[0, 1]$, so $L''(\rho) \in [-1, 1]$ and $|L'(\rho)| \le 2$. Taylor's integral remainder, followed by expectation, yields

$$\mathcal{K}_C(\alpha, \rho u) \le \mathcal{K}_C(\alpha, 0) - \rho a_{\mathrm{I}} + \rho^2/2 = \mathcal{K}_C(\alpha, 0) - \Delta_{\mathrm{I}}. \tag{42}$$

If $a_{\mathrm{I}} > 0$, the guaranteed gain is positive for $0 < \rho < 2a_{\mathrm{I}}$ and equals $a_{\mathrm{I}}^2/2$ at the feasible choice $\rho = a_{\mathrm{I}}$. The regional objective need not be convex: $a_{\mathrm{I}} \le 0$ means that this bound does not certify a positive gain, not that every positive interaction strength must fail. □

The comparison is against the same frozen PMI baseline. It does not require that fitted interactions approximate an unknown true coupling matrix. A direction learned from labels must nevertheless be fixed independently of the data used for its single-direction statistical certificate, unless simultaneous coverage is provided.

C.8 Composition of the finite-MC risk budget

Proof of Theorem 4.1. All component results refer to the same task distribution, draws, calibration map, contrast parameters, and region partition. Applying them in order gives

$$\mathcal{K}_C(\alpha, K) \le \mathcal{K}_C(\alpha, 0) - \Delta_{\mathrm{I}} \tag{43}$$

$$\le \mathrm{TC}_{\mathcal{D}} + \sum_h \mathcal{K}_h(\alpha_h) - \Delta_{\mathrm{I}} \tag{44}$$

$$\le \mathrm{TC}_{\mathcal{D}} + \sum_h \mathcal{K}_h(0) - \sum_h \Delta_{\mathrm{P},h} - \Delta_{\mathrm{I}} \tag{45}$$

$$\le \overline{\mathrm{TC}} + \sum_h \mathcal{B}_h^0(n) - \sum_h \Delta_{\mathrm{P},h} - \Delta_{\mathrm{I}} = \mathcal{B}_{\mathrm{reg}}(n). \tag{46}$$

The first three steps use Proposition 3.3, Lemma 3.2, and Proposition 3.2, respectively. The final step uses Lemma 3.1, Proposition 3.1, and the assumed total-correlation bound. Alternatively, any valid finite upper bounds on the same baseline risks $\mathcal{K}_h(0)$ suffice for that final step. Every term already includes the finite deployment MC; no second MC error radius is added. □

Any simultaneously valid lower bound on a module gain may replace that gain, yielding a conservative bound. If a lower bound is nonpositive, a module can be disabled and its gain set to zero only by actually making that change and evaluating subsequent terms for the resulting frozen model. In particular, the Ising alignment signal depends on the chosen contrast baseline. Under valid assumptions, $\mathcal{B}_{\mathrm{reg}}$ and each asserted local KL upper bound are nonnegative. A negative estimated budget signals an invalid bound, selection event, or model contract; truncating it to zero does not repair certification.

C.9 From regional KL to dangerous-state probability and log odds

The probability and optional log-odds certificates are stated together in Corollary 4.1; the latter requires its additional interior-probability condition.

Proof of Corollary 4.1 and its log-odds extension. Because U is a union of cells of the fixed partition, another deterministic map sends the region label to $Y_U = \mathbf{1}\{S \in U\}$. Data processing gives

$$\mathbb{E}\,\mathrm{KL}\big(\mathrm{Ber}(p_U^\star)\|\,\mathrm{Ber}(\widehat{p}_U)\big) \le \mathcal{K}_C(\alpha, K) \le \mathcal{B}_{\mathrm{reg}}(n). \tag{47}$$

Bernoulli Pinsker gives $\mathrm{KL}(\mathrm{Ber}(p)\|\,\mathrm{Ber}(q)) \ge 2(p-q)^2$. Taking expectations, then applying Markov's inequality to the squared error, proves

$$\begin{aligned} \mathbb{E}(\widehat{p}_U - p_U^\star)^2 &\le \frac{\mathcal{B}_{\mathrm{reg}}(n)}{2}, \\ \Pr_{X,\Xi}\left(|\widehat{p}_U - p_U^\star| > \sqrt{\frac{\mathcal{B}_{\mathrm{reg}}(n)}{2\delta}}\right) &\le \delta. \end{aligned} \tag{48}$$

If the budget is zero, the squared error is zero almost surely and the same conclusion holds directly.

For the log-odds version, suppose both $p_U^\star$ and $\widehat{p}_U$ belong to $[\varepsilon, 1-\varepsilon]$ almost surely. Every point on the segment between $\ell^\star = \operatorname{logit} p_U^\star$ and $\widehat{\ell} = \operatorname{logit} \widehat{p}_U$ then satisfies $\psi'' \ge \varepsilon(1-\varepsilon)$. The reverse curvature bound to Equation (29) yields

$$\mathrm{KL}\big(\mathrm{Ber}(p_U^\star)\|\,\mathrm{Ber}(\widehat{p}_U)\big) \ge \frac{\varepsilon(1-\varepsilon)}{2}(\widehat{\ell} - \ell^\star)^2. \tag{49}$$

Combining this with Equation (47) and Markov gives

$$\begin{aligned} \mathbb{E}(\widehat{\ell} - \ell^\star)^2 &\le \frac{2\mathcal{B}_{\mathrm{reg}}(n)}{\varepsilon(1-\varepsilon)}, \\ R_\ell(\delta; n) &= \sqrt{\frac{2\mathcal{B}_{\mathrm{reg}}(n)}{\varepsilon(1-\varepsilon)\delta}}, \\ \Pr_{X,\Xi}(|\widehat{\ell} - \ell^\star| > R_\ell) &\le \delta. \end{aligned} \tag{50}$$

□

The log-odds constant follows from logistic strong convexity, not from simply composing Pinsker with a logit Lipschitz bound. The probability result does not need this interior-probability assumption. Clipping only the prediction does not establish the condition on the true posterior. Both certificates concern the joint task–MC distribution, rather than conditional coverage for every fixed input.

C.10 Margin-protected decisions

Proof of Corollary 4.2. Let $\mathcal{E}_\delta = \{|\widehat{p}_U - p_U^\star| \le R_p(\delta; n)\}$, with coverage from Corollary 4.1. On this event, a true margin $M_p(X) = |p_U^\star - \tau| > R_p$ prevents the estimate from crossing the fixed threshold τ. With a common tie convention,

$$\{\widehat{a} \ne a^\star\} \subseteq \mathcal{E}_\delta^c \cup \{M_p(X) \le R_p(\delta; n)\}. \tag{51}$$

The union bound proves

$$\Pr_{X,\Xi}(\widehat{a} \ne a^\star) \le \Pr_X(M_p(X) \le R_p(\delta; n)) + \delta. \tag{52}$$

Replacing probability by log odds, τ by $t = \operatorname{logit} \tau$, and R_p by R_ℓ proves the corresponding log-odds version under its additional conditions. Independence of the error and low-margin events is not needed.

At $\tau = 1/2$, $a^\star$ is a Bayes classifier for Y_U. Pointwise,

$$\mathbf{1}\{\widehat{a} \ne Y_U\} \le \mathbf{1}\{a^\star \ne Y_U\} + \mathbf{1}\{\widehat{a} \ne a^\star\}. \tag{53}$$

Define $R_{0\text{–}1}(\widehat{a}) = \Pr(\widehat{a} \ne Y_U)$ and $R_{\mathrm{Bayes}} = \Pr(a^\star \ne Y_U)$. Taking expectations gives $R_{0\text{–}1}(\widehat{a}) \le R_{\mathrm{Bayes}} + \eta_{\mathrm{margin}} + \delta$ whenever $\Pr_X(M_p(X) \le R_p) \le \eta_{\mathrm{margin}}$. □

An output-based certificate is also possible: if $|\widehat{p}_U - \tau| > R_p$ (or $|\widehat{\ell} - t| > R_\ell$), any disagreement with the corresponding true-posterior action requires failure of the coverage event. Hence the population probability of a wrong certified action is at most δ. The conditional error rate among certified outputs is not automatically bounded by δ; that statement additionally depends on the probability of certification.

C.11 Finite calibration, estimands, and scope

Domain of the binary-state analysis. The distribution $\mathcal{D}$ in these results is the analysis branch on which all twelve heads have admitted binary semantics. If this branch is obtained by an admission condition fixed before scoring, all expectations, calibration coverage, and risk guarantees concern that conditional population. Selecting admitted inputs using the scoring draws can change their conditional law and requires a separate argument. An inapplicable or insufficient-evidence predicate is not silently assigned probability $1/2$, converted into a negative label, or removed from the twelve-head model. Such inputs follow the explicit policy path, and full-input admission, abstention, and coverage rates must be reported separately. The present branch-level certificate does not automatically extend to the unconditional input population.

A finite-data certificate for contrast alignment. Fix the model, affine calibration, NULL construction, and sampling law independently of the following calibration tasks. Assume a known deterministic bound $|D_{h,n}| \le M_h < \infty$. Use $m_{\mathrm{P}} \ge 1$ iid calibration tasks from $\mathcal{D}$, each with an independent run of the same n-draw protocol. A superscript (b) denotes the quantities on calibration task b. The empirical alignment is

$$\widehat{a}_{\mathrm{P},h} = \frac{1}{m_{\mathrm{P}}} \sum_{b=1}^{m_{\mathrm{P}}} D_{h,n}^{(b)} \big(p_{h,0,n}^{(b)} - Y_h^{(b)}\big). \tag{54}$$

Each summand lies in $[-M_h, M_h]$. For a chosen failure probability $\delta_{\mathrm{P},h} \in (0,1)$, Hoeffding's inequality and $V_{\mathrm{P},h} \le M_h^2$ give

$$\underline{a}_{\mathrm{P},h} = \widehat{a}_{\mathrm{P},h} - M_h \sqrt{\frac{2\log(1/\delta_{\mathrm{P},h})}{m_{\mathrm{P}}}}, \tag{55}$$

$$\underline{\Delta}_{\mathrm{P},h}(\alpha_h) = \alpha_h \underline{a}_{\mathrm{P},h} - \frac{\alpha_h^2 M_h^2}{8}. \tag{56}$$

With probability at least $1 - \delta_{\mathrm{P},h}$, $\Delta_{\mathrm{P},h}(\alpha_h) \ge \underline{\Delta}_{\mathrm{P},h}(\alpha_h)$ simultaneously for all nonnegative strengths. Strength selection within this envelope is therefore allowed. Searching new NULL constructions or calibration maps requires independent selection data or a valid simultaneous bound. An observed maximum of unbounded NLL-derived scores is not by itself a deterministic bound M_h.

A finite-data certificate for interaction alignment. Freeze the complete uncoupled baseline, including α, the affine calibration, and the scoring protocol, as well as the direction u, independently of these calibration tasks. For $m_{\mathrm{I}} \ge 1$ iid region-labeled tasks, define

$$A_b = \mathbb{E}_{\widehat{q}_0^{(b)}}[T_u \mid U_{C^{(b)}}] - \mathbb{E}_{\widehat{q}_0^{(b)}} T_u \in [-2,2], \qquad \widehat{a}_{\mathrm{I}} = \frac{1}{m_{\mathrm{I}}} \sum_{b=1}^{m_{\mathrm{I}}} A_b. \tag{57}$$

Each task includes a fresh run of the same n-draw protocol. For $\delta_{\mathrm{I}} \in (0,1)$, Hoeffding's inequality gives

$$\underline{a}_{\mathrm{I}} = \widehat{a}_{\mathrm{I}} - \sqrt{\frac{8\log(1/\delta_{\mathrm{I}})}{m_{\mathrm{I}}}}, \qquad \underline{\Delta}_{\mathrm{I}}(\rho) = \rho \underline{a}_{\mathrm{I}} - \rho^2/2. \tag{58}$$

With probability at least $1 - \delta_{\mathrm{I}}$, $\Delta_{\mathrm{I}}(\rho) \ge \underline{\Delta}_{\mathrm{I}}(\rho)$ simultaneously for every $\rho \ge 0$. In particular, selecting α using the same tasks changes the baseline of this certificate: a split between contrast selection and interaction certification, or a valid bound simultaneous over the searched baselines, is required. Both gain certificates assume calibration labels follow the stated task-label distribution; agreement among model annotators alone does not establish that premise.

Joint coverage and model selection. Let $\mathcal{F}_{\mathrm{cal}}$ be the event that all used candidate budgets, semantic reference-KL bounds, the total-correlation bound, and module-gain bounds hold for the final frozen model. Suppose $\Pr(\mathcal{F}_{\mathrm{cal}}) \geq 1 - \delta_{\mathrm{cal}}$, with $\delta_{\mathrm{cal}} \in (0, 1)$, and deployment tasks and draws are fresh and independent of calibration. For every calibration realization in $\mathcal{F}_{\mathrm{cal}}$, the cascade and deployment guarantees then apply to its selected, frozen model. If $\Pr_X(M_p(X) \leq R_p(\delta; n)) \leq \eta_{\mathrm{margin}}$ also holds for that realization, integrating over calibration gives an overall disagreement bound of

$$\delta_{\mathrm{cal}} + \eta_{\mathrm{margin}} + \delta. \tag{59}$$

The coverage failure δ_{cal} includes all estimated prerequisites, not just the two alignment signals. A union bound over valid component events is sufficient; independence between those events is not necessary. A radius chosen using calibration data must be interpreted conditionally on the frozen model, with a corresponding valid margin-tail control.

Independent statistical units. The draw count $n = n_{\mathrm{mc}}$ is distinct from the numbers m_{P} and m_{I} of independent calibration tasks. Additional masks reduce within-task sampling uncertainty but do not create new independent semantic or safety labels. Correlated traces from a common source require a group-level sampling assumption and a specified bounded group loss, or another valid dependence-aware concentration argument. A group-level estimand is not automatically the trace-weighted deployment risk.

Identifiable budgets and computational comparisons. The quantity $\mathrm{TC}_{\mathcal{D}}$ depends on the true conditional joint predicate distribution; a small set of regional labels does not identify it. A structural assumption, valid statistical enclosure, or independently justified upper bound is required. A distribution-free coarse bound such as $H \log 2$ is valid but can make the resulting certificate uninformative. Likewise, fitting logits on the evaluation data does not by itself establish the population reference-KL bound $\kappa_h^2/8$. Larger n decreases the explicit candidate variance term, but the contrast and interaction alignment signals also depend on the deployment sampling protocol; the entire selected-model budget is not automatically monotone in n. The contrast comparison holds the REAL sample count fixed and includes an additional NULL computation cost. A matched-compute comparison must account for that cost explicitly.

Relation to executable policy. The analyzed output is the model's dangerous-region posterior and a frozen single-threshold action. Hard triggers, abstention, two-threshold decisions, or region-size adjustments are additional policy operations. Their semantics must be connected to the safety label and their complete frozen decision rule must be analyzed or independently calibrated before transferring a guarantee to the full policy layer. Deterministic execution and auditability do not alone establish correctness of a hard rule. In particular, a nonvacuous model-risk certificate is neither an unconditional proof of safety for every trace nor a substitute for measured coverage and end-to-end safety performance.

D Independent calibration of a complete policy

Policy as Code (PAC) specifies an executable decision procedure. The following result describes how a complete procedure can additionally receive a statistical risk bound; it is distinct from the cascade analysis of Section 4. Let Π be a finite family of $M_\pi \geq 1$ complete policies, fixed independently of the calibration data. For each prespecified constraint $q \in \{1, \ldots, Q\}$, with $Q \geq 1$, let $Z_{q,1}, \ldots, Z_{q,n_q}$ be a fixed number $n_q \geq 1$ of independent and identically distributed calibration units from a target distribution P_q. A unit may be a task, or an independently sampled group of related tasks with a specified group loss. Any randomized policy draws are included in the unit and follow the same distribution at deployment. Define a fixed loss $L_q(\pi; Z) \in [0, 1]$, its population risk $R_q(\pi) = \mathbb{E}_{Z \sim P_q}[L_q(\pi; Z)]$, and its empirical mean $\widehat{R}_q(\pi) = n_q^{-1} \sum_{b=1}^{n_q} L_q(\pi; Z_{q,b})$. Samples and losses may be shared across policies and constraints; independence is required across units within each constraint.

Proposition D.1 (Simultaneous policy-risk bounds)**.** *For $\delta_{\mathrm{pol}} \in (0, 1)$, set*

$$U_q(\pi) = \min\left\{1, \widehat{R}_q(\pi) + \sqrt{\frac{\log(M_\pi Q/\delta_{\mathrm{pol}})}{2n_q}}\right\}. \tag{60}$$

Then, with probability at least $1 - \delta_{\text{pol}}$ *over the calibration data,* $R_q(\pi) \le U_q(\pi)$ *simultaneously for every* $\pi \in \Pi$ *and every* q*. Consequently, any policy selected from* $\widehat{\Pi} = \{\pi \in \Pi : U_q(\pi) \le \epsilon_q \text{ for every } q\}$ *satisfies all prespecified risk tolerances* $\epsilon_q \in [0, 1]$ *on this event. If* $\widehat{\Pi}$ *is empty, no policy is certified.*

Proof. For a fixed (π, q) and $t > 0$, the bounded iid losses satisfy $\Pr(R_q(\pi) - \widehat{R}_q(\pi) > t) \le \exp(-2n_q t^2)$ by Hoeffding's inequality (Hoeffding, 1963). Substituting the square-root term in Equation 60 bounds this probability by $\delta_{\text{pol}}/(M_\pi Q)$. A union bound over all $M_\pi Q$ pairs yields the simultaneous event. Clipping an upper bound at one preserves validity because every population risk is at most one. On that event, $R_q(\pi) \le U_q(\pi) \le \epsilon_q$ holds for every selected policy and constraint. □

The policy includes preprocessing, scoring, risk inference, thresholds, hard checks, approval, abstention, and fallback; its loss must evaluate the operational consequences of these choices. Coverage or approval burden requires an additional explicit constraint if it is part of the intended guarantee. Correlated traces cannot be counted as independent units, and selecting a certified policy does not permit refitting its components on the same calibration data. Other risk-control procedures can replace this bound under their own assumptions (Bates et al., 2021; Angelopoulos et al., 2025). Section 5 reports detection and latency point estimates; it does not instantiate this independent policy-certification procedure.

E Benchmark implementation and additional results

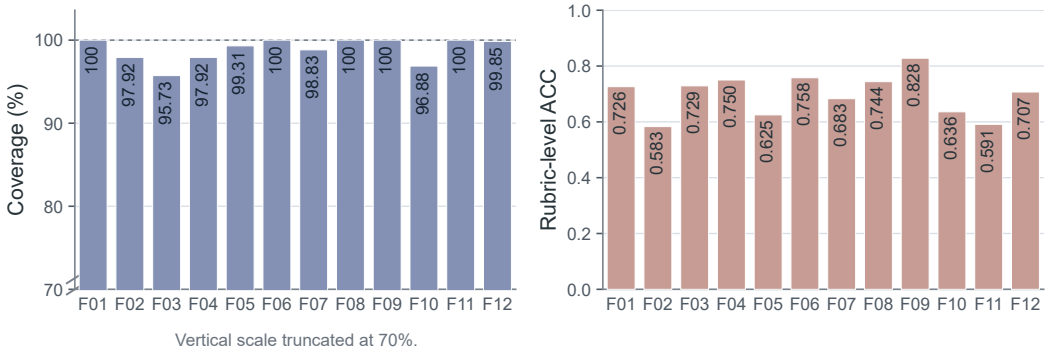
This appendix specifies the reporting conventions and numerical values for Section 5. Benchmark definitions and test-set sizes appear in Section 5.1.

Runtime implementation and timing. The benchmark configuration is frozen LLaDA-8B on one NVIDIA H100, with $\alpha = 0.5$ and $n_{\text{mc}} = 16$, rather than the 32-draw grid maximum. Latency (Lat.) is mean per-trajectory service time in seconds; lower is preferable. For AEGIS, timing covers all four online stages: evidence extraction, MAGIC, Ising inference, and PAC; offline annotation and policy development are excluded. Its 200 timing trajectories are sampled separately from each benchmark and need not coincide with a baseline's full evaluation set. Local execution and commercial API timings include different serving, queueing, and network effects, so they are not hardware-normalized compute or monetary-cost scorings. For Agent-SafetyBench, FORMALJUDGE with Qwen3-14B/32B/80B uses means from three timing repetitions with one worker; the other baseline means come from their full experiments. FORMALJUDGE uses thinking-off with GPT-5.5 and Opus-4.8. For Mixed-SafetyClaw and Upward Deception, Qwen3-80B denotes Qwen3-Next-80B-A3B-Instruct. Across benchmark-matched comparisons, AEGIS takes 9.26–28.33% of direct-LLM/CoT service time, equivalent to the reported 3.53–10.80× speedups. Relative to direct GPT-5.5 alone, the speedups are 3.81×, 3.53×, and 3.95×.

Metric denominators and abstention. For trajectory-level detection, unsafe behavior is the positive class. Let TP and FN count unsafe trajectories predicted unsafe and safe, respectively; FP and TN count safe trajectories predicted unsafe and safe. On valid predictions, the reported percentages are

$$\text{Prec.} = 100\frac{\text{TP}}{\text{TP} + \text{FP}}, \quad \text{Rec.} = 100\frac{\text{TP}}{\text{TP} + \text{FN}}, \quad \text{FPR} = 100\frac{\text{FP}}{\text{FP} + \text{TN}}. \tag{61}$$

Higher precision and recall and lower FPR are preferable; no metric alone resolves all safety trade-offs. UNKNOWN outputs are excluded from these denominators. Valid-prediction coverage is the fraction of evaluated trajectories receiving a non-UNKNOWN verdict and is distinct from precision and recall. For AEGIS, the 22, 18, and 7 UNKNOWN outputs yield 90.39%, 96.50%, and 97.27% coverage on Agent-SafetyBench, Mixed-SafetyClaw, and Upward Deception, respectively. FORMALJUDGE with Opus-4.8 has 32.68% coverage on Mixed-SafetyClaw and 51.56% on Upward Deception. Conditional metrics can therefore describe different accepted subsets; they are not unconditional detection rates. We report the supplied point estimates without inferring integer confusion counts, paired confidence intervals, or significance from aggregate percentages.



(a) Supplied agreement percentages.

(b) Rubric-level classification accuracy.

Figure 5: Rubric study on Mixed-SafetyClaw. Left: supplied agreement percentages, pending reconciliation with the confirmed cohort denominator; the vertical axis is truncated. Right: frozen LLaDA-8B accuracy against unanimous valid model-generated references.

Table 5: Supplied values underlying the rubric plots. Agreement percentages require the reconciliation described above; ACC uses admitted reference labels.

Head	Agreement (%)	ACC (%)	Head	Agreement (%)	ACC (%)
F01	100.00	72.6	F07	98.83	68.3
F02	97.92	58.3	F08	100.00	74.4
F03	95.73	72.9	F09	100.00	82.8
F04	97.92	75.0	F10	96.88	63.6
F05	99.31	62.5	F11	100.00	59.1
F06	100.00	75.8	F12	99.85	70.7

E.1 Rubric agreement and scoring accuracy

Let $\ell_{ih}^{(m)}$ denote annotator $m \in \{1, 2, 3\}$'s label for trace i and rubric $h \in \{1, \ldots, 12\}$, and let N_{ann} be the full Mixed-SafetyClaw cohort size specified in Section 5.1. The intended headwise agreement statistic is

$$A_h^{\text{ann}} = \frac{1}{N_{\text{ann}}} \sum_{i=1}^{N_{\text{ann}}} \mathbf{1}\{\ell_{ih}^{(1)} = \ell_{ih}^{(2)} = \ell_{ih}^{(3)}\}. \tag{62}$$

The indicator is one when the three labels agree and zero otherwise; the panel comprises GPT-5.6-sol, Grok 4.6, and Gemini-3.7-flash. This measures unanimous interpretation, not human-validated correctness, joint twelve-head coverage, or verdict coverage.

Agreement reporting status. Figure 5(a) and Table 5 retain the supplied agreement percentages: 95.73–100%, with an unweighted mean of 98.87% and five heads at 100%. The full annotation cohort is confirmed, but the percentages for F02, F03, F04, F05, F10, and F12 cannot arise by rounding integer unanimous-trace counts under its common denominator. They therefore require reconciliation against per-head counts or the actual aggregation convention before interpretation under Equation 62. The plotting source contains supplied percentages only; it does not establish raw counts. We do not infer replacement counts from the nearest compatible percentages.

For accuracy, let $\mathcal{I}_h$ contain evaluated traces with a unanimous, admissible binary reference label y_{ih}^{ref}, and let $\widehat{y}_{ih}$ be the predicted binary predicate label. Then $\text{ACC}_h = 100|\mathcal{I}_h|^{-1} \sum_{i \in \mathcal{I}_h} \mathbf{1}\{\widehat{y}_{ih} = y_{ih}^{\text{ref}}\}$ when $|\mathcal{I}_h| > 0$. Here satisfaction is positive; it is not the unsafe-outcome label in Equation 61. The rubric-accuracy study uses 192 sampled Mixed-SafetyClaw trajectories with rubric-specific prompts and evidence extraction. Its unweighted mean accuracy is 69.67%, ranging from 58.3% for F02 to 82.8% for F09. These model-generated references may share systematic errors.

Correction and sampling grid. The correction/sampling study uses the full Agent-SafetyBench test set and admits only unanimous valid reference labels. The tested values are $\alpha \in$

Table 6: MaGiC accuracy across the supplied correction/sampling grid (fractions).

α	$n_{\mathrm{mc}} = 8$	16	32	64
0.0	0.549	0.683	0.711	0.708
0.3	0.482	0.655	0.763	0.739
0.5	0.676	0.744	**0.799**	0.797
1.0	0.418	0.596	0.685	0.664

$\{0, 0.3, 0.5, 1.0\}$ and $n_{\mathrm{mc}} \in \{8, 16, 32, 64\}$. The autoregressive (AR) reference uses Qwen3-8B-Instruct with a class-token prompting interface and reports accuracy 0.705 as a fraction. This comparison changes both model family and scoring interface, so it does not identify architectural causality on its own. Table 6 provides the exact plotted values. The best observed setting exceeds AR prompting by 9.4 percentage points (13.33% relative); its gain over no correction at the same budget is 8.8 points. The observed best is a grid maximum, not an independently selected test guarantee.

Ising controls and interpretation. The Ising ablation uses Agent-SafetyBench with common inputs, data partitions, calibration, and decision thresholds across variants. Without Ising, precision, recall, and FPR are 73.43%, 70.15%, and 11.31%; learned interactions yield 76.64%, 72.21%, and 8.35%. Random Sparse combines a sparse graph with random coupling weights, yielding 54.14%, 32.19%, and 48.57%, respectively. The comparison tests the reported learned readout against absent and random interactions; it does not establish robustness over every random graph or instantiate the theoretical risk certificate. Per-head admitted reference counts, the hyperparameter-selection split, and the random-graph seed distribution remain unspecified.