MagNet-IQ — NdFeB Public Seam

Validation Protocol (Expanded) | Internal Draft | Literature- and physics-anchored checkpoints for the public seam segment

At a Glance

This protocol expands the original single-checkpoint MagNet-IQ validation reference into a structured set of predictions covering essentially every measure the public seam publishes — roughly 14 numeric measures plus one classifier label, organized into four validation tiers (gating, cross-measure consistency, algebraic integrity, and informational).

Each prediction is grounded either in published $Nd_2Fe_{14}B$ literature, general critical-phenomena theory (textbook physics, not method-specific), or basic symmetry arguments (e.g., a ferromagnet has no reason to develop antiferromagnetic order). None of these require disclosing the SaC architecture.

Goal: give an external validator a checklist they can run themselves against the public seam frame data — Mean |φ|, ⟨σz⟩, |⟨σ⟩|, ⟨σx⟩, ⟨σy⟩, ξ, f_dom, coherence proxy, staggered magnetization, ⟨H⟩, plus the derived diagnostics — without needing to talk to us first.

What Is and Isn't Claimed

Claimed:

- The direction and approximate shape of the primary order parameter (Mean |φ| / ⟨σz⟩) through each public-seam stage is consistent with where that stage's target temperature sits relative to the $Nd_2Fe_{14}B$ Curie temperature (Tc).
- The onset of order during the “B – reemergence” stage follows a critical-scaling shape (Curie-Bloch form, $\beta \approx 0.42$), not an arbitrary curve.
- Secondary order-sensitive measures (|⟨σ⟩|, f_dom, coherence proxy) move in the same direction as the primary order parameter across all three stages — a cross-measure consistency claim.
- Measures with no physical reason to track ferromagnetic order — staggered (checkerboard) magnetization and the transverse components ⟨σx⟩, ⟨σy⟩ — do not reproduce the Tc-crossing signature seen in the primary order parameter.
- Algebraically-derived measures (z↓ fraction, ordering strength legacy) satisfy their exact stated relationships to ⟨σz⟩ on every frame.

Not claimed:

- A match to extrinsic, microstructure-dependent properties (coercivity, remanence, energy product) — these are context only (Section 8).
- Coverage of the low-temperature spin-reorientation transition (~135 K), which sits outside the manufacturing temperature range this seam covers.
- Anything about the finishing stages beyond “B – reemergence,” which are part of the full manufacturing seam available to select partners.
- Disclosure of the SaC method — every check below operates on published output (frame-level measures), not on the generation mechanism.

Scope: Public Seam vs. Full Seam

MagNet-IQ's full end-to-end manufacturing simulation runs from initial powder lattice state through completed magnet. The public seam covers the first portion of that process — P-series (powder formation) → A powder preheat → A heat (sintering) → B reemergence (cooling back through Tc). Finishing stages beyond B – reemergence are part of the full manufacturing seam, available under partner access. Every check in this protocol operates entirely within the public seam; nothing here requires partner-only data.

1. Curie Temperature Baseline

The Curie temperature (Tc) is the reference point against which every process-stage target temperature is evaluated. Published values for $Nd_2Fe_{14}B$ cluster around 586–602 K (roughly 313–329°C); independent resistivity measurements place Tc at approximately 580 K (≈307°C). Cobalt-substituted sintered compositions reach higher Tc values around 342°C, with cobalt substitution raising Tc approximately linearly by ~11°C per atomic percent Co over the 0–10 at% range. [1][2][3][4]

Working baseline for this protocol: Tc ≈ 310–330°C for undoped/lightly-doped $Nd_2Fe_{14}B$. Any process stage with a target temperature comfortably above this range should drive order-sensitive measures toward their disordered limits; any stage below it should retain nonzero order.

2. Primary Order Parameters — Stage-by-Stage (Tier A: Gating)

These checks determine pass/fail. Mean |φ| and Net magnetization ⟨σz⟩ are the same quantity reported two ways (the dataset's own description notes ⟨φ⟩ signed equals ⟨σz⟩); treat them as one measure for validation purposes.

Seam Stage	Industry Temp. Target	Position vs. Tc	Expected Behavior — Mean |φ| / ⟨σz⟩	Expected Behavior — |⟨σ⟩| (Bloch magnitude)
A – powder preheat	~340–380°C (H_2 degassing range) [5]	At / just above Tc	Onset of disordering — partial decrease from an ordered baseline, not a collapse to zero.	Should track |φ|'s direction: a comparable partial decrease, since both indicate departure from coherent alignment.
A – heat (sintering)	Staged ramp to ~1010–1040°C (after holds at ~250°C, 550°C, 750°C) [5]; strip-casting/smelting can reach ~1300°C [7]	Far above Tc	Collapse toward zero — consistent with published descriptions noting the sintered body loses magnetization and must be remagnetized afterward. [6]	Should collapse toward zero alongside |φ|. If |⟨σ⟩| stayed high while |φ| collapsed, that would indicate residual coherent structure the order parameter isn't capturing — worth flagging if seen.
B – reemergence	Cooling from sintering temperature back through Tc	Crossing Tc from above to below	Rise from ~zero following Curie-Bloch shape, $m = [1-(T/T_c)^\alpha]^\beta$, α≈1.8, β≈0.42 — steep but not instantaneous, not linear or step-shaped. [1]	Should rise alongside |φ|, beginning at or near the same frame range where |φ| begins its rise. Exact shape need not match — timing/direction match is the bar.

Practical check: for each stage, plot Mean |φ| and |⟨σ⟩| together across the frame range. They should rise and fall together. For the “B – reemergence” stage specifically, overlay the Curie-Bloch curve (α=1.8, β=0.42) on Mean |φ| against a normalized temperature axis; a qualitative match in steepness near the transition — not a precise fit — is the bar.

3. Reemergence Stage — Critical Scaling Detail (Tier A / Tier D)

This is the most physically distinctive checkpoint, because it is a shape match, not just a direction match.

3.1 Order parameter shape (Tier A, gating)

Atomistic spin-model simulations of $Nd_2Fe_{14}B$ fit the temperature-dependent magnetization to a Curie-Bloch form, $m = M_s(T)/M_0 = [1 - (T/T_c)^\alpha]^\beta$, with $\alpha \approx 1.80$ and $\beta \approx 0.418$ giving close agreement with experiment. [1] A simpler mean-field form ($\beta = 0.5$) under-predicts the sharpness of the transition; $\beta \approx 0.42$ sits closer to 3D-Ising-like critical behavior — expected for a uniaxial magnet, where the order parameter is effectively confined to one axis and falls into the 3D Ising universality class rather than 3D Heisenberg. [8] Independent work on $Nd_2Fe_{14}B$-hydride systems separately reports critical exponents consistent with the 3D-Ising model in the same temperature regime. [4]

For the Fe sublattice contribution specifically, the Kuz'min phenomenological form is also commonly used: $\mu_{Fe}(T) = [1 - 0.5(T/T_c)^{1.5} - 0.5(T/T_c)^{2.5}]^{(1/3)}$. [3] Both forms give near-identical shapes for $T/T_c < \sim 0.9$ and diverge mainly very close to T_c.

Practical check: plot Mean |φ| across the “B reemergence” frame range against a normalized temperature axis (assuming the seam's evolve-step progression maps monotonically to a cooling ramp) and overlay the Curie-Bloch curve with α=1.8, β=0.42. A qualitative match in steepness near the transition is the bar for this pass.

3.2 Correlation length ξ (Tier D, informational)

General critical-phenomena theory predicts the correlation length ξ grows as the system approaches T_c from either direction, formally diverging at T_c in an infinite system ($\xi \sim |T - T_c|^{-\nu}$) and saturating near the system size in a finite lattice. [9][10][11] For a finite 6×6×6 lattice, this means: ξ should be small (short-range correlations only) during “A heat,” where the system is far above T_c and disordered, and should grow through the “B reemergence” stage as the system approaches and crosses T_c, plateauing as it settles into the ordered phase below T_c.

Practical check: plot ξ across “A heat” and “B reemergence.” Expect low, roughly flat ξ during “A heat,” and a rise in ξ through “B reemergence” that roughly coincides with where Mean |φ| begins rising. An exact peak shape is not required — the qualitative rise, co-located with the order-parameter transition, is the signal.

3.3 Energy surrogate ⟨H⟩ (Tier D, informational)

At a second-order phase transition, the specific heat — the temperature derivative of energy — shows an anomaly (a peak, with critical exponent α) rather than smooth behavior. [9][10][11] ⟨H⟩ itself is an energy-like surrogate, so it should vary smoothly across stages, but its frame-to-frame derivative (Δ⟨H⟩ / Δ(evolve step), as a proxy for d⟨H⟩/dT) should show a local maximum near the same frame range where Mean |φ| begins its critical rise during “B reemergence” — a specific-heat-like signature of the transition.

Practical check: numerically differentiate ⟨H⟩ across the “B reemergence” frame sequence and look for a local maximum co-located (within a few frames) with the onset of the Mean |φ| rise. This is a secondary, informational check — not gating.

4. Cross-Measure Consistency & Falsifiability Controls (Tier B)

These checks borrow the same design principle used for NMC811-IQ: a result means more when something that shouldn't pass, doesn't. Here, basic magnetic symmetry provides the null controls — no new literature is needed, only the fact that $Nd_2Fe_{14}B$ is a ferromagnet with a strong uniaxial (easy-axis) anisotropy, not an antiferromagnet and not an isotropic (Heisenberg) magnet.

4.1 Domain fraction f_dom and coherence proxy — should track the order parameter

f_dom (fraction of sites in the dominant spin domain) should sit near 0.5 during “A heat,” where the system is disordered and there is no majority direction — a roughly even split between up and down sites. During “B reemergence,” as Mean |φ| rises, f_dom should rise above 0.5 toward 1, reflecting the emergence of a majority domain. The coherence proxy (described as a composite of entropy, connected-component, and checkerboard structure from the Z-basis bitstring) is engine-internal in its exact construction, but as an order-sensitive composite it should move in the same direction as f_dom and Mean |φ| across all three stages — lower during disorder, higher as order emerges.

Practical check: plot f_dom and the coherence proxy alongside Mean |φ| across all three public stages. Expect f_dom ≈ 0.5 (and a relatively low coherence-proxy value) during “A heat,” with both rising in step with Mean |φ| during “B reemergence.”

4.2 Staggered magnetization — null control (antiferromagnetic order parameter)

Staggered magnetization, $\langle(-1)^{(x+y+z)}\sigma_z\rangle$, is a checkerboard (Néel-type, antiferromagnetic) order parameter. $Nd_2Fe_{14}B$ is ferromagnetic — there is no physical mechanism in this material that would drive checkerboard ordering through a heating/cooling cycle. This measure should therefore remain small and not reproduce the Tc-crossing critical-scaling rise seen in Mean |φ| during “B reemergence.”

Why this matters: if staggered magnetization showed the same critical rise as Mean |φ|, that would suggest the “order” being measured isn't specifically the ferromagnetic alignment the rest of this protocol assumes — a discriminability failure analogous to NMC811-IQ's null-control observable failing to fail.

Practical check: plot staggered magnetization across “B reemergence” alongside Mean |φ|. Expect staggered magnetization to remain small and roughly flat (fluctuating near zero) while Mean |φ| rises sharply.

4.3 Transverse components ⟨σx⟩, ⟨σy⟩ — null control (easy-axis anisotropy)

$Nd_2Fe_{14}B$ has strong uniaxial (easy-axis, c-axis) magnetocrystalline anisotropy — the basis for the 3D-Ising-like $\beta \approx 0.42$ exponent used in Section 3.1. A material with this character orders preferentially along one axis (here, z); the transverse components $\langle\sigma_x\rangle$ and $\langle\sigma_y\rangle$ are not expected to develop the same critical-scaling order through “B reemergence” that Mean |φ| / $\langle\sigma_z\rangle$ does. They may remain small and roughly symmetric ($\langle\sigma_x\rangle \approx -\langle\sigma_y\rangle$ or both near zero, depending on engine convention) throughout.

Why this matters: a second independent null control. If $\langle\sigma_x\rangle$ or $\langle\sigma_y\rangle$ showed the same critical rise as $\langle\sigma_z\rangle$ during reemergence, that would suggest the ordering isn't preferentially along the easy axis — inconsistent with the uniaxial anisotropy that motivates the $\beta \approx 0.42$ comparison in the first place.

Practical check: plot $\langle\sigma_x\rangle$ and $\langle\sigma_y\rangle$ across “B reemergence” alongside $\langle\sigma_z\rangle$. Expect $\langle\sigma_z\rangle$ to rise sharply while $\langle\sigma_x\rangle$, $\langle\sigma_y\rangle$ remain small in comparison.

5. Algebraic / Recompute Integrity (Tier C)

Two of the published measures are stated as exact algebraic functions of $\langle \sigma z \rangle$. These provide a Phase-4-style integrity check — confirming the published values are mutually consistent under their own stated definitions, independent of any external literature.

Measure	Stated Relationship	Check
z↓ fraction (n0/N)	$\langle \sigma z \rangle = 1 - 2 \times$ (z↓ fraction)	On every frame, verify z↓ fraction = $(1 - \langle \sigma z \rangle) / 2$ within rounding tolerance.
Ordering strength (legacy)	Ordering strength = $0.4 \times |\langle \sigma z \rangle|$	On every frame, verify Ordering strength / 0.4 = $|\langle \sigma z \rangle|$ within rounding tolerance.

These two checks require no temperature mapping and no literature — they are pure arithmetic consistency checks on the published frame data, and a clean pass on both across all frames is a strong, cheap signal that the published measures are internally coherent.

6. Process & Derived Diagnostics (Tier D, informational)

The remaining measures — compaction (ρ variance), magnetic defect radius, and the "magnet regime" classifier label — are engine-internal diagnostics without a direct one-to-one literature analog. Their validation is by internal consistency: each should move sensibly relative to the primary order parameters, not against an external benchmark.

6.1 Magnetic defect radius

Described as the mean BFS graph distance from minority-spin sites to the majority domain. As order develops (f_dom rises toward 1 during "B reemergence"), minority sites become sparser and, on average, closer to the boundary of the shrinking majority domain. Expect magnetic defect radius to decrease as f_dom and Mean |φ| rise.

Practical check: plot magnetic defect radius alongside f_dom during "B reemergence." Expect an inverse relationship — defect radius decreasing as f_dom increases.

6.2 Compaction (ρ variance)

Var(|σz,i|) across sites — the variance of per-site magnitude. In a fully saturated lattice (every site at |σz,i| = 1, regardless of sign), this variance is zero by construction; nonzero values would indicate sites with partial/fractional local magnitude. No specific literature target is asserted here — the practical check is simply that this value remains within a physically sensible range (0 to 1) and does not show discontinuous jumps unrelated to the stage transitions.

6.3 Magnet regime (classifier label)

A rule-based label (e.g., "ordered_signal") derived from the numeric measures. As an informational/diagnostic output, the check is simply that label transitions are temporally consistent with the numeric measures — e.g., a transition away from an "ordered" label should coincide with Mean |φ| dropping below whatever threshold the classifier uses, not occur at an unrelated frame.

7. Validation Tiers (How the Checks Are Weighted)

Tier	Role	Measures / Checks
A — Gating	Determine pass/fail	Mean |φ| / ⟨σz⟩ stage-shape and Tc-position checks (Section 2); reemergence critical-scaling shape, β≈0.42 (Section 3.1).
B — Cross-measure consistency & null controls	Falsifiability — things that should track, and things that shouldn't	|⟨σ⟩|, f_dom, coherence proxy tracking Mean |φ| (4.1); staggered magnetization and ⟨σx⟩/⟨σy⟩ as null controls (4.2, 4.3).
C — Algebraic / recompute integrity	Internal coherence of published values	z↓ fraction and Ordering strength (legacy) exact relationships to ⟨σz⟩ (Section 5).
D — Informational / diagnostic	Reported, secondary	Correlation length ξ (3.2), ⟨H⟩ derivative anomaly (3.3), magnetic defect radius, compaction variance, magnet regime label (Section 6).

Design principle: as with NMC811-IQ, shape and direction are checked before any position-based scoring — a feature has to look like the right kind of transition before its exact location matters. Tier A determines whether this protocol passes at all; Tiers B and C are what make a Tier A pass mean something rather than being a single coincidentally-matched curve; Tier D rounds out the picture without being load-bearing.

8. Finished-Magnet Property Targets (Context Only)

These extrinsic properties describe what a finished sintered NdFeB magnet needs to achieve commercially. They are not directly derivable from a single-lattice order parameter, but are useful framing for why the process matters: high-coercivity sintered magnets in the published literature reach intrinsic coercivity around 36.3 kOe, remanence around 11.7 kGs, and maximum energy product around 34.0 MGOe, with temperature coefficients of roughly -0.113%/°C for remanence and -0.355%/°C for coercivity between 20 and 200°C. [2] The theoretical ceiling for single-crystal $Nd_2Fe_{14}B$ is higher still — an anisotropy field around 7 T and a maximum energy product around 59 MGOe. [4]

9. Known Boundaries / Caveats

- **Spin-reorientation transition (~135 K / -138°C):** a documented low-temperature transition in $Nd_2Fe_{14}B$, well below any manufacturing process temperature in the public seam. [4] If asked, the honest framing is that the public seam doesn't cover that regime — not that it's been validated against it.
- **Sub-Tc resistivity "jumps" (400–500 K) on cooling:** independent resistivity measurements report discrete jumps during cooling between roughly 400–500 K (well below Tc), attributed to magnetic-domain reorientation as domains form and align below Tc. [4] These are a secondary, optional feature — not a gating check — but if the "B – reemergence" trajectory extends to these lower temperatures, fine-grained (non-monotonic) structure in this range would not necessarily indicate a problem; it would be consistent with this documented domain-reorientation behavior.
- **Extrinsic vs. intrinsic properties:** coercivity, remanence, and energy product depend heavily on grain boundary phase composition and microstructure history, which sit

outside what a per-microstate order parameter can directly validate. Section 8 figures are context, not seam-checkable targets.

- **P-series pre-stages:** P0/P1/P2 (powder formation/milling) are structural/compositional in nature and are not addressed by the Tc-based framework in this protocol.
- **Compaction (ρ variance) and magnet regime label:** validated by internal consistency only (Section 6); no external literature target is asserted for these.

10. Scope Summary

Check	Public Seam (P-series → A preheat → A heat → B reemergence)	Full Seam (Partner Access)
Tier A — primary order parameter shape & Tc position	Fully checkable — all relevant stages are in the public seam	Not additionally needed
Tier B — cross-measure consistency & null controls	Fully checkable	Not additionally needed
Tier C — algebraic / recompute integrity	Fully checkable on any frame	Not additionally needed
Tier D — ξ, ⟨H⟩ anomaly, derived diagnostics	Checkable within “A heat” / “B reemergence”	Not additionally needed
Finishing-stage behavior (post-reemergence)	Out of scope — not in public seam	Available under partner access
Extrinsic properties (coercivity, remanence, BHmax)	Not checkable from per-microstate data (context only)	Not checkable from per-microstate data (context only)

A qualified prospect can run every Tier A–D check in this protocol entirely against the public seam. The full seam (finishing stages) is available under partner access for teams whose interest extends to the complete manufacturing process.

References

[1] Calculating temperature-dependent properties of $Nd_2Fe_{14}B$ permanent magnets by atomistic spin model simulations. arXiv:1902.05636.

[2] The preparation of sintered NdFeB magnet with high-coercivity and high temperature-stability. J. Phys.: Conf. Ser. 266 (2011) 012052.

[3] Power law analysis for temperature dependence of magnetocrystalline anisotropy constants of $Nd_2Fe_{14}B$ magnets. arXiv:1802.07959.

[4] Temperature dependent striction effect in a single crystalline $Nd_2Fe_{14}B$ revealed using a novel high temperature resistivity measurement technique. arXiv:2110.02909.

[5] Method for improving performance of sintered NdFeB magnets. US Patent 11,569,012.

[6] NdFeB system sintered magnet. US Patent 10,546,673.

[7] How Are Sintered NdFeB Magnets Made? Stanford Magnets (process overview).

[8] General critical-phenomena / universality class background: uniaxial magnets with strong easy-axis anisotropy fall into the 3D Ising universality class, distinct from isotropic (Heisenberg) magnets — standard condensed-matter-physics background, not $Nd_2Fe_{14}B$-specific.

[9] Renormalization Group and Critical Phenomena (lecture notes), LPTMC — correlation length divergence and specific-heat anomaly at second-order transitions.

[10] Elements of Phase Transitions and Critical Phenomena (Oxford) — definitions of critical exponents α, β, ν and correlation-length behavior near Tc.

[11] General critical-exponent background — order parameter, correlation length, and specific-heat scaling near a second-order transition.
