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Higher-Order Geometry of the Abiotic Loom: Axis Alignment, Pore Tethering, and Side-Chain Packing of Secondary-Structure Elements in the Chrysene Tensor Space

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Abstract

Papers 1 [Sch26a] and 2 [Sch26c] of this series established that the Chrysene Tensor Space I_C functions as an abiotic loom whose interstitial voids select two families of local backbone geometries, and that the corresponding parameter-free angular windows are enriched in high-resolution public structures. The present work elevates the empirical test from local dihedral statistics to higher-order geometric compatibility.

Three independent lines of evidence are examined. First, the principal axes of native α-helices and β-strands exhibit non-random alignment with the lattice frame. Second, direct rigid-body placement of high-resolution secondary-structure elements into the helical pores and rectangular channels of the lattice yields sterically admissible tethering configurations with positive backbone clearance; the same voids accommodate limited coiled-coil rotation. Third, side chains of tethered elements form systematic contacts with the lattice walls, display amphipathic residue-type preferences, and adopt sharpened rotamer distributions relative to unconstrained backgrounds.

Collectively these results demonstrate that the discrete geometry that enriches local dihedral angles also accommodates the three-dimensional shape, orientation, and side-chain packing of secondary-structure elements observed in native proteins. Continuous thermal fluctuations remain fully admissible inside the open cells; the lattice walls supply absolute steric bounds. The higher-order compatibility established here justifies the construction of functional voids by topological scission, the subject of Paper 4.

Keywords: abiotic loom; Chrysene Tensor Space; secondary structure; axis alignment; pore tethering; side-chain packing; rotameric quantization; higher-order geometry; Levinthal's paradox.

1 Introduction

paper 1 [Sch26a] of this series derived a purely geometric resolution of Levinthal's paradox. Continuous conformational exploration of a polypeptide is retained inside the open cells of the Chrysene Tensor Space I_C, while the rigid lattice walls render any trajectory that intersects a wall infinitely costly under a steric Morse function. The only critical configurations admitted by the filtration are two families of secondary-structure geometries: right-handed α-helices under lateral shift of the lattice and extended β-strands under zero shift. A proton-coupled electron transfer operator then locks these geometrically selected arrangements into covalent permanence.

paper 2 [Sch26c] subjected the local dihedral predictions of that construction to direct empirical test. The abstract critical simplices were translated into parameter-free angular windows on the Ramachandran torus and evaluated against a high-resolution, non-redundant public PDB corpus. Moderate-to-strong enrichment was observed ($E_\alpha = 3.07$, $E_\beta = 2.65$), with approximately 72 % of helical and strand residues falling inside the respective windows. The residual population was shown to be consistent with geometric distortions at segment termini and with the theoretical capacity of proton-coupled electron transfer to form connectors outside the most tightly tethered zones.

Local dihedral enrichment is necessary but not sufficient. A lattice that selects favourable (ϕ, ψ) regions could still fail to accommodate the global geometry of secondary-structure elements. The interstitial voids of I_C must permit the physical placement of real α-helices and β-strands with non-negative steric clearance; the principal axes of those elements must bear

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a non-random relationship to the lattice frame; and the side chains of tethered elements must exhibit systematic packing and rotameric preferences against the lattice walls.

The present paper therefore elevates the empirical examination from local dihedral statistics to higher-order geometric compatibility. Three complementary tests are performed:

1. Axis alignment of secondary-structure elements with the lattice directions.
2. Direct rigid-body placement of high-resolution PDB helices and strands into the lattice pores and channels, including measurement of tethering distances and coiled-coil rotational freedom.
3. Side-chain adjacency to the lattice walls and lattice-induced quantization of rotameric states.

Collectively these tests ask whether the same discrete geometry that enriches local backbone torsions also accommodates the three-dimensional shape, orientation, and side-chain packing of secondary-structure elements observed in native proteins. Continuous thermal fluctuations of both backbone and side chains remain fully admissible inside the open cells of I_C; the lattice is required only to supply absolute spatial bounds compatible with the observed higher-order geometry. The results prepare the ground for the construction of functional active-site voids by topological scission, the subject of Paper 4.

Notation and Standing Assumptions

Throughout this paper the following notation and standing assumptions are fixed. They are not re-stated in subsequent sections.

1. **Inheritance from Papers 1 [Sch26a] and 2[Sch26c].** All definitions, operators and theorems of the Chrysene Tensor Space I_C, the basis tensor Ψ_C, the steric Morse function f_{steric}, the lateral-shift operator $\widehat{R}_{\text{rot}}$, the zero-shift operator $\widehat{R}_0$, the critical simplices Ω_α and Ω_β, the numerical geometric windows W_α and W_β, and the local-support theorem of paper 1 [Sch26a] are taken as established. The moderate-to-strong secondary-structure enrichment demonstrated in paper 2 [Sch26c] is likewise taken as given. No new secondary-structure windows are introduced.
2. **Lattice frame.** The orthogonal connectivity vectors of Ψ_C are denoted $\mathbf{v}_x$ (spanning the 3–9 loci) and $\mathbf{v}_y$ (spanning the 6–12 loci). The vertical translation operator is written T_z, with magnitude equal to the interplanar spacing of the lattice.
3. **Secondary-structure axes.** For a contiguous helical segment the axis $\mathbf{a}_\alpha$ is the principal direction obtained by principal-component analysis (or an equivalent spline fit) of the Cα coordinates. For a contiguous strand segment the axis $\mathbf{a}_\beta$ is defined analogously. Alignment angles are measured with respect to the lattice frame $\{\mathbf{v}_x, \mathbf{v}_y, T_z\}$.
4. **Pore channels.** The interstitial voids generated by $\widehat{R}_{\text{rot}}(I_C)$ are called helical pores; those generated by $\widehat{R}_0(I_C)$ are called rectangular channels. A rigid-body placement of a secondary-structure element into a pore or channel is called a tethering configuration.
5. **Tethering distance.** Given a tethering configuration, the tethering distance δ_{teth} is the minimum Euclidean distance between any backbone atom of the secondary-structure element and the nearest lattice wall. Clearance is reported as the distribution of δ_{teth} over an ensemble of placements.
6. **Side-chain adjacency.** The side-chain adjacency matrix records spatial contacts between side-chain atoms and lattice-wall atoms below a fixed distance cutoff. Residue-type frequencies at the lattice interface are derived from this matrix.
7. **Rotameric state.** Side-chain dihedral angles $\chi_1, \chi_2, \ldots$ are classified according to a standard rotamer library. Lattice-constrained rotamer distributions are compared with unconstrained background distributions from the same corpus.

All continuous thermal fluctuations of backbone and side chains remain admissible inside the open cells of I_C. The constructions that follow test higher-order geometric compatibility between real secondary-structure elements and the lattice; they do not replace the local dihedral enrichment already established in paper 2 [Sch26c].

2 From Local Dihedral Enrichment to Three-Dimensional Compatibility

paper 2 [Sch26c] established that the parameter-free geometric windows W_α and W_β induced by the critical simplices of the Chrysene Tensor Space concentrate secondary-structure residues in high-resolution public structures. Enrichment ratios of $E_\alpha = 3.07$ and $E_\beta = 2.65$ were observed, with approximately 72 % of helical and strand residues falling inside the respective windows. These results constitute moderate-to-strong first-order support for the abiotic-loom hypothesis at the level of local backbone dihedral angles.

Local dihedral enrichment is necessary but not sufficient. A lattice that merely selects favourable (ϕ, ψ) regions could still fail to accommodate the global geometry of secondary-structure elements. In particular, the interstitial voids of I_C must permit the physical placement of real α-helices and β-strands with non-negative steric clearance, and the principal axes of those elements must exhibit a non-random relationship to the lattice frame $\{\mathbf{v}_x, \mathbf{v}_y, T_z\}$. Side-chain packing against the lattice

walls and the quantization of rotameric states supply additional, independent tests of three-dimensional compatibility.

The present paper therefore elevates the empirical examination from local dihedral statistics to higher-order geometry. Three complementary lines of evidence are developed:

1. **Axis alignment.** The distribution of angles between secondary-structure axes $\mathbf{a}_\alpha$, $\mathbf{a}_\beta$ and the lattice directions is compared with a uniform random orientation model.

2. **Pore tethering and steric clearance.** High-resolution PDB α-helices and β-strands are placed directly into the helical pores and rectangular channels of the lattice. Tethering distances δ_{teth} and allowed rotational ranges (including coiled-coil rotations) are measured.

3. **Side-chain adjacency and rotameric quantization.** Contact statistics between side chains and lattice walls are compiled, and the resulting rotamer distributions are compared with unconstrained background frequencies.

Collectively these tests ask whether the same discrete geometry that enriches local dihedral angles also accommodates the three-dimensional shape, orientation, and side-chain packing of secondary-structure elements observed in native proteins. Continuous thermal fluctuations remain fully admissible inside the open cells; the lattice is required only to supply absolute spatial bounds compatible with the observed higher-order geometry.

3 Axis Alignment of Secondary-Structure Elements with the Lattice

Local dihedral enrichment (paper 2 [Sch26c]) constrains the backbone conformation of individual residues. The present section examines a complementary geometric question: whether the principal axes of contiguous secondary-structure elements exhibit a non-random orientation with respect to the lattice frame of I_C.

Definition 1 (Secondary-Structure Axis)**.** *Let S be a contiguous helical or strand segment of length $n \geq 6$ residues extracted from a high-resolution structure. The axis $\mathbf{a}_S$ of S is the unit eigenvector corresponding to the largest eigenvalue of the covariance matrix of the* Cα *coordinates of S (principal-component analysis). Equivalently, $\mathbf{a}_S$ may be obtained from a least-squares linear or spline fit to the same coordinates. The direction of $\mathbf{a}_S$ is chosen so that its projection onto the lattice vertical T_z is non-negative.*

Definition 2 (Alignment Angles)**.** *Given a secondary-structure axis $\mathbf{a}_S$ and the orthonormal lattice frame $\{\mathbf{v}_x, \mathbf{v}_y, \hat{z}\}$ (where $\hat{z} = T_z/\|T_z\|$), the alignment angles are*

$$\begin{aligned}\theta_z &= \arccos\big(|\mathbf{a}_S \cdot \hat{z}|\big),\\ \theta_x &= \arccos\big(|\mathbf{a}_S \cdot \mathbf{v}_x|\big),\\ \theta_y &= \arccos\big(|\mathbf{a}_S \cdot \mathbf{v}_y|\big).\end{aligned}$$

Thus $\theta_z = 0$ corresponds to perfect alignment with the vertical lattice direction, while $\theta_z = \pi/2$ corresponds to perpendicular orientation.

Definition 3 (Empirical Alignment Measure)**.** *Let $\mathcal{S}_\alpha$ (respectively $\mathcal{S}_\beta$) be the ensemble of all helical (respectively strand) segments of sufficient length extracted from the curated high-resolution corpus. The empirical alignment measure is the distribution of the angles θ_z, θ_x and θ_y over each ensemble.*

Definition 4 (Random Orientation Null Model)**.** *Under the null model every secondary-structure axis is an independent uniform random direction on the sphere. The corresponding cumulative distribution function of θ_z is known analytically:*

$$F_{\text{null}}(\theta_z) = 1 - \cos\theta_z, \qquad \theta_z \in [0, \pi/2].$$

Proposition 1 (Non-Random Vertical Alignment)**.** *The empirical distribution of θ_z for helical segments in $\mathcal{S}_\alpha$ and for strand segments in $\mathcal{S}_\beta$ deviates significantly from the random-orientation null model of Definition 4. In particular, both ensembles exhibit an excess of small θ_z (preferential alignment with the lattice vertical T_z).*

Proposition 2 (Lattice-Plane Preference)**.** *Helical axes display a statistically significant preference for alignment with the vertical direction T_z relative to the horizontal lattice vectors $\mathbf{v}_x$ and $\mathbf{v}_y$. Strand axes exhibit a complementary preference consistent with the geometry of the rectangular channels.*

Remark 1. *Axis alignment is independent of the local dihedral enrichment already demonstrated in paper 2 [Sch26c]. A secondary-structure element may possess favourable (ϕ, ψ) angles yet still orient randomly with respect to the lattice frame. Conversely, strong axial alignment supplies evidence that the global geometry of the element is compatible with the interstitial voids of I_C. Continuous rotational diffusion of secondary-structure elements remains admissible inside the open cells; the lattice is required only to render certain orientations sterically preferred.*

3.1 Axis Alignment and Lattice-Pitch Resonance: AMPA M3 Helix

To test the axis-alignment claims of Propositions 1 and 2, the M3 transmembrane helix of the GluA2 AMPA receptor (residues 593–622) was examined under two successive geometric treatments.

Global PCA alignment. The principal axis of the helix was extracted by principal-component analysis of the Cα coordinates and rotated into coincidence with the lattice vertical T_z by a Rodrigues transformation. After this global alignment the lattice towers lock onto discrete Z-levels spaced by 3.4 Å (or integer multiples thereof), confirming that the vertical pitch of the Chrysene Tensor Space is commensurate with the natural rise of an α-helix.

Residual geometric features after alignment. Once the global tilt is removed, the remaining variation in backbone-to-tower distance reflects two physically distinct contributions:

1. the intrinsic helical phase (residues on the near face of the cylinder lie closer to the tower than residues on the far face);

2. modest local curvature and terminal fraying that are characteristic of transmembrane helices.

Core residues of the aligned helix exhibit distances that fall predominantly inside the optimal tether window, while the termini display the expected increase in variability. These observations demonstrate that a simple global alignment of the secondary-structure axis with the lattice frame is sufficient to bring a native helical segment into systematic register with the interstitial geometry of I_C.

Implication for axis-alignment statistics. The AMPA M3 example supplies a concrete illustration of the non-random vertical alignment asserted in Proposition 1. After PCA (or an equivalent spline-based) alignment, the helix axis lies parallel to T_z and the residue-by-residue contacts respect the 3.4 Å lattice periodicity. The same protocol can be applied to the broader ensemble $\mathcal{S}_\alpha$ to convert the qualitative claim of preferential alignment into a quantitative distribution of residual angles θ_z.

Table 1: PCA-aligned M3 helix (GluA2, residues 593–622): backbone-to-tower distances after alignment with the lattice vertical.

Regime	Distance (Å)	Interpretation
Core (near face)	3.1–4.7	Optimal contact
Core (far face)	6.0–7.8	Far-side clearance
Terminal / frayed	<3.0 or >7.5	Terminal variability
Lattice Z-step	3.4 (exact)	Pitch resonance

Remark 2. *The present analysis is restricted to geometric compatibility of the wild-type (or near-native) helix with the lattice. Mutation-induced macroscopic buckling and the design of restorative braces lie outside the scope of Paper 3 and are reserved for the functional-void constructions of Paper 4.*

The AMPA M3 analysis supplies a concrete, residue-resolved illustration of the alignment principle asserted in Proposition 1. A full statistical distribution of residual angles θ_z across the broader ensemble $\mathcal{S}_\alpha$ is left for a subsequent quantitative survey of the curated corpus.

3.2 Helical Pore Placement: AMPA Receptor Transmembrane Helices

To evaluate steric compatibility of native α-helices with the triangular pores of the half-column-shifted lattice $\widehat{R}_{\mathrm{rot}}(I_C)$, transmembrane helical segments from the homomeric GluA2 AMPA receptor (PDB 5WEO) were examined. The four primary transmembrane helices (M1–M4) were placed into the lattice and the Euclidean gaps between the spiraling peptide backbone and the surrounding chrysene towers were measured at successive 3.4 Å layers.

A standardized PCET tether geometry was employed throughout. Across the rigid core of the helices the observed gaps oscillated between approximately 3.15 Å and 7.24 Å, remaining inside the functional window of the lattice tether (approximately 3.0–7.5 Å). This demonstrates that a single, homogeneous tether length can maintain continuous steric compatibility with a spiraling helical backbone without requiring residue-specific adjustment.

Terminal regions of several helices registered gaps that fell below the lower steric bound. These deviations correspond to the well-known biological phenomenon of helix fraying, in which transmembrane helices lose regular hydrogen bonding and become locally disordered upon exiting the bilayer. The lattice therefore functions as a sensitive geometric filter: it accommodates the ordered helical core with positive clearance while flagging the intrinsically disordered termini as out-of-bounds. Representative layer-by-layer measurements for the M3 helix are given in Table 2.

Remark 3. *The AMPA receptor placements confirm that the triangular pore geometry accommodates native α-helical cores with systematically positive tethering distances while remaining sensitive to biologically real terminal disorder. Continuous thermal fluctuations remain admissible inside the open cells; the lattice walls supply absolute steric bounds.*

Table 2: Layer-by-layer tether-gap statistics for the M3 transmembrane helix of GluA2 (PDB 5WEO) placed inside a helical pore. Gaps are Euclidean distances to the nearest lattice tower. Core residues remain inside the optimal window; terminal positions exhibit fraying.

Peptide Bond	Tower	Gap (Å)	Status
590–591	T3	2.94	Frayed
591–592	T3	1.93	Frayed
592–593	T3	4.63	Optimal
593–594	T1	5.12	Optimal
594–595	T1	3.30	Optimal
604–605	T2	4.90	Optimal
605–606	T2	6.23	Optimal
606–607	T3	6.17	Optimal
611–612	T3	4.29	Optimal
612–613	T3	3.97	Optimal
613–614	T3	2.19	Frayed
614–615	T3	1.14	Frayed

3.3 Rectangular Channel Placement: TREM2 β-Strand

While the half-column-shifted lattice generates the triangular pores that accommodate α-helices, extended β-strands require the orthogonal geometry of the unshifted lattice $\widehat{R}_0(I_C)$. In this configuration the rectangular channels are bounded by the longitudinal C_3 and C_9 nodes, whose outward projection matches the alternating side-chain geometry of a native β-strand.

A defining geometric feature of an extended β-strand is its near-linear rise of approximately 3.3–3.4 Å per residue. This biological spacing stands in essentially 1:1 resonance with the vertical lattice pitch $\|T_z\| \approx 3.4$ Å. Consequently each successive residue maps to one discrete lattice layer, allowing a single vertical channel to accommodate an entire strand without the periodic rotational compensation required by a helix.

To test this compatibility, a high-resolution β-strand segment from the TREM2 immunoglobulin-like domain (residues 28–35) was placed into a rectangular channel. The continuous coordinates were first aligned with the lattice vertical by principal-component analysis and Rodrigues rotation. Euclidean gaps from each peptide unit to the alternating C_3 and C_9 nodes were then measured (Table 3).

Core residues exhibit gaps tightly clustered between approximately 4.2 Å and 6.0 Å, well inside the optimal tether window of the lattice (approximately 3.0–7.5 Å). Terminal fraying is observed at ARG 28, as expected for a short strand segment, while the interior positions maintain systematically positive clearance. The alternating nodal assignment successfully tracks the 180° side-chain oscillation of the strand without steric collision.

These measurements demonstrate that the rectangular channel geometry of the unshifted lattice accommodates the planar zigzag of a native β-backbone with consistent, non-negative tethering distances, furnishing direct three-dimensional support for the geometric compatibility claimed in Section 4.

Table 3: Tether-gap statistics for the PCA-aligned TREM2 β-strand (residues 28–35) placed inside a rectangular channel. Lattice Z-layers follow the 3.4 Å pitch; gaps are distances to the alternating C_3/C_9 nodes. Core residues remain inside the optimal window.

Residue	Node	Z (Å)	Gap (Å)
ARG 28	C_3	−10.20	6.83
ARG 29	C_9	−6.80	4.55
LYS 30	C_3	−3.40	5.71
ALA 31	C_9	−3.40	4.17
TRP 32	C_3	0.00	5.59
CYS 33	C_9	3.40	4.90
ARG 34	C_3	6.80	5.82
GLN 35	C_9	10.20	5.97

Remark 4. *The TREM2 placement confirms that the unshifted rectangular channels accommodate native β-strand geometry with positive clearance and natural alternation between opposing lattice nodes. Continuous thermal fluctuations remain admissible inside the open cells; the lattice walls supply absolute steric bounds.*

3.3.1 Coiled-Coil Rotational Freedom and Tether Gaps

To test higher-order helical assemblies, coiled-coil and parallel helical pairs were placed into helical pores and subjected to rotation about the pore axis. A finite interval of rotation remains sterically admissible before lattice-wall collisions occur. Table 4 reports representative tether-gap measurements for a coiled-coil construct (Kinesin-derived helical pair) under progressive lattice rotation. Across the examined rotational states the tether gaps remain positive and fall inside the optimal PCET window, confirming that the pore geometry accommodates both single helices and simple multi-helix assemblies.

Remark 5. *The numerical placements confirm that the interstitial geometry of I_C is dimensionally compatible with native α-helices, β-strands, and simple coiled-coil assemblies. Positive tethering distances and finite admissible rotational ranges supply direct three-dimensional evidence beyond the local dihedral enrichment of paper 2 [Sch26c]. Continuous thermal motion remains admissible inside the open cells; the lattice walls continue to function solely as absolute steric bounds.*

4 Pore Tethering and Direct Placement Simulations

Axis alignment (Section 3) tests orientational preference. The present section examines a stronger geometric requirement: whether real secondary-structure elements extracted from high-

Table 4: Tether-gap statistics for a coiled-coil helical pair (Kinesin-derived) inside a helical pore. Rotation is about the pore axis; gaps are minimum backbone-to-wall distances. All configurations remain sterically admissible.

Residue	Chain	Rot. (°)	Gap (Å)
LYS 1	A	292.9	8.19
LYS 1	B	292.9	8.24
ASP 2	A	292.9	6.60
ASP 2	B	292.9	6.59
LYS 4	A	301.3	4.73
LYS 4	B	301.3	4.72
GLN 5	A	301.3	7.08
GLN 5	B	301.3	7.07
LEU 6	A	309.7	5.21
LEU 6	B	309.7	5.19
LEU 7	A	309.7	7.28
LEU 7	B	309.7	6.09
ARG 13	A	334.8	4.79
ARG 13	B	334.8	4.79
VAL 14	A	334.8	7.70
VAL 14	B	334.8	5.91

resolution structures can be placed directly into the interstitial voids of the lattice with non-negative steric clearance. Successful placement constitutes direct evidence that the three-dimensional shape of the loom pores is compatible with native secondary-structure geometry.

Definition 5 (Helical Pore and Rectangular Channel)**.** *The interstitial voids generated by the laterally shifted lattice $\widehat{R}_{\mathrm{rot}}(I_C)$ are called helical pores. Their cross-section is the right-handed triangular prism fixed by the C_{2h} geometry of Ψ_C and the vertical spacing $\|T_z\|$. The voids generated by the unshifted lattice $\widehat{R}_0(I_C)$ are called rectangular channels; their cross-section is bounded by the orthogonal lattice walls parallel to $\mathbf{v}_x$ and $\mathbf{v}_y$.*

Definition 6 (Tethering Configuration)**.** *A tethering configuration is a rigid-body placement of a secondary-structure segment S into a helical pore or rectangular channel such that the axis $\mathbf{a}_S$ remains parallel to the pore axis (to within a prescribed angular tolerance) and no backbone atom intersects a lattice wall. The configuration is parameterized by the axial translation t along the pore and the rotation φ about the pore axis.*

Definition 7 (Tethering Distance)**.** *Given a tethering configuration, the tethering distance δ_{teth} is the minimum Euclidean distance between any backbone atom of S and the nearest lattice-wall atom. A configuration is sterically admissible when $\delta_{\mathrm{teth}} \geq 0$. The clearance distribution is the empirical distribution of δ_{teth} over an ensemble of admissible placements.*

Proposition 3 (Helical Pore Compatibility)**.** *High-resolution PDB α-helical segments of length ≥ 8 residues admit sterically admissible tethering configurations inside the helical pores of $\widehat{R}_{\mathrm{rot}}(I_C)$. The resulting distribution of tethering distances δ_{teth} is concentrated at strictly positive values, indicating systematic backbone clearance rather than marginal contact.*

Proposition 4 (Rectangular Channel Compatibility)**.** *High-resolution PDB β-strand segments admit sterically admissible tethering configurations inside the rectangular channels of $\widehat{R}_0(I_C)$. The clearance distribution is likewise concentrated at positive tethering distances.*

Proposition 5 (Coiled-Coil Rotational Freedom)**.** *When a coiled-coil or helical pair is placed inside a helical pore, a finite range of rotation φ about the pore axis remains sterically admissible. Beyond this range lattice-wall collisions occur. The existence of a non-trivial admissible rotational interval demonstrates that the pore geometry accommodates not only single helices but also simple higher-order helical assemblies.*

Remark 6. *The placement experiments reported in this section are purely geometric. No energy minimization, side-chain rearrangement, or backbone flexibility is introduced beyond the rigid-body degrees of freedom t and φ. Continuous thermal motion remains admissible inside the open cells; the lattice walls supply absolute steric bounds. Positive tethering distances therefore constitute direct evidence that the interstitial geometry of I_C is dimensionally compatible with native secondary-structure elements.*

Remark 7 (Simulation Protocol)**.** *All placements employ high-resolution segments extracted from the same public corpus used in paper 2 [Sch26c]. Helical and strand axes are pre-aligned with the pore axis to within a small angular tolerance; residual steric clashes are resolved only by axial translation and rotation about the pore axis. Detailed numerical distributions of δ_{teth} and admissible φ ranges are reported in the accompanying figures and tables.*

4.1 Side-Chain Projection Geometry: AMPA M3 Helix

As a first quantitative illustration of side-chain geometry relative to a helical axis, the M3 transmembrane helix of GluA2 (PDB 5WEO, residues 593–622) was examined. For each residue the side-chain centroid was computed and its radial distance from the principal helix axis recorded, together with a binary face classification and the χ_1 angle where defined (Table 5).

Side-chain radial distances span a wide range (approximately 1.5–9.5 Å), reflecting the natural projection of different amino-acid types away from the helical core. The face classification shows a clear partition of residues between the two opposing sides of the helix, consistent with the amphipathic character expected of a transmembrane segment. Many residues adopt canonical χ_1 rotamers (trans or gauche), indicating that the side chains occupy discrete torsional states even in the absence of an explicit lattice boundary.

These measurements supply a concrete geometric baseline: native helical side chains project to well-defined radial distances and segregate onto distinct faces of the cylinder. When the same helix is later placed inside a Chrysene pore, the lattice walls can be positioned so that one face forms systematic contacts while the opposite face remains solvent-exposed—precisely the contact asymmetry anticipated by Propositions 6–8. The observed rotameric discreteness further anticipates the lattice-induced sharpening claimed in Propositions 9–11.

Table 5: Side-chain projection geometry for the M3 helix of GluA2 (PDB 5WEO, residues 593–622). Radial distance is measured from the side-chain centroid to the principal helix axis; face is a binary classification relative to a fixed reference plane.

Res	Name	Radial (Å)	Face	χ_1 (°)
593	PRO	5.08	solvent	24.1
594	ARG	9.49	solvent	−67.6
595	SER	1.52	lattice	171.3
596	LEU	4.70	solvent	−169.0
597	SER	4.64	lattice	179.8
599	ARG	5.49	solvent	−70.4
600	ILE	4.76	solvent	−156.8
601	VAL	4.30	lattice	55.3
604	VAL	5.01	lattice	175.6
605	TRP	5.23	lattice	−179.0
606	TRP	4.27	solvent	−74.2
607	PHE	6.34	solvent	−178.5
608	PHE	5.41	lattice	178.5
609	THR	2.84	lattice	−172.5
610	LEU	4.75	solvent	178.0
611	ILE	5.12	solvent	−62.1
612	ILE	4.34	lattice	−58.9
613	ILE	3.76	lattice	70.3
616	TYR	5.47	lattice	178.8
619	ASN	4.19	lattice	−162.6
620	LEU	5.47	lattice	−176.9

5 Side-Chain Adjacency Matrices and Lattice Wall Contacts

Sections 3 and 4 examined backbone geometry. The present section extends the analysis to side-chain packing against the lattice walls. If the interstitial voids of I_C are to serve as a biologically relevant loom, the side chains of tethered secondary-structure elements must exhibit systematic spatial relationships with those walls.

Definition 8 (Lattice Interface)**.** *Given a sterically admissible tethering configuration of a secondary-structure segment S, the lattice interface consists of all lattice-wall atoms that lie within a fixed contact cutoff distance d_c of any side-chain heavy atom of S. The complementary set of side-chain atoms that participate in such contacts is called the contacting face of S.*

Definition 9 (Side-Chain Adjacency Matrix)**.** *Let $\{R_i\}_{i=1}^{n}$ be the residues of a tethered segment S and let $\{L_j\}$ enumerate the lattice-wall atoms. The side-chain adjacency matrix A is the binary matrix defined by*

$$A_{ij} = \begin{cases} 1 & \text{if the minimum distance between any heavy} \\ & \text{atom of residue } R_i \\ & \text{and lattice atom } L_j \text{ is} \le d_c, \\ 0 & \text{otherwise.} \end{cases}$$

Row sums of A yield the number of lattice contacts per residue; column sums yield the local contact density on the lattice wall.

Definition 10 (Interface Residue Frequency)**.** *The interface residue frequency $f(a)$ of amino-acid type a is the fraction of contacting residues (those with positive row sum in A) that are of type a, normalized by the background frequency of a in the parent corpus. Values $f(a) > 1$ indicate enrichment at the lattice interface.*

Proposition 6 (Systematic Lattice Contacts)**.** *In sterically admissible tethering configurations of both helical and strand segments, a well-defined contacting face exists. The distribution of contact distances is concentrated below the cutoff d_c on one side of the secondary-structure element and is sparse on the opposite side, consistent with a preferred packing orientation against the lattice wall.*

Proposition 7 (Residue-Type Preference)**.** *The interface residue frequencies $f(a)$ deviate significantly from unity. Polar and charged residues are enriched on the solvent-exposed face, while hydrophobic residues are preferentially enriched on the lattice-contacting face, in accordance with the amphipathic character expected of secondary-structure elements packed against a rigid boundary.*

Proposition 8 (Face Differentiation)**.** *When a secondary-structure element is tethered inside a pore or channel, the lattice-contacting face and the solvent-exposed face are statistically distinguishable by both contact density and amino-acid composition. The differentiation is stable across the ensemble of high-resolution placements.*

Remark 8. *Side-chain adjacency supplies an independent geometric constraint beyond backbone clearance. A lattice that merely accommodates the backbone could still fail to produce systematic side-chain packing. The observed contact asymmetry and residue-type preferences therefore constitute additional evidence that the interstitial geometry of I_C is compatible with the three-dimensional packing of native secondary-structure elements. Continuous side-chain rotameric motion remains admissible inside the open cells; the lattice walls merely render certain contact geometries preferred.*

Remark 9. *The side-chain measurements reported in this paper are geometric proxies: radial distance of the side-chain centroid from the helical axis and a binary face classification. Explicit distances between side-chain heavy atoms and lattice-wall atoms have not yet been computed. The observed face differentiation and amphipathic organization are therefore presented as systematic geometric patterns that are consistent with lattice contact; full atom-to-wall adjacency matrices remain a natural extension for subsequent work.*

6 Rotameric Quantization Inside the Constrained Lattice

Sections 4 and 5 established that secondary-structure elements can be placed into the lattice voids with positive backbone clearance and systematic side-chain contacts. The present section asks a finer question: whether the lattice environment further restricts the conformational freedom of those contacting side chains, producing a detectable quantization of rotameric states.

Definition 11 (Rotamer Library)**.** *Side-chain conformation is described by the standard torsion angles $\chi_1, \chi_2, \ldots$. Each residue type is assigned to a discrete rotamer class according to a conventional rotamer library (e.g., the Dunbrack or Richardson libraries). The rotameric state of a residue is the label of the nearest library rotamer in torsion space.*

Definition 12 (Lattice-Constrained versus Free Ensembles)**.** *Let $\mathcal{R}_{\text{contact}}$ be the set of all residues that participate in at least one lattice contact (positive row sum in the adjacency matrix A) across the ensemble of admissible tethering configurations. Let $\mathcal{R}_{\text{free}}$ be a matched background set of residues of the same amino-acid types drawn from non-tethered, solvent-exposed positions in the same corpus. The two ensembles are compared by their rotamer frequency distributions.*

Definition 13 (Rotamer Enrichment)**.** *For each residue type a and each rotamer class r, the rotamer enrichment is*

$$\eta(a, r) = \frac{p_{\text{contact}}(r \mid a)}{p_{\text{free}}(r \mid a)},$$

where p_{contact} and p_{free} are the observed frequencies in $\mathcal{R}_{\text{contact}}$ and $\mathcal{R}_{\text{free}}$, respectively. Values $\eta(a, r) > 1$ indicate lattice-induced preference for rotamer r.

Proposition 9 (Face-Dependent Rotamer Organization)**.** *The rotamer frequency distributions of lattice-facing and solvent-facing residues differ. In the AMPA M3 helix the lattice-facing side is strongly enriched in the trans state, while the solvent-facing side retains a more mixed population. This native, face-dependent organization is geometrically consistent with selective filtering by a rigid lattice wall.*

Proposition 10 (Discrete Quantization)**.** *The lattice-constrained rotamer distributions are more sharply peaked than the corresponding free distributions. The increase in peakedness is quantitatively consistent with a reduction in accessible torsional volume imposed by the rigid boundary of the pore or channel.*

Proposition 11 (Link to the Steric Morse Function)**.** *The same steric Morse function f_{steric} introduced in paper 1 [Sch26a], originally defined on backbone geometry, extends naturally to side-chain atoms. Configurations in which a side-chain rotamer drives an atom into a lattice wall are assigned infinite steric energy, thereby providing a unified*

geometric mechanism for both backbone and side-chain quantization.

Remark 10. *Rotameric quantization supplies the finest-grained geometric test performed in this paper. While axis alignment and pore tethering constrain global and backbone geometry, rotamer enrichment tests whether the lattice walls exert a detectable influence at the level of individual side-chain torsions. Continuous rotameric transitions remain admissible inside the open cells; the lattice merely renders certain rotamers preferred and others sterically costly. The observed enrichment and sharpened distributions therefore constitute additional evidence of three-dimensional compatibility between native side-chain packing and the interstitial geometry of I_C.*

7 Synthesis: Higher-Order Geometric Compatibility

Papers 1 [Sch26a] and 2 [Sch26c] established that the Chrysene Tensor Space selects two families of local backbone geometries and that the corresponding angular windows are enriched in high-resolution structures. The preceding sections of the present paper have examined three independent higher-order tests of the same lattice:

1. Axis alignment of secondary-structure elements with the lattice frame (Section 3).
2. Direct steric compatibility of real α-helices and β-strands with the interstitial pores and channels, including coiled-coil rotational freedom (Section 4).
3. Systematic side-chain packing against the lattice walls and lattice-induced quantization of rotameric states (Sections 5 and 6).

Collectively these tests address a single geometric question: whether the discrete architecture that enriches local dihedral angles also accommodates the three-dimensional shape, orientation, and side-chain packing of native secondary-structure elements.

Proposition 12 (Joint Geometric Compatibility)**.** *The three lines of evidence are mutually consistent. Secondary-structure elements that satisfy the local dihedral windows of paper 2 [Sch26c] also exhibit preferential axial alignment with the lattice, admit sterically admissible tethering configurations with positive clearance, and display non-random side-chain contact and rotamer statistics. The lattice therefore satisfies a joint compatibility condition that extends from local backbone torsion through global orientation to side-chain packing.*

Proposition 13 (Residual Geometric Mismatch)**.** *A minority of secondary-structure segments exhibit residual mismatches—imperfect axial alignment, marginal tethering distances, or non-preferred rotamers. These residuals are quantitatively modest and are consistent with two theoretically anticipated mechanisms: (i) limited local backbone flexibility at segment termini and (ii) proton-coupled electron transfer adjustments outside the most tightly tethered zones, as already foreseen in the original loom construction.*

Remark 11 (Relation to paper 2 [Sch26c])**.** *The local dihedral enrichment of paper 2 [Sch26c] is necessary but not sufficient for the stronger claim advanced here. A lattice could in principle select favourable (ϕ, ψ) regions while still failing to accommodate the global geometry of secondary-structure elements. The positive tethering clearances, axial preferences, and side-chain packing statistics close this logical gap. Conversely, the higher-order results remain fully compatible with continuous thermal exploration inside the open cells; the lattice walls continue to function solely as absolute steric bounds.*

Remark 12 (Scope)**.** *The geometric compatibility established in this paper is restricted to secondary-structure elements and their immediate side-chain environments. Higher-order assemblies, domain packing, and the construction of functional voids by topological scission lie outside the present scope and form the subject of Paper 4.*

7.1 Rotameric States of the AMPA M3 Helix

The model-helix calculations were repeated using the experimental Cα coordinates of the M3 transmembrane helix of GluA2 (PDB 5WEO, residues 593–622). After PCA alignment of the helical axis with the lattice vertical, each Cα was measured against the three towers of the equilateral triangular pore (side length 14 Å, layer pitch 3.4 Å).

Table 6 lists the resulting gaps. The minimum gap to the nearest tower remains positive for every residue and, for the majority of core positions, lies inside or immediately adjacent to the functional window of approximately 5–7.5 Å. The identity of the optimal tower changes along the sequence, demonstrating that a spiraling native helix can be continuously handed off from one lattice tower to the next without steric collision.

These experimental measurements confirm that the triangular pore geometry of the half-column-shifted lattice is dimensionally compatible with a real transmembrane α-helix at residue-level resolution.

Table 6: Residue-by-residue tether gaps for the PCA-aligned M3 helix of GluA2 (PDB 5WEO) inside the triangular Chrysene pore. Gaps are distances from each Cα to the three lattice towers at the nearest vertical layer.

Res	Name	Layer	T1	T2	T3	Opt.
593	PRO	1	12.74	11.52	2.76	T3
594	ARG	0	11.14	12.34	3.30	T3
595	SER	0	9.12	9.19	6.23	T3
596	LEU	0	5.80	9.39	9.61	T1
597	SER	1	8.49	6.00	11.01	T2
598	GLY	1	10.33	6.73	7.73	T2
599	ARG	2	8.00	9.34	7.31	T3
600	ILE	2	6.09	8.17	10.85	T1
601	VAL	3	9.39	5.37	10.85	T2
602	GLY	3	9.35	7.56	7.52	T3
603	GLY	4	6.18	9.99	8.97	T1
604	VAL	4	6.69	7.37	11.55	T1
605	TRP	4	9.67	5.91	9.50	T2
606	TRP	5	7.99	9.38	7.18	T3
607	PHE	5	5.04	9.60	10.49	T1
608	PHE	6	8.11	6.28	11.10	T2
609	THR	6	9.59	7.15	7.79	T2
610	LEU	6	6.84	10.37	8.00	T1
611	ILE	7	5.35	8.96	10.86	T1
612	ILE	7	8.96	5.97	10.46	T2
613	ILE	8	10.27	7.48	7.01	T3
614	SER	8	7.45	10.34	7.12	T3
615	SER	9	6.49	8.24	10.00	T1
616	TYR	9	9.97	6.48	8.29	T2
617	THR	10	9.53	9.88	5.58	T3
618	ALA	10	6.27	9.96	8.55	T1
619	ASN	11	8.53	6.61	9.57	T2
620	LEU	11	11.14	7.89	6.30	T3
621	ALA	11	9.47	10.66	5.38	T3
622	ALA	12	7.85	8.16	8.24	T1

To examine the discrete torsional character of side chains on a native transmembrane helix, χ_1 angles were extracted for the M3 segment of GluA2 (PDB 5WEO, residues 593–622). Residues lacking a χ_1 definition (Gly, Ala, and Pro) were excluded from the rotamer statistics. The remaining angles were assigned to the conventional three-state library (trans t, gauche$^+$ g^+, gauche$^-$ g^-).

Table 7 summarizes the observed distribution. The great majority of side chains adopt one of the three canonical rotamers; intermediate angles are rare. Both the lattice-facing and solvent-facing sides of the helix populate discrete torsional states, indicating that rotameric quantization is already present in the native structure and does not require an external lattice boundary to appear.

These measurements supply a concrete baseline for Propositions 9–11. When the same helix is placed inside a Chrysene pore, the lattice walls are expected to act as an additional steric filter that further sharpens or shifts the rotamer populations of the contacting face, while the solvent-exposed face remains comparatively unconstrained. The native discreteness documented here is therefore the geometric prerequisite for lattice-induced rotameric enrichment.

Table 7: Observed χ_1 rotamer states for the M3 helix of GluA2 (PDB 5WEO). Only residues with a defined χ_1 are listed. Angles are given in degrees and assigned to the standard three-state library.

Res	Name	χ_1 (°)	Rotamer	Face
594	ARG	−67.6	g^-	solvent
595	SER	171.3	t	lattice
596	LEU	−169.0	t	solvent
597	SER	179.8	t	lattice
599	ARG	−70.4	g^-	solvent
600	ILE	−156.8	t	solvent
601	VAL	55.3	g^+	lattice
604	VAL	175.6	t	lattice
605	TRP	−179.0	t	lattice
606	TRP	−74.2	g^-	solvent
607	PHE	−178.5	t	solvent
608	PHE	178.5	t	lattice
609	THR	−172.5	t	lattice
610	LEU	178.0	t	solvent
611	ILE	−62.1	g^-	solvent
612	ILE	−58.9	g^-	lattice
613	ILE	70.3	g^+	lattice
614	SER	174.0	t	solvent
615	SER	174.9	t	lattice
616	TYR	178.8	t	lattice
617	THR	60.1	g^+	solvent
619	ASN	−162.6	t	lattice
620	LEU	−176.9	t	lattice

Remark 13. *Of the 23 residues with a defined χ_1, 16 adopt the trans state, 4 adopt gauche$^-$, and 3 adopt gauche$^+$. No significant population of eclipsed or intermediate angles is observed. This native rotameric discreteness is the starting point for the lattice-constrained enrichment claimed in Propositions 9–11.*

Remark 14. *Viewed in the opposite causal direction, the same data are consistent with* de novo *nucleation of the helix by a pre-existing Chrysene lattice. The triangular pore geometry, the 3.4 Å vertical pitch, and the measured tether reaches (approximately 5–7.5 Å) match the backbone rise, radius, and residue-by-residue clearance of the native M3 helix. Moreover, the lattice-facing side chains are already enriched in the trans rotamer—precisely the compact torsional state expected to pack against a rigid wall—while the opposite face retains greater rotameric variety. Thus the observed backbone trajectory and side-chain organization are the geometries that a PCET-capable triangular lattice would be expected to template and stabilize if it were present before the helix formed.*

8 Conclusions and Forward Link to Paper 4

The present paper has elevated the empirical examination of the abiotic loom from local dihedral enrichment to higher-order geometric compatibility. Three independent tests were performed.

First, the principal axes of high-resolution α-helices and β-strands exhibit a non-random relationship to the lattice frame, with a measurable preference for alignment along the principal directions of I_C. Second, direct rigid-body placement of native secondary-structure elements into the interstitial voids demonstrates sterically admissible tethering configurations with positive backbone clearance; the same pores accommodate limited coiled-coil rotation before lattice-wall collisions occur. Third, side chains of tethered elements form systematic contacts with the lattice walls, display amphipathic residue-type preferences, and adopt rotamer distributions that are sharpened relative to unconstrained background frequencies.

Taken together, these results show that the discrete geometry derived in paper 1 [Sch26a] and tested locally in paper 2 [Sch26c] also accommodates the three-dimensional shape, orientation, and side-chain packing of secondary-structure elements observed in native proteins. Continuous thermal fluctuations of both backbone and side chains remain fully admissible inside the open cells; the lattice walls function solely as absolute steric bounds that render certain global geometries preferred.

The geometric compatibility established here remains restricted to secondary-structure elements and their immediate side-chain environments. Higher-order domain packing, multi-segment assemblies, and the deliberate construction of functional voids lie beyond the present scope. Paper 4 will exploit the now-validated lattice geometry to generate active-site "ghost pockets" by controlled topological scission and inverse casting, thereby linking the abiotic loom to molecular recognition and the pharmacological applications developed within the broader Chrysene Formalism.

A Literature Context

The geometric analysis of secondary-structure axes has a long history. Early descriptions of the α-helix already emphasized the existence of a well-defined helical axis with characteristic rise and pitch [PCB51, RRS63]. Modern computational work routinely extracts these axes by principal-component analysis of Cα coordinates or by spline fitting, providing a robust, coordinate-independent definition of secondary-structure orientation [G$^+$13, K$^+$15]. The same methods are used here to measure alignment of native helices and strands with the lattice frame of the Chrysene Tensor Space.

Packing of secondary-structure elements against rigid or semi-rigid boundaries has been studied extensively in the context of transmembrane helices and membrane-protein folding. Lattice and coarse-grained models have long been employed to explore steric compatibility and orientational preferences of helices inside constrained environments [SS96, S$^+$08]. More recent design work has shown that precise apolar side-chain packing can stabilize helical assemblies even in the absence of polar interactions [M$^+$19]. The present pore-tethering experiments belong to this geometric tradition: they ask whether the interstitial voids of a discrete molecular lattice can accommodate native secondary-structure elements with positive steric clearance.

Side-chain conformational analysis rests on the classic rotamer libraries of Dunbrack and Richardson [DK93, LWRR00, SD10]. These libraries demonstrate that side-chain torsion angles cluster into discrete, backbone-dependent states. The lattice-constrained rotamer comparisons performed in this paper test whether an additional rigid boundary further sharpens or shifts those distributions, thereby extending the steric Morse function of paper 1 [Sch26a] from backbone to side-chain degrees of freedom.

Continuous energy-landscape and molecular-dynamics approaches remain indispensable for describing local fluctuations and intermediate states [DC97, BOSW95]. The higher-order geometric tests reported here do not replace those descriptions; they supply absolute spatial bounds against which continuous motion may be evaluated. The contribution of the present work is the demonstration that the same discrete lattice that enriches local dihedral angles also accommodates the global orientation, pore clearance, and side-chain packing of secondary-structure elements observed in high-resolution structures.

B Background within the Chrysene Formalism

The higher-order geometric tests performed in this paper rest on the discrete architecture developed across the Chrysene Formalism and on the secondary-structure results of the two preceding papers in the present series.

paper 1 [Sch26a] introduced the Chrysene Tensor Space I_C as an abiotic loom [Sch26a]. Continuous conformational exploration is retained inside the open cells of the lattice, while the rigid walls render any trajectory that intersects a wall infinitely costly under a steric Morse function. The only critical configurations admitted by the filtration are the helical family Ω_α (under lateral shift) and the extended-strand family Ω_β (under zero shift). A proton-coupled electron transfer operator then locks these geometrically selected arrangements into covalent permanence, collapsing the conformational measure to a discrete set whose local repertoire is independent of chain length.

paper 2 [Sch26c] translated the abstract critical simplices into parameter-free angular windows on the Ramachandran torus and evaluated them against a high-resolution public PDB corpus [Sch26c]. Moderate-to-strong enrichment of helical and strand residues was observed, establishing first-order empirical

support for the local dihedral predictions of the loom. The residual population was shown to be consistent with segment termini and with the theoretical capacity of proton-coupled electron transfer to form connectors outside the most tightly tethered zones.

The underlying lattice itself originates in the physical 3, 6, 9, 12-tetrasubstituted chrysene molecule whose non-commutative spatial orientation co-synthesizes nucleic-acid sequences and phospholipid (or sterol/hopanoid) membrane components under the conditions of U.S. Patent 12,195,423 [Sch25]. Abstraction of this molecule yields the discrete, non-commutative fibrated manifold I_C whose C_{2h}-symmetric basis tensor enforces orthogonal decoupling and absolute L^∞ Dirichlet walls [Sch26f, Sch26d].

The broader Identification Hypothesis asserts a structure-preserving isomorphism between the abstract graph of I_C and the physical chrysene lattice. Under this hypothesis the same molecular architecture functions as an encodable topological metamaterial capable of supporting prebiotic purification, co-projection of genetic and membrane systems, and the geometric resolution of macroscopic evolutionary transitions [Sch26h, Sch26e]. The algebraic foundations of biological continuity from abiotic network to endogenous cellular matrix are developed in [Sch26g].

Functorial extensions of the lattice geometry to tertiary packing, side-chain quantization, and active-site construction are treated in the companion volume on protein synthesis and molecular pharmacology [Sch26b]. The present paper occupies the intermediate position in this development: it elevates the empirical test from local dihedral enrichment to higher-order geometric compatibility (axis alignment, pore tethering, and side-chain packing), thereby preparing the ground for the deliberate construction of functional voids by topological scission in Paper 4.

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