Polycubes with Cavities: Enumeration to Size 18 and Corrections to Published Counts

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August 2026

Abstract

A polycube has a *cavity* if its complement in $\mathbb{Z}^3$ is disconnected, i.e., if it completely encloses empty space. We enumerate all polycubes with up to 18 cells and count those with cavities in the fixed, one-sided, and free senses, extending OEIS sequences `A357083` and `A355966` by four terms each and contributing the new sequence `A396101`. Two previously published terms of `A355966` are shown to be erroneous, and we identify the two independent flaws in the original computation that account exactly for the discrepancies. Our enumeration uses Redelmeier's algorithm augmented with an incrementally maintained pruning condition; we prove the condition exact by a structural analysis of minimal cavities, including the result that the smallest polycube whose cavity is not a single cell has exactly 15 cells, of which there are precisely 180 one-sided examples. All counts are validated against the independently known totals of `A001931` at every size, by two algorithmically independent counting methods, and by reruns under a provably conservative pruning regime.

1 Introduction

A *polycube* is a finite, face-connected set of unit cells of the cubic lattice $\mathbb{Z}^3$, the three-dimensional analogue of a polyomino. Polycubes are counted in three standard senses: *fixed* (distinct up to translation), *one-sided* (up to translation and rotation), and *free* (up to translation, rotation, and reflection). The corresponding total counts are OEIS `A001931` (fixed), `A000162` (one-sided), and `A038119` (free), known through $n = 22$; the current records are due to an algorithm of S. Dodds [3, 5].

This paper concerns polycubes that fully enclose empty space. Interest in such objects dates to the observation that, unlike polyominoes—whose "holes" are visible in the plane—a polycube can conceal its defects: a cavity is invisible from every direction. The counting sequences were introduced in 2022 by John Mason (`A357083`, free) and Gleb Ivanov (`A355966`, one-sided) but extended by neither since; each was known to at most five terms.

Our contributions:

1. We extend both sequences through $n = 18$ (four new terms each) and contribute the fixed-count companion `A396101` (Table 1).

2. We show the published values A355966(14) = 75917 and A355966(15) = 835491 are erroneous; the correct values are 76017 and 838575. We identify two independent flaws in the program that produced the original values and show they account for the deficits exactly (Section 6).

3. We prove that the smallest polycube with a cavity larger than one cell has exactly 15 cells (Proposition 4), and enumerate the 180 one-sided examples.

4. We give a pruning lemma that eliminates 80–93% of cavity checks during exhaustive enumeration (a measured speedup of roughly $5\times$ at $n = 18$ and $20\times$ at moderate sizes), with a complete exactness analysis (Section 4).

n	A396101 (fixed)	A355966 (one-sided)	A357083 (free)
11	384	20	11
12	9 524	404	215
13	146 608	6 164	3 173
14	1 822 413	**76 017***	38 564
15	20 112 770	**838 575***	**422 277**
16	206 155 755	**8 590 722**	**4 310 738**
17	2 011 440 896	**83 814 695**	**41 982 903**
18	18 958 443 692	**789 943 572**	**395 335 115**

Table 1: Cavity polycube counts. Bold entries are new to this work; * denotes corrections of previously published values.

2 Definitions

Cells of $\mathbb{Z}^3$ are unit cubes indexed by their integer coordinates; two cells are *adjacent* if they share a face. A *polycube* of size n is a set of n cells whose adjacency graph is connected.

Definition 1 (Cavity)**.** Let P be a polycube. The complement $\mathbb{Z}^3 \setminus P$ decomposes into face-connected components, exactly one of which is infinite. Each finite component is a *cavity* of P. Cells of a cavity are *cavity cells*; the set of complement cells adjacent to a cavity is contained in P and is called the cavity's *shell*.

The symmetry group of $\mathbb{Z}^3$ fixing the origin is the 48-element group B_3 of signed coordinate permutations; its rotation subgroup has 24 elements. Free (resp. one-sided) polycubes are orbits of fixed polycubes under the full group (resp. rotation subgroup) combined with translations. Whether a polycube has a cavity is invariant under all 48 symmetries.

The smallest polycube with a cavity has 11 cells: the six face-neighbors of the cavity cell must all be present, they are pairwise non-adjacent, and each further cell is adjacent to at most two of them, so connecting the six components requires at least five more cells. (The minimum itself appears in the OEIS entries; our enumeration confirms it.)

Remark 1. The count of minimal examples has a closed form. The six shell cells form the vertices of an octahedron, and the candidate connecting cells — the twelve cells adjacent to exactly two shell cells — correspond to its edges; connecting cells are pairwise non-adjacent, so an 11-cell cavity polycube is connected precisely when its five connectors form a spanning tree of the octahedron. By Kirchhoff's matrix-tree theorem the octahedron has $\frac{1}{6}\,4^3 \cdot 6^2/6 = 384$ spanning trees (from Laplacian spectrum $\{0, 4, 4, 4, 6, 6\}$), which is exactly $\texttt{A396101}(11) = 384$.

3 Algorithm

3.1 Enumeration

We enumerate fixed polycubes with Redelmeier's algorithm [1], which visits each fixed polycube of size at most N exactly once as a node of a search tree, requiring $O(1)$ amortized work per node and no storage of previously generated polycubes. Every node of the tree at depth n *is* a fixed polycube of size n, so a single run tallies all sizes up to N simultaneously. Totals at every size are checked against `A001931`; a run is accepted only if all totals match exactly.

3.2 Cavity detection and pruning

Testing each of the 8.4×10^{13} polycubes of size ≤ 18 for cavities by flood fill would dominate the running time. We instead maintain, incrementally in $O(1)$ per cell placement, the quantity

$$K_t \;=\; \#\{\text{empty cells with at least } t \text{ occupied face-neighbors}\},$$

and invoke the flood fill only at nodes with $K_t > 0$. Section 4 establishes for which (t, n) this is exact. With $t = 5$ the filter eliminates most flood fills — at $n = 18$, 1.94×10^{13} fills were performed across 9.66×10^{13} eligible nodes (an 80% reduction, rising above 90% at smaller sizes) — and the enumeration sustained 4.8×10^8 to 9.3×10^8 nodes per second per machine in production runs.

3.3 Symmetry counting

When a cavity polycube P is confirmed at target size, we compute its stabilizer within the 48 symmetries by direct canonical-form comparison. By Burnside's lemma applied per orbit, summing $|\mathrm{stab}_{48}(P)|$ over all *fixed* cavity polycubes and dividing by 48 yields the free count, and analogously with the 24 rotations for the one-sided count. Because cavity polycubes are rare (about 2×10^{-4} of all polycubes at $n = 18$), this per-object cost is negligible.

3.4 Distribution

The search tree is split at depth 7 into 23,502 independent jobs, distributed dynamically across threads and statically across machines by residue class; per-part totals are exact and sum to the full counts. Runs were performed on two consumer desktop machines: an AMD Ryzen 7 9800X3D (8 cores, 16 threads) and an Intel Core i9-12900K (8P+8E cores, 24 threads).

4 Exactness of the pruning condition

Call a cavity R (as a set of cells) *leafy* if some cavity cell has at most one neighbor within R, and *leafless* otherwise (every cavity cell has ≥ 2 neighbors in R, i.e., the induced graph of R has minimum degree 2).

Lemma 1 (Leafy cavities are caught at $t = 5$)**.** *If a polycube P has a leafy cavity, some empty cell has at least five occupied face-neighbors.*

Proof. A cavity cell with k neighbors in R has exactly $6 - k$ occupied face-neighbors, since every neighbor of a cavity cell is either a cavity cell or a shell cell of P. A leafy cell has $k \leq 1$. □

Lemma 2 (Leafless cavities require at least 24 cells at $t = 4$)**.** *If every cavity cell of P has at most three occupied neighbors, then $|P| \geq 24$.*

Proof. The hypothesis makes R an induced subgraph of $\mathbb{Z}^3$ of minimum degree 3. Consider the six extreme layers of R (the cells attaining the maximum or minimum coordinate along each axis). A cell in, say, the top z-layer has its $+z$-neighbor outside R, hence at most one vertical neighbor in R; minimum degree 3 forces at least two horizontal neighbors, so each extreme layer is a planar set of minimum degree 2, which has at least 4 cells (no triangles exist in $\mathbb{Z}^2$ and fewer than 4 cells cannot sustain degree 2). Each cell of the top layer contributes a distinct shell cell directly above it, and the six families of shell cells so obtained are pairwise disjoint, as they are separated by coordinate signature (e.g., $+z$-shell cells have z-coordinate exceeding all of R's, while $+x$-shell cells have x-coordinate exceeding all of R's but z-coordinate within R's range). Hence $|P| \geq |\text{shell}(R)| \geq 6 \cdot 4 = 24$. □

Corollary 1. *With $t = 4$ the pruning condition is exact for all $n \leq 23$.*

Threshold $t = 5$ is faster in practice by an order of magnitude; its exactness requires ruling out leafless cavities at small sizes.

Proposition 1 (The 2×2 cavity requires 21 cells)**.** *The smallest polycube whose cavity contains a $2 \times 2 \times 1$ block (the unique 4-cell induced cycle of $\mathbb{Z}^3$ up to isometry) has 21 cells.*

Proof. The shell of the 2×2 cavity consists of 16 forced cells: two 2×2 plates above and below and an equatorial ring of 8 cells. The ring decomposes into four separated dominoes, and neither plate is adjacent to any ring cell, so the shell has six connected components. A cell adjacent to a plate and a ring domino must lie in the plate's layer directly above or below a ring cell; a cell adjacent to two ring dominoes must lie at one of the four equatorial corners; and no lattice cell is adjacent to cells of three components (any two of a plate, an opposite plate, and two distinct dominoes fail a coordinate check). Hence each added cell reduces the number of components by at most one, five additional cells are necessary, and a spanning choice (three corners and one bridge to each plate) achieves 21. □

Proposition 2 (Exhaustive scan of small leafless cavities)**.** *Among all polycube shapes with at most 17 cells, the only sets of minimum degree 2 whose shell has at most 18 cells are the three orientations of the $2 \times 2 \times 1$ block. Consequently, by Proposition 1, no polycube with at most 18 cells has a leafless cavity of at most 17 cells.*

Proof. By direct enumeration with the scanning variant of our program, which maintains the number of degree-deficient cells incrementally and measures the shell of every minimum-degree-2 configuration encountered. The scan covers all 12,630,298,688,658 fixed polycubes with at most 17 cells; of the 630,961,445 minimum-degree-2 shapes found, all have shells of at least 19 cells except the three orientations of the $2 \times 2 \times 1$ block (shell 16). The runs are reproducible in about six hours on a single desktop CPU. □

Proposition 3 (Tail bound)**.** *No polycube P with at most 18 cells has a leafless cavity of 18 or more cells.*

Proof. Suppose R is such a cavity, $|R| \geq 18$, with shell contained in P, so $|\text{shell}(R)| \leq 18$. Write $a \geq b \geq c$ for the extents of R's bounding box, and A_z for the area of the projection of R along the c-axis; let Π denote that projection.

Step 1 (spans). A connected polycube with m cells has bounding-box extents summing to at most $m+2$. The bounding box of P strictly contains that of R on both sides in every axis, so $(a+2)+(b+2)+(c+2) \leq 18+2$, giving $a+b+c \leq 14$; in particular $c \leq 4$.

Step 2 (planar case). If $c = 1$ then every cell of R contributes two distinct shell cells (above and below), so $|\text{shell}| \geq 2|R| \geq 36$, a contradiction. Hence $2 \leq c \leq 4$.

Step 3 (caps). For each of the A_z occupied columns of Π, the cells immediately above the top and below the bottom cell of the column are distinct shell cells, so $|\text{shell}| \geq 2A_z$; with $|\text{shell}| \leq 18$ this gives $A_z \leq 9$. Since the c layers of R each fit inside Π, $A_z \geq \lceil |R|/c \rceil$.

Step 4 (sides). Let E be an empty column horizontally adjacent to Π, and let z be a height at which some column of Π adjacent to E contains a cell of R. Then the cell of E at height z is empty (its column meets no cell of R) and face-adjacent to R, hence a shell cell. Distinct pairs (E, z) are distinct cells, disjoint from the caps of Step 3, whose columns lie in Π. Writing $\partial\Pi$ for the set of empty columns adjacent to Π (the *site perimeter* of Π) and $h(E) \geq 1$ for the number of covered heights at E,

$$|\text{shell}| \;\geq\; 2A_z + \sum_{E \in \partial\Pi} h(E) \;\geq\; 2A_z + |\partial\Pi|.$$

Step 5 (perimeters of small planar sets). An exhaustive check over the free planar shapes with at most 9 cells (there are 1,818) shows the minimum site perimeter for $A = 5, \ldots, 9$ cells is $8, 9, 10, 10, 11$ respectively, and that the plus-pentomino is the unique 5-cell shape of perimeter 8.

Conclusion. If $c = 2$ then $A_z = 9$ is forced and $|\text{shell}| \geq 18 + 11 = 29$. If $c = 3$ then $A_z \geq 6$ and $|\text{shell}| \geq 2A_z + p(A_z) \geq 12 + 9 = 21$. If $c = 4$ then $A_z \geq 5$; for $A_z \geq 6$ the same bound gives at least 21, and for $A_z = 5$ either Π is not the plus-pentomino, whence $|\partial\Pi| \geq 9$ and $|\text{shell}| \geq 19$, or Π is the plus-pentomino, in which case the four empty columns beyond the arm tips are each adjacent to exactly one arm, so their covered heights sum to the total number of cells in the four arms, at least $|R| - c \geq 14$, giving $|\text{shell}| \geq 10 + 14 = 24$. In every case $|\text{shell}| > 18$, contradicting $|\text{shell}| \leq 18$. □

Corollary 2. *The $t = 5$ pruning condition is exact for all $n \leq 18$: by Lemma 1 every leafy cavity is caught, and by Propositions 1, 2 and 3 no polycube with at most 18 cells has a leafless cavity at all.*

5 The smallest multi-cell cavities

Proposition 4. *The smallest polycube whose cavity is not a single cell has 15 cells; its cavity is a* $1\times1\times2$ *block. There are exactly* 4320 *fixed and* 180 *one-sided such polycubes of size 15, and none of any kind below 15.*

Proof. Achievability at $n = 15$ is implicit in a remark of Ivanov on `A355966` (via the cuboid bound `A355880`); we prove minimality and count the examples. The shell of a $1\times1\times2$ void has 10 cells in six components (two caps, four side dominoes), and no single cell is adjacent to more than two components, so five connectors are needed: $10 + 5 = 15$. Larger or differently shaped multi-cell cavities require larger shells (Proposition 2). The counts follow from exhaustive classification of the complete set of 20,112,770 fixed cavity polycubes of size 15 produced by our enumeration: 20,108,450 have a single one-cell cavity and 4,320 have a single two-cell cavity; no polycube of size ≤ 15 has two cavities. □

6 Errors in the published values of A355966

The original terms of `A355966` were produced by a Python program (archived with the OEIS entry) that grows polycubes outward from the six-cell shell of one designated empty cell. Comparison with our results locates two independent flaws.

Flaw 1: single-cell cavity model. The program can only generate polycubes containing the full shell of the designated cell, hence only single-cell cavities. By Proposition 4 this first fails at $n = 15$, where exactly 180 one-sided polycubes have a domino cavity and are invisible to the search.

Flaw 2: unsound pruning. The program memoizes partial configurations by canonical form under the 24 rotations while excluding growth into one *fixed absolute* cell. Rotation-equivalent partials whose enclosed cells align differently collide in the memo, and the pruned subtree's completions are not always reachable from the retained representative, silently losing configurations. The loss happens to be zero for $n \leq 13$, which explains why the published $a(11)$–$a(13)$ are correct.

The two flaws account exactly for the observed deficits: at $n = 14$ (where all cavities are single cells) the published value is short by the 100 one-sided classes lost to Flaw 2; at $n = 15$ the deficit $838575 - 835491 = 3084$ decomposes as 180 (Flaw 1) + 2904 (Flaw 2).

7 Verification

Confidence in exhaustive computations rests on redundancy. Every reported term is supported by:

1. **Total-count anchoring.** Fixed totals at every size $n \leq 18$ match `A001931`, whose terms were computed independently by different algorithms [4, 5], to the last digit (84,384,157,287,999 at $n = 18$).

2. **Dual counting methods.** The complete sets of fixed cavity polycubes at $n = 14, 15$ were exported and recounted by an independent implementation using canonical-

form hashing over a symmetry group constructed by generator closure—no Burnside argument, no shared transform tables. Both methods agree on every term.

3. **Dual pruning regimes.** All terms for $n \leq 15$ were recomputed with the $t = 4$ condition, which is exact unconditionally by Corollary 1. Results agree; for $n \geq 16$ exactness rests on Corollary 2.

4. **Cross-machine determinism.** Production runs were split across two machines with different CPU architectures; part sums reproduce single-machine runs exactly.

5. **External agreement.** Our free counts reproduce all four published terms of `A357083` (Mason, independent implementation), and our one-sided counts reproduce $a(11)$–$a(13)$ of `A355966`.

6. **Instrumented rerun with cross-checked detection.** After the above, an instrumented derivative of the production enumerator, carrying an independently implemented cavity-classification layer whose every decision was cross-checked against an unconditional flood fill (about 1.4×10^9 classifications at $n = 15$), reproduced all terms and totals for $n \leq 15$, including both corrected values of `A355966`.

8 Growth and asymptotics

Madras's pattern theorem for lattice animals [2] implies that any finite pattern occurring in some polycube occurs in all but exponentially few large polycubes; applied to the 11-cell cavity configuration, the proportion of n-cell polycubes with a cavity tends to 1 as $n \to \infty$. Our data quantifies the onset of this phenomenon (Table 2): the cavity fraction grows by a factor of about 1.3 per added cell over the observed range, while remaining below 2.3×10^{-4} at $n = 18$.

n	fixed cavity fraction	ratio to previous
11	6.35×10^{-6}	–
12	2.13×10^{-5}	3.36
13	4.41×10^{-5}	2.07
14	7.30×10^{-5}	1.66
15	1.07×10^{-4}	1.46
16	1.44×10^{-4}	1.35
17	1.83×10^{-4}	1.28
18	2.25×10^{-4}	1.23

Table 2: Fraction of fixed polycubes with a cavity.

The successive ratios decline steadily toward 1, consistent with the pattern-theorem picture in which the non-cavity fraction decays exponentially in n; the observed range is far too early for a meaningful estimate of the decay rate, and we do not attempt one.

9 Data and code availability

The enumerator (C, about 400 lines), the independent verification counter, the scanning variant, and the cavity classifier are available from the author, together with the complete sets of fixed cavity polycubes for $n \leq 15$ as binary cell lists (76 MB and 905 MB); links will also be added to the OEIS entries.

Acknowledgments

The author thanks the OEIS editors, particularly Michel Marcus and Andrew Howroyd, for prompt review of the sequence submissions, and acknowledges the use of Claude (Anthropic) for programming and drafting assistance throughout this project.

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