other, and otherwise LD was tested pairwise such that the r2 cannot be above 0.8 and significant at alpha = 0.05.

These filters result in 541 taxa and 13,964 sites. Only 14 of the 15 Turkey Pen samples passed filtering due to coverage.

Unique Hardy-Weinberg without LD filtered set (population cores)

This dataset was filtered as above, but omitting step 6 that filtered out SNPs in LD. These filters result in 565 taxa and 23,056 sites, where only 14 of the 15 Turkey Pen samples passed filtering. This filtered set was subject to additional taxa filtering using Silhouette scoring (*45*) to generate genetically unique populations. Firstly, maize and teosinte populations were defined based on species, subspecies, geographic distribution, elevation and cultural context (details can be found in Table S3). From those, individuals that were more similar to members of any other population than to their own were filtered out. To that end, a matrix of genetic distances (identity by sequence - IBS) was computed using plink toolset (*46*). Silhouette scores were calculated with formula (1). For each individual *i*, where *s* is a silhouette score, *a* is the average genetic distance to members of the same population and *b* is the average genetic distance to members of the closest, foreign population.

(1) $s(i) = [b(i)-a(i)]/max\{a(i),b(i)\}$

Populations that had most negative effect on average silhouette scores of adjacent populations were removed. At this stage the populations: 'US - Athabaskan', 'South America - Lowlands', 'Parviglumis - Huehuetenangensis', 'Mexico - N. Midlands', 'US - SW Highlands', 'Parviglumis - C. Highlands and 'Parviglumis - C. Midlands' were removed. Additionally, populations that were characterized by very small sample size were filtered out: 'US - Texas Low' and 'US - Gaspé Flint'. From the remaining populations, individuals with negative silhouette scores were removed iteratively, with re-calculation of the IBS matrix and scores after each iteration, until all individuals were characterized with scores higher than 0.01. This dataset contains 328 individuals, 23,056 SNPs and is referred to as 'population scores'.

Landrace Hybrid design and phenotyping

Landrace hybrids were generated at the Native Seeds/SEARCH farm in Patagonia, Arizona, in the summer of 2013 by crossing as many individuals as possible from 108 landrace accessions onto the inbred line PHZ51, chosen for good agronomic performance and disease resistance. PHZ51 plantings were staggered once a week for a month to encourage floral synchronization, and the earliest estimated landrace accessions were planted in the second planting. The individuals with attempted crosses were preferentially genotyped for population genetic analysis.

In the summer of 2015, the progeny from 111 hybrid individuals with sufficient seed return representing 80 accessions and 10 PHZ51xB73 checks were grown in an
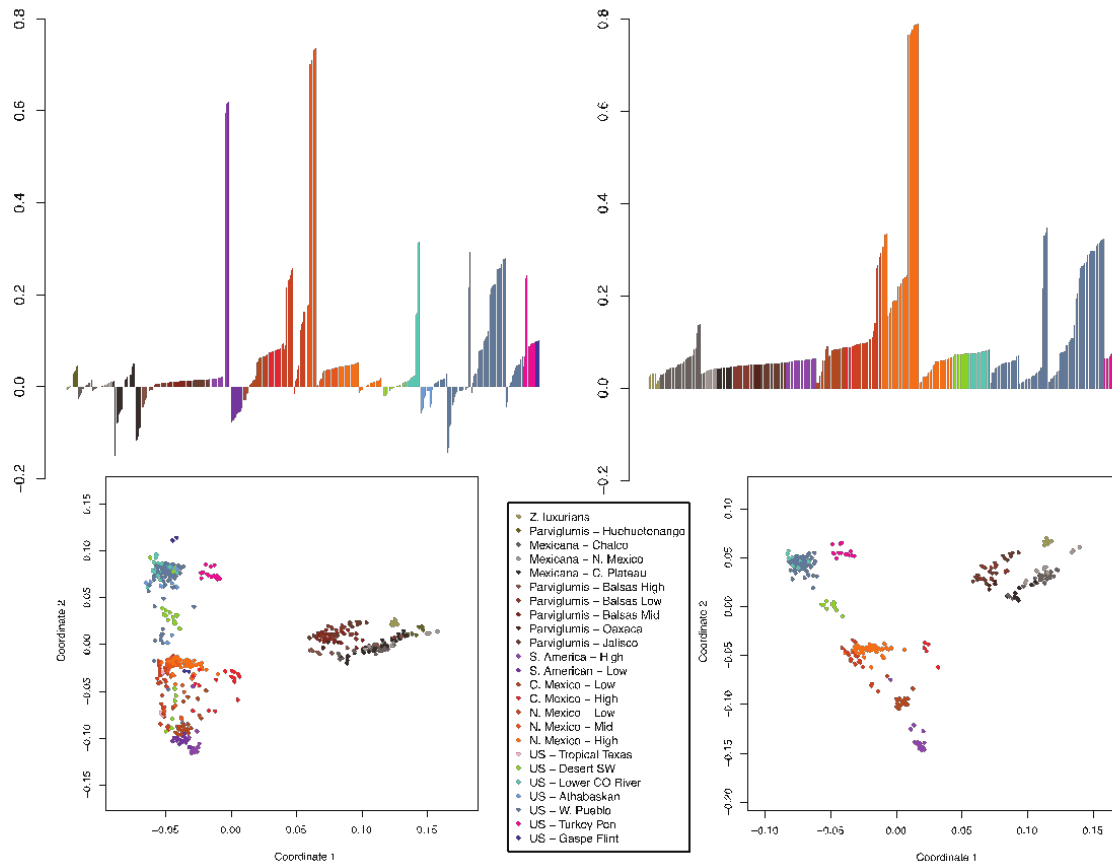
Figure S11: Effect of filtering for core samples. Isolation of core populations from the geographic/cultural subsets and filtering of individuals in each core population was carried out using silhouette scoring. In top panel we show individual silhouette scores before (left) and after (right) filtering out samples with negative scores. In the bottom panel we show MDS plot before (left) and after (right) filtering.
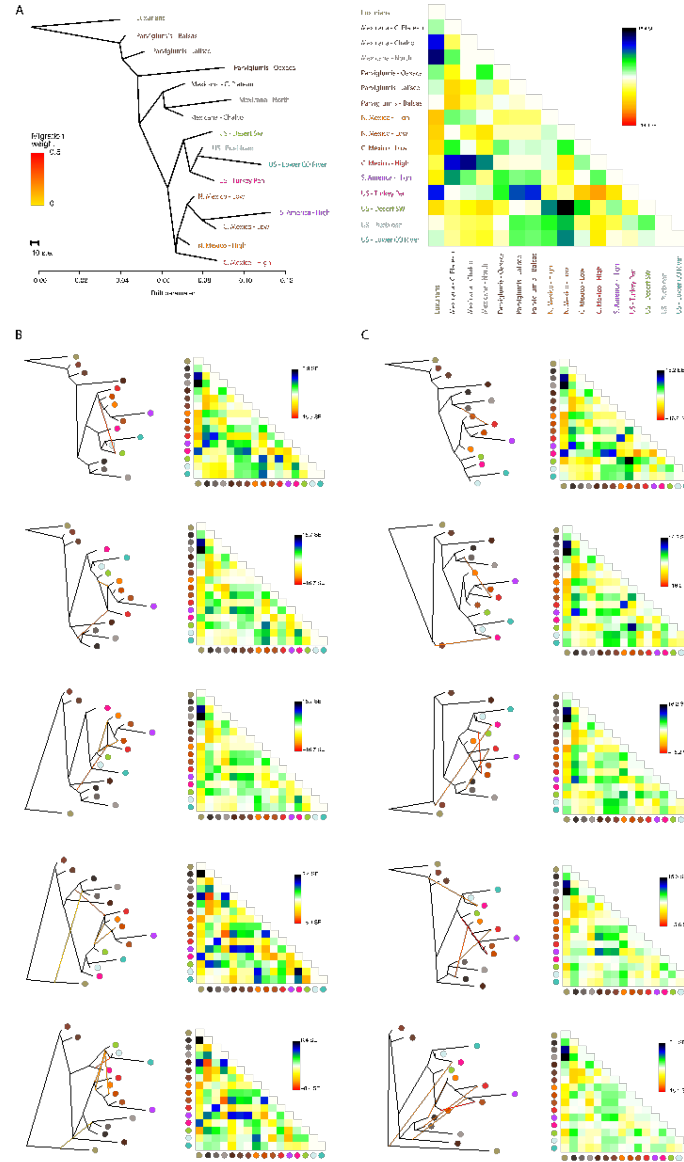
Figure S17: Admixture modelling with TreeMix. (A) Population tree without admixture edges (left) and residual fit of the tree as standard errors. (B) Population trees with 1-5 modeled admixture edges, allowing the admixture to vary freely and residual heatmaps. (C) Population trees with 1-5 modeled admixture edges, forcing the first edge between the C. Mexican Highlands and Mexicana together with subsequent residual heatmaps. Colors of dots match population colors. All analyses use the HWE filtered SNP set of the core population.
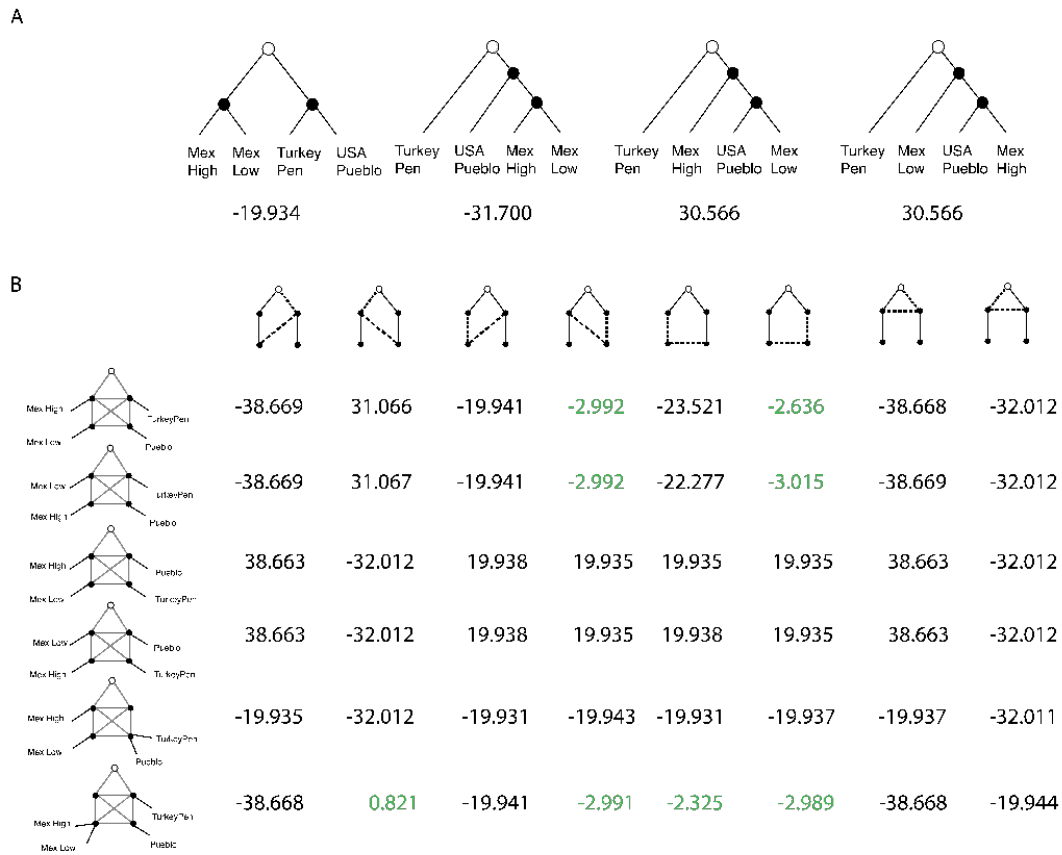
Mex High | Mex Low | Turkey Pen | USA Pueblo   Turkey Pen | USA Pueblo | Mex High | Mex Low   Turkey Pen | Mex High | USA Pueblo | Mex Low   Turkey Pen | Mex Low | USA Pueblo | Mex High

-19.934   -31.700   30.566   30.566

B

-38.669	31.066	-19.941	-2.992	-23.521	-2.636	-38.668	-32.012
-38.669	31.067	-19.941	-2.992	-22.277	-3.015	-38.669	-32.012
38.663	-32.012	19.938	19.935	19.935	19.935	38.663	-32.012
38.663	-32.012	19.938	19.935	19.938	19.935	38.663	-32.012
-19.935	-32.012	-19.931	-19.943	-19.931	-19.937	-19.937	-32.011
-38.668	0.821	-19.941	-2.991	-2.325	-2.989	-38.668	-19.944

Figure S13: Model space explored in AdmixtureGraph for four populations. Four simple ancestry models (A) and 48 admixture models (B) that are the extension of three population models (Fig. S12) were tested. Numbers represent maximum z-score calculated for all possible f(4) statistic combinations; values highlighted in green show model that best fits the data. Leafs of the graphs represent sampled populations. Filled black circles represent internal nodes (unsampled populations), while empty circles represent roots. Continuous black lines denote direct ancestry, dotted lines denote admixture event. (B) Rows show various arrangements of sampled populations, columns show different admixture events.
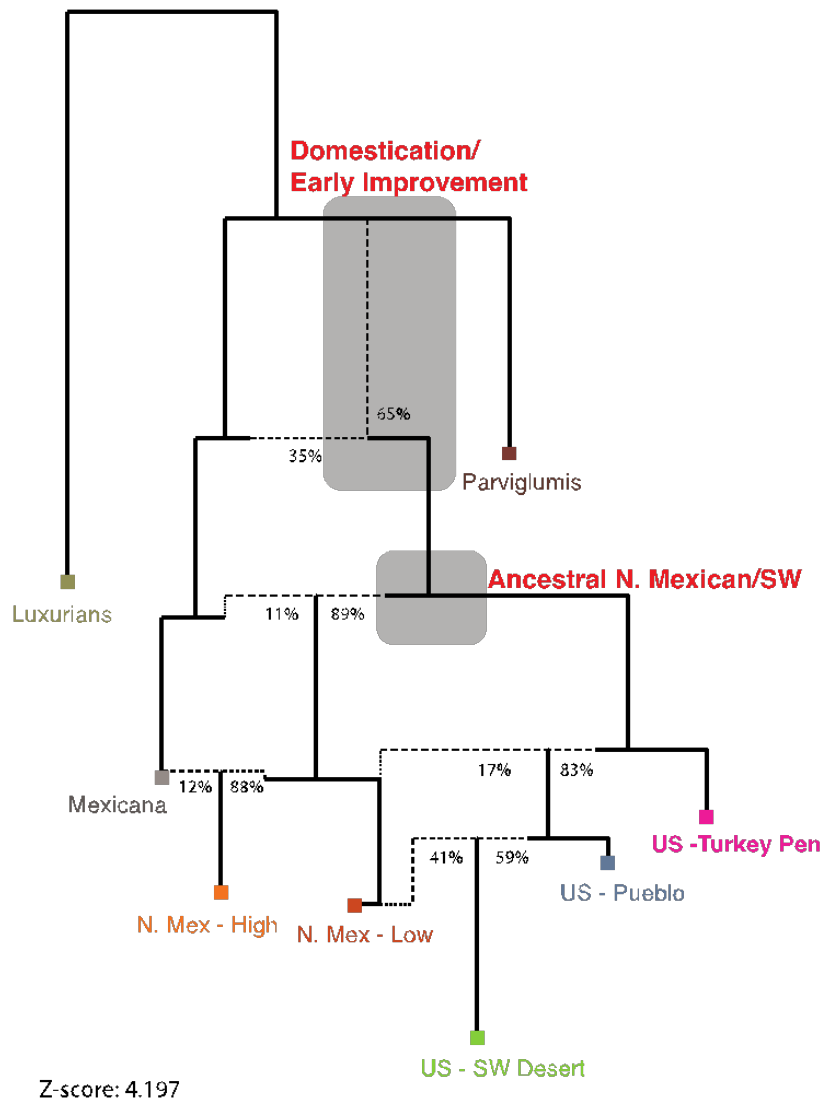
Figure S19: AdmixtureGraph analysis modelling drift among seven populations.
This analysis extends 5 population model to include Mexicana introgression. *Z. luxurians* is used as an outgroup. The Z-score for this model was 4.197.