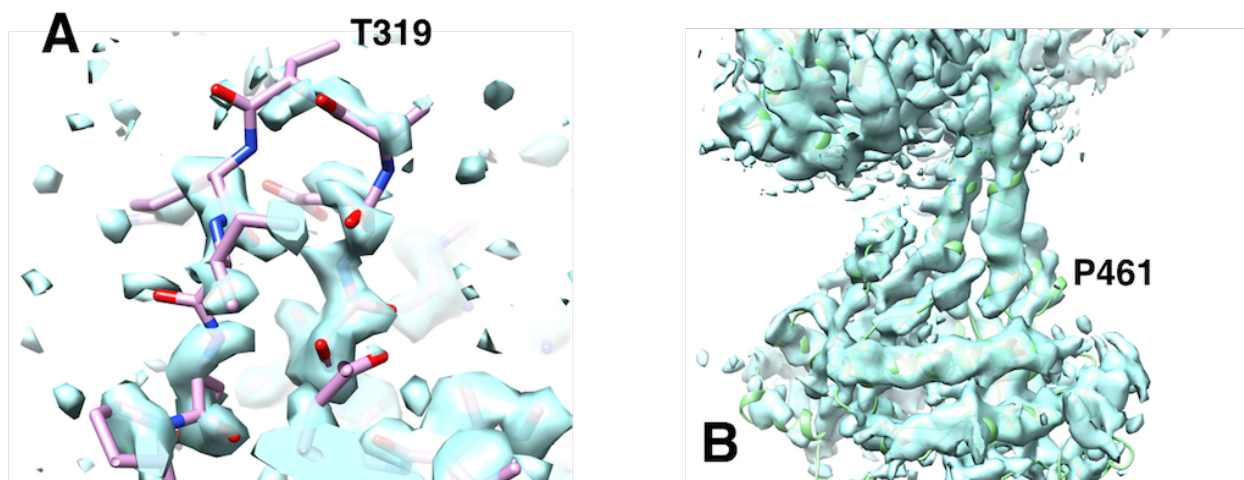# Improvement of cryo-EM maps by density modification

Thomas C. Terwilliger, Steven J. Ludtke, Randy J. Read, Paul D. Adams, Pavel V. Afonine
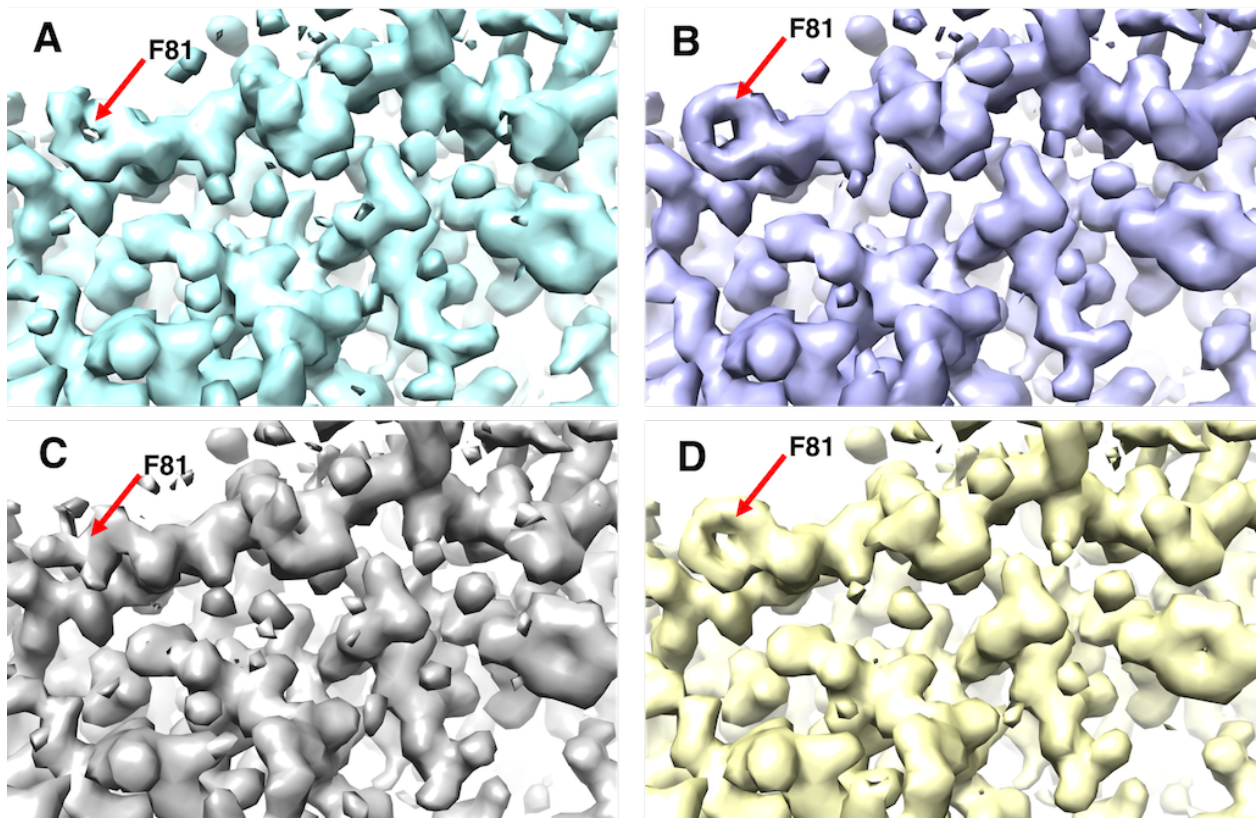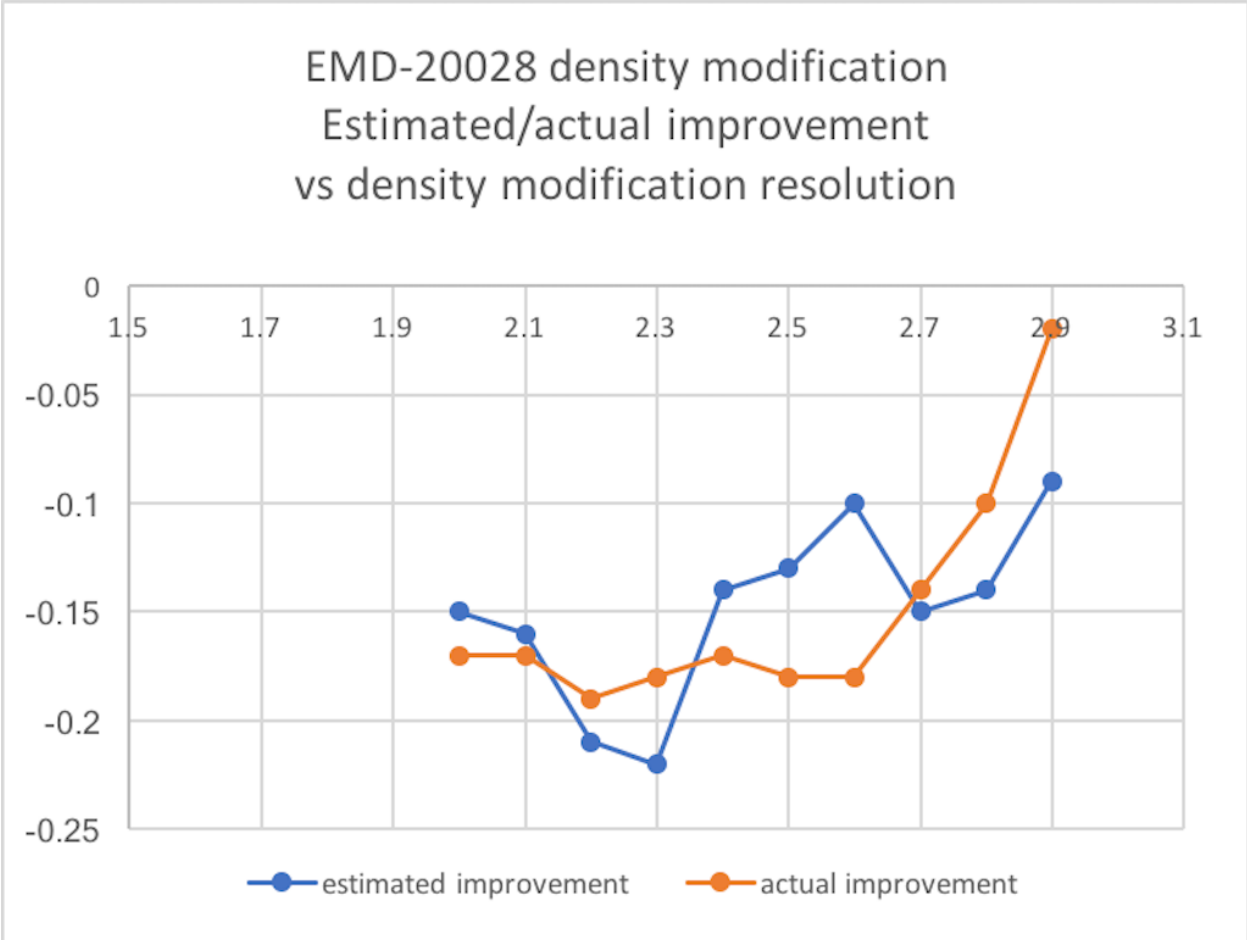
Supplementary Figures

Supplementary Fig. S1. Analysis of non-density-modified maps to examine whether simple modifications (sharpening, using deposited maps) would yield maps that appear similar to the density-modified maps. A. Deposited map showing the same region as depicted in Fig. 2C. This map also shows poor density for the loop. Varying the sharpening of the map did not yield connected density as in Fig. 2D.   B. Sharpened version of the original map shown in Fig. 2E.
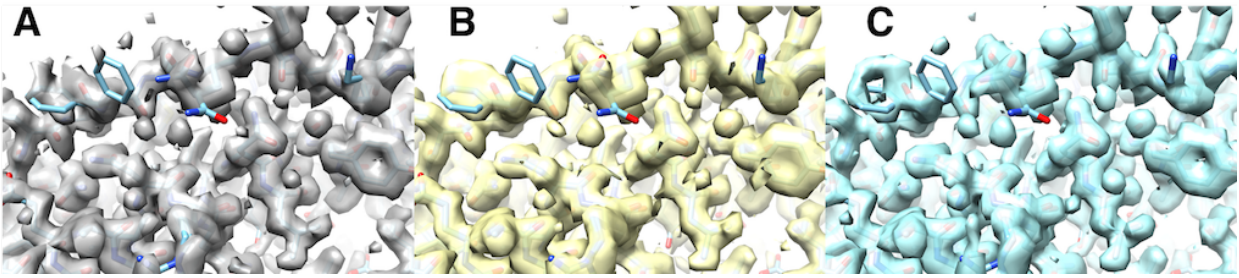
Supplementary Fig. S2. Histogram matching of emd-20026. A. Average of half-maps, sharpened to match density-modified map in C. B, histogram-matched version of map in A, sharpened as in A. C, Density-modified map. All contours set to enclose equal volumes. Maps masked around atoms in model.

Supplementary Fig. S3. Comparison of half-maps 1 and 2 for density modification shown in Fig. S2. All maps masked and sharpened to match density-modified map in Fig. S2C. A and C, half maps 1 and 2. B and D, density-modified half-maps 1 and 2.
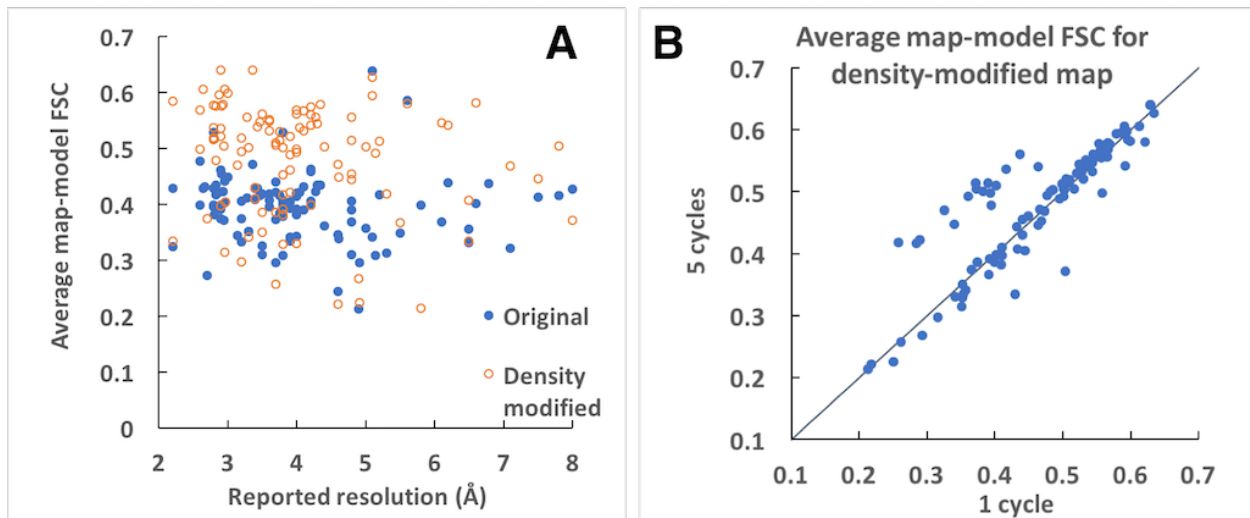
Supplementary Fig. S4. Effect of density modification resolution on actual and estimated change in resolution where FSC is ½. Half-dataset maps for EMD-20028 were density modified as in Fig. 1, but varying the resolution for density modification from 2 to 2.9 Å. The estimate change in resolution (calculated from the error analysis) and the actual change in resolution (calculated from the FSC to the high-resolution EMD-20026 map) are shown.
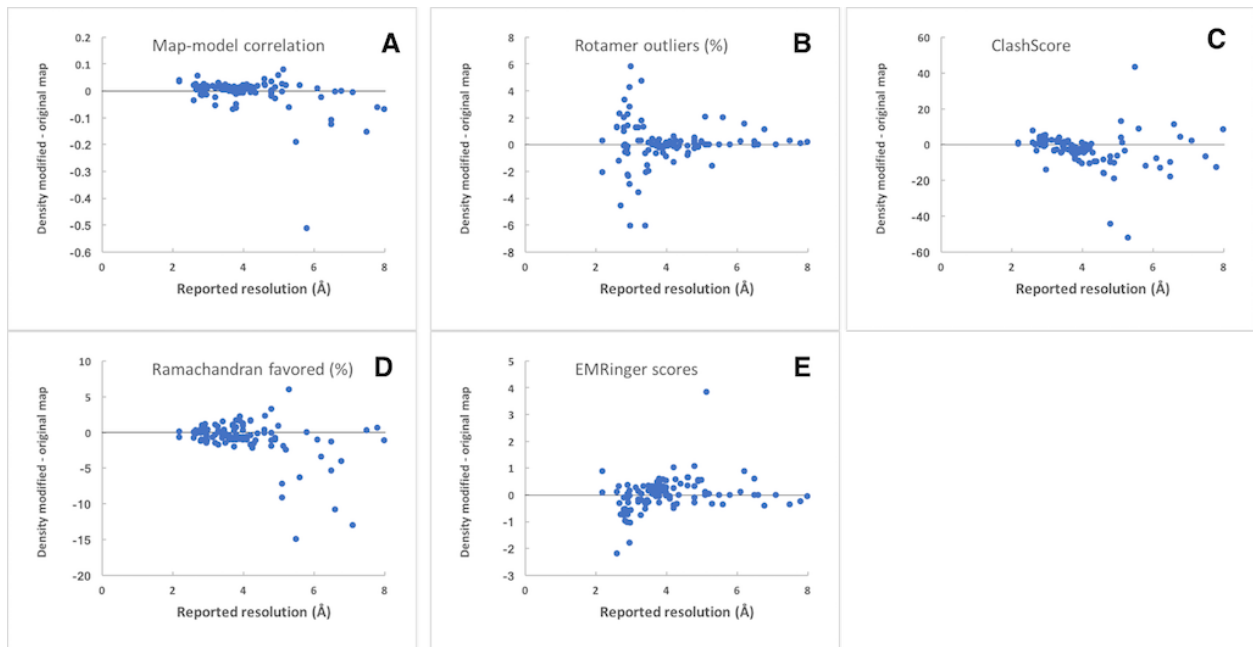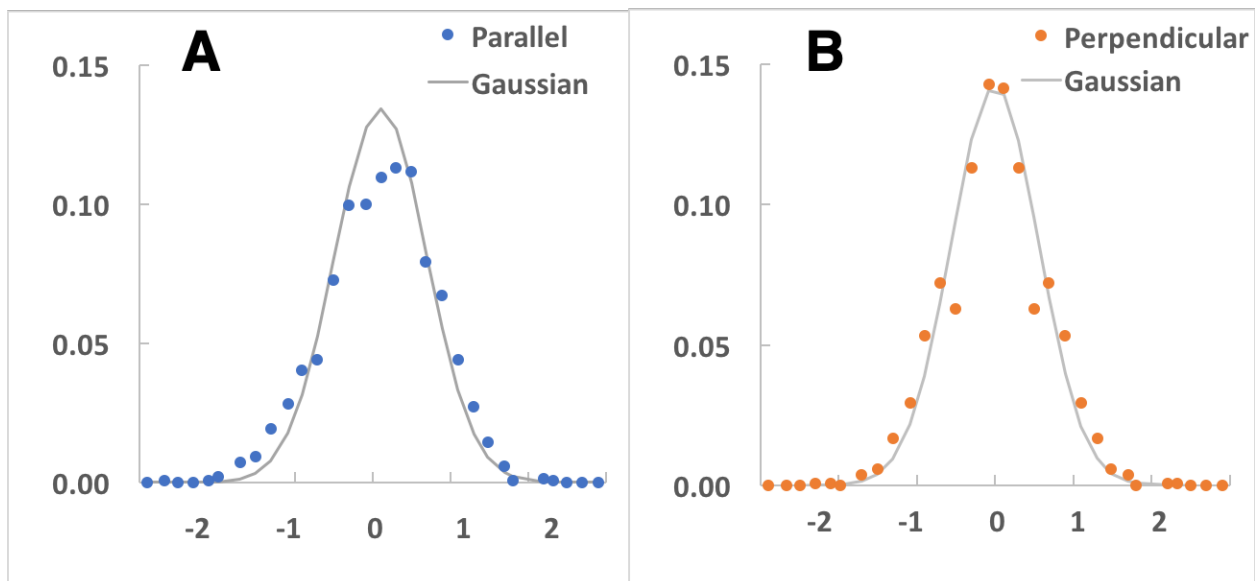
Supplementary Fig. S5. Change in model/map metrics after density modification. Analyses are plotted as a function of resolution for the 104 datasets shown in Fig. 2. A. Map-model correlation, B. Rotamer outliers, C. ClashScore, D. Ramachandran percentage in favored region, E, EMRinger scores.
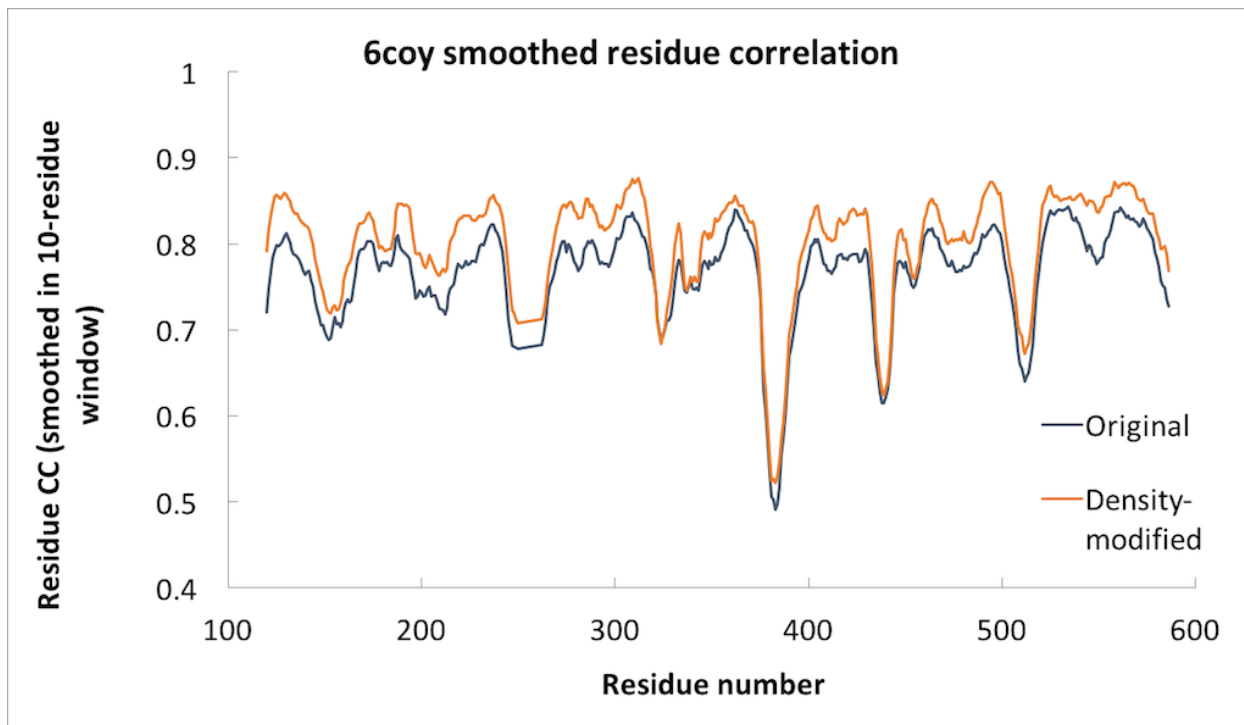
Supplementary Fig. S6. Map-model residue correlation smoothed in 10-residue windows for EMD-7544 (PDB entry 6coy).

Supplementary Fig. S7. Effect of applying 5 cycles of density modification vs 1. A. Average map-model FSC after 5 cycles of density modification (compare with Fig. 2B). B. Change in average map-model FSC between one cycle of density modification and 5 cycles.

Supplementary Figure S8. Flow chart of density modification process (see text). Operations in real-space are in blue and those in reciprocal-space are in green.

Supplementary Figure S9. Analysis of distribution of errors in Fourier coefficients for apoferritin 3.1 Å map. A. Estimated errors in Fourier coefficients parallel to coefficients for 3.1 Å map. B. Errors perpendicular to coefficients for 3.1 Å map. Solid lines in each case correspond to a Gaussian fitted to the values shown (see text).