Assessment of density maps by analyzing their dissimilarities and the dissimilarities among Gaussian-based approximations of the maps

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This assessment is based on the use of unfiltered maps. One of the maps was used as the reference map to align (rigid-body alignment) all other maps and the maps were re-sampled on the grid of the reference map (the alignment and re-sampling of the maps was done in Chimera). The re-sampled maps have the size (in voxels) and the voxel size of the reference map. Pearson correlation coefficient (CC) was then computed (in Spider) among the maps and among their approximations with 3D Gaussian functions. The maps were approximated with Gaussian functions (in Xmipp), using the same standard deviation of Gaussian functions and the same desired approximation error for each map of a target. Gaussian functions were computed inside a mask that was the same for all density maps in a target data set. This mask was created (in Xmipp) based on one of the density maps, using a threshold and morphological operators. The dissimilarities (distances) among maps and their Gaussian-based approximations (1-CC) were projected onto a low-dimensional (here, 3D) space (in Matlab, using nonmetric multidimensional scaling of the n-by-n dissimilarity matrix, where n is the number of density maps). The maps and their Gaussian-based approximations were visualized in this 3D space of distances, which helps understand how different actually these maps are. Figures showing this low-dimensional space of distances among the maps and among their Gaussian-based approximations, for each target set of maps, are provided below (after References).

This assessment method is inspired by the method proposed in [1] from which it differs because it is based on rigid-body instead of flexible alignment of density maps. Additionally, here, we assess not only the density maps but also their Gaussian-based approximations [2]. The Gaussian-based approximations can be seen as denoised [3] or, generally, as simplified (approximate) versions of the given density maps.

Computation of Gaussian-based approximations of density maps:

BetaGal: Density maps were aligned with respect to emcd106 and resampled on its grid to the size $196^3$ voxels (voxel size = 1.275 Å). Also, the mask was created based on emcd106 (threshold = 0.0161). Standard deviation of Gaussian functions was 0.6 voxels. Desired approximation error was 10%.

BMV: Density maps were aligned with respect to emcd102 and resampled on its grid to the size $210^3$ voxels (voxel size = 0.99 Å). Also, the mask was created based on emcd102 (threshold = 0.00682). Standard deviation of Gaussian functions was 1.5 voxels. Desired approximation error was 10%.

Ferritin: Density maps were aligned with respect to emcd122 and resampled on its grid to the size $132^3$ voxels (voxel size = 1.346 Å). Also, the mask was created based on emcd122 (threshold = 0.0313). Standard deviation of Gaussian functions was 1.5 voxels. Desired approximation error was 10%.

GroEL: Density maps were aligned with respect to emcd104 and resampled on its grid to the size $200^3$ voxels (voxel size = 1.42 Å). Also, the mask was created based on emcd104 (threshold = 0.0132). Standard deviation of Gaussian functions was 1.5 voxels. Desired approximation error was 10%.

Proteasome: Density maps were aligned with respect to emcd107 and resampled on its grid to the size $240^3$ voxels (voxel size = 1.315 Å). Also, the mask was created based on emcd107 (threshold = 0.00675). Standard deviation of Gaussian functions was 0.6 voxels. Desired approximation error was 10%.
Ribosome: Density maps were aligned with respect to emcd114 and resampled on its grid to the size 190$^3$ voxels (voxel size = 2.68 Å). Also, the mask was created based on emcd114 (threshold = 0.0684). Standard deviation of Gaussian functions was 1.2 voxels. Desired approximation error was 10%.

TRPVI: Density maps were aligned with respect to emcd101 and resampled on its grid to the size 256$^3$ voxels (voxel size = 1.2 Å). Also, the mask was created based on emcd101 (threshold = 0.00959). Standard deviation of Gaussian functions was 1 voxels. Desired approximation error was 10%.

References


GroEL density maps

GroEL Gaussian-based density maps