DeepQs: Local quality assessment of cryo-EM density map by deep learning map-model fit score

Journal of Structural Biology

Q-score

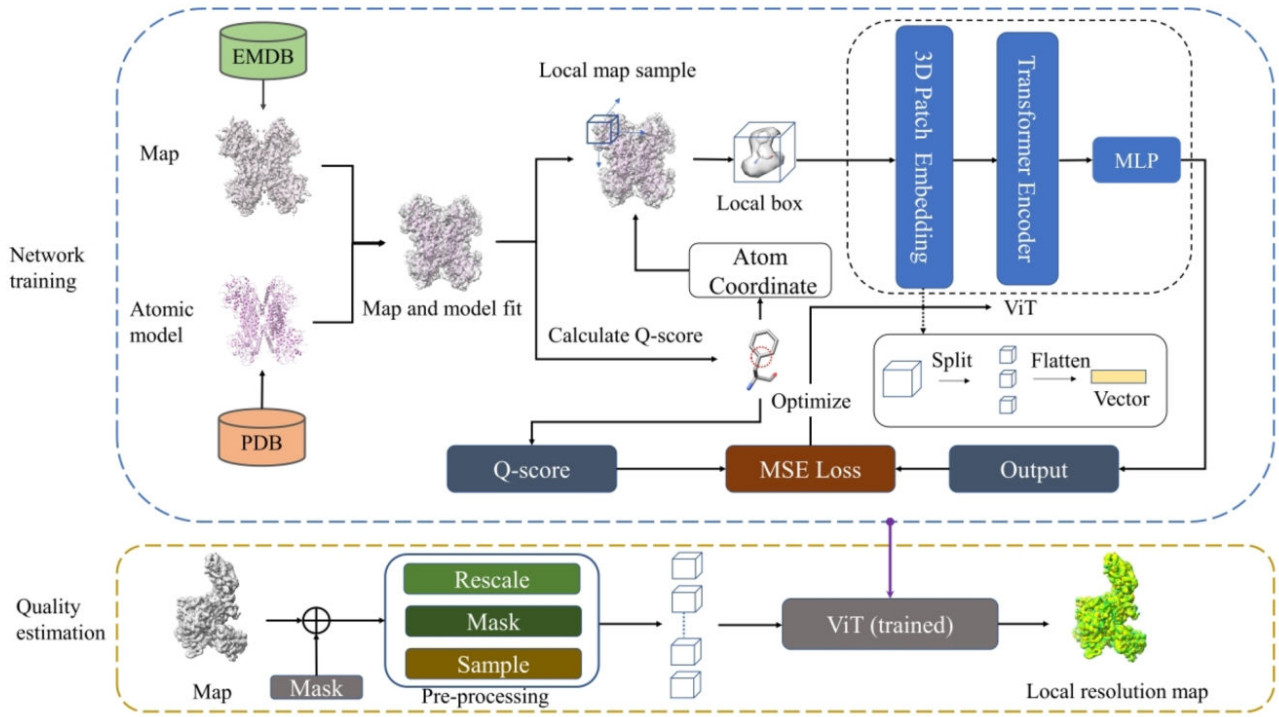
- 刻画一个原子在密度图上的可分辨程度的量。
- v表示某原子周围若干点上的理论电子密度值。$\mu = 0, \sigma = 0.6A.$

$$
\begin{aligned}
y &= Ae^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} + B \\
A &= avg_M + 10\sigma_M \\
B &= avg_M - \sigma_M
\end{aligned}
$$

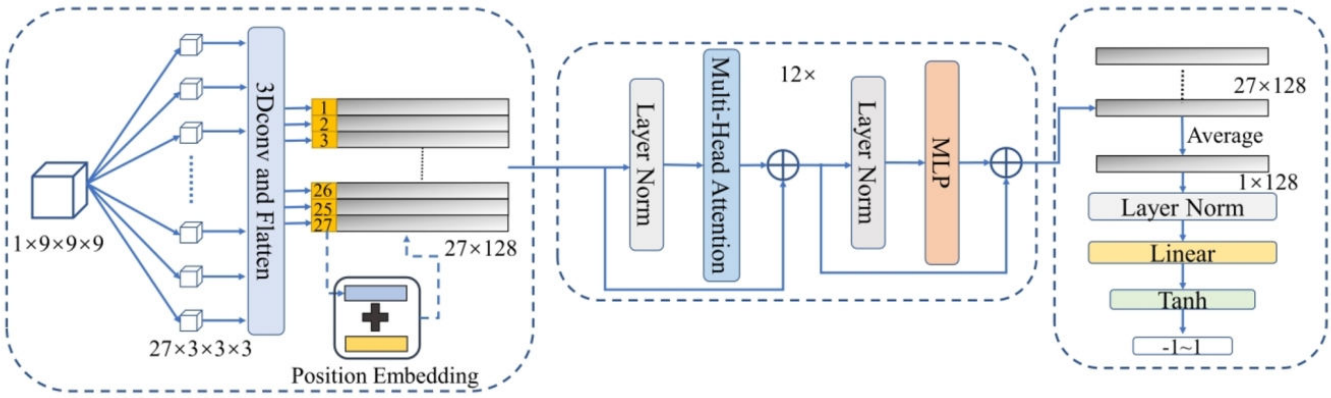
- u表示对应点上的观测密度值（密度图上对应点处的值）。
- 两个向量的互相关系数就是Q-score

$$
\begin{aligned}
\bar{u} &= (u_1 - u_{\text{mean}}, u_2 - u_{\text{mean}}, \cdots, u_n - u_{\text{mean}}) = (\bar{u}_1, \bar{u}_2, \cdots, \bar{u}_n) \\
\bar{v} &= (v_1 - v_{\text{mean}}, v_2 - v_{\text{mean}}, \cdots, v_n - u_{\text{mean}}) = (\bar{v}_1, \bar{v}_2, \cdots, \bar{v}_n) \\
Q - \text{score} &= \frac{\bar{u} \cdot \bar{v}}{|\bar{u}| * |\bar{v}|} = \frac{\sum_{i=1}^{n} \bar{u}_i^* \bar{v}_i}{\sqrt{\sum_{i=1}^{n} \bar{u}_i^2} * \sqrt{\sum_{i=1}^{n} \bar{v}_i^2}}
\end{aligned}
$$

Workflow



Network



- $\tanh(x) = (e^{x} - e^{-x}) / (e^{x} + e^{-x})$

Result

- 在高于6A的密度图中，网络返回的Q-score中位数和分辨率之间有明显相关性(p=0.9).

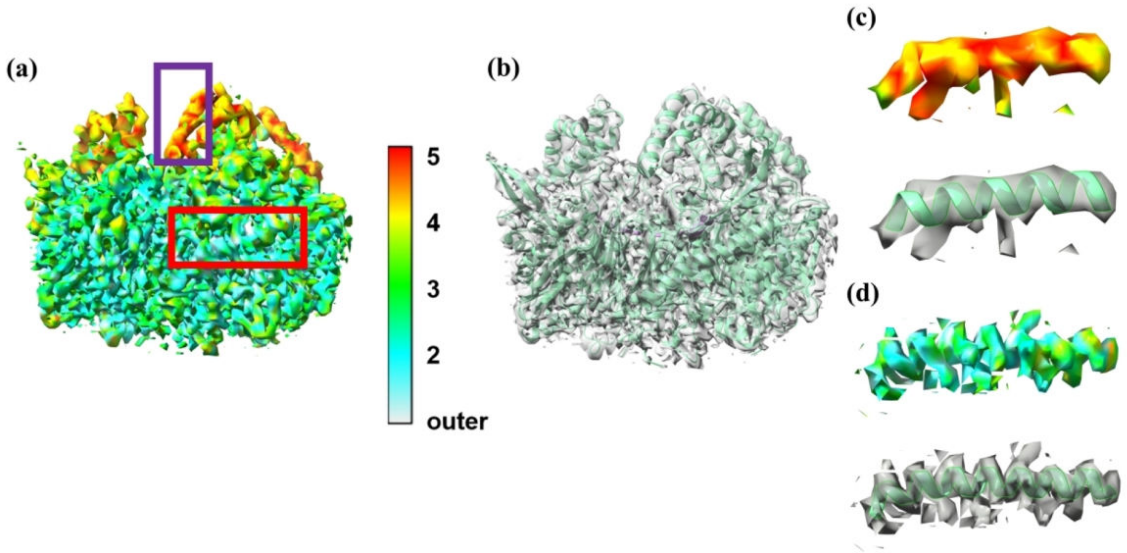
$$R = -3.816^{*} D_o + 5.679$$

Table 1
Summary of quality estimation for the experimental cases for comparing the FSC and local resolution median value.

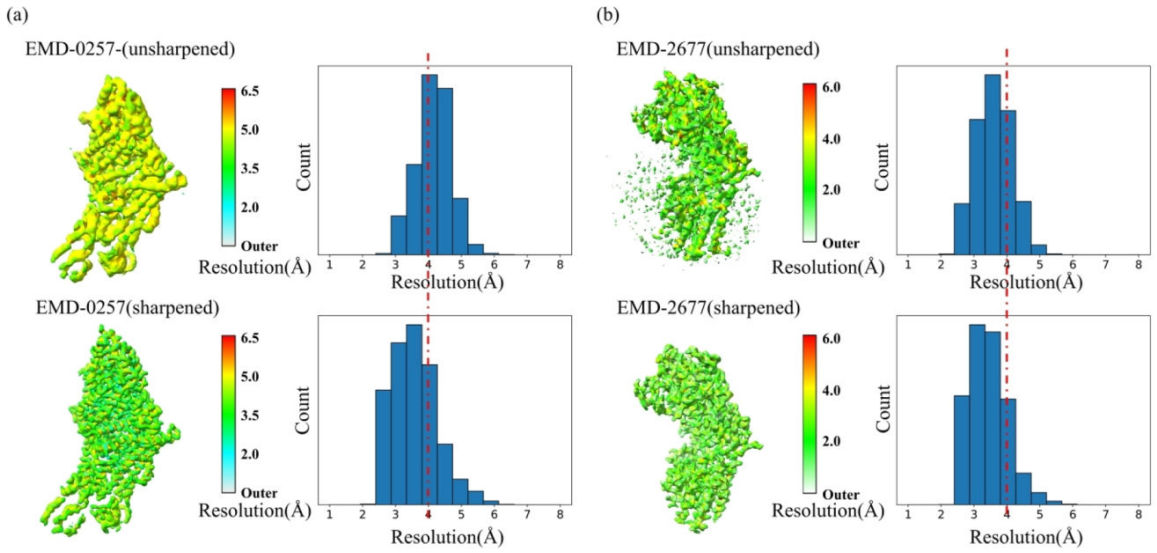
EMDB code	FSC (Å) [a]	ResMap median (Å)	MonoRes median(Å)	DeepRes median (Å)	DeepQs median (Corresponding resolution) [b] (Ours)
23282	3.07	3.50	3.51	3.45	0.694(3.03 Å)
12581	3.5	2.80	3.99	2.80	0.625(3.29 Å)
24304	4.5	5.01	5.76	5.18	0.288(4.58 Å)

[a] 0.143 is used as the threshold.
[b] Corresponding resolution is derived from equation (8).

- DeepQs能反应出局部的分辨率信息。



- DeepQs可以用来检测锐化算法的效果。



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