These **remarks** are to answer how close does Qnet come to RMSF.

Qnet is the linear combination of all weighted square cPCA modes from HPCA.
Vnet is the linear combination of all weighted square cPCA modes from JED

From JED we typically plot normalized squared eigenvectors given as (normalized V^2).
we typically plot weighted squared eigenvectors as Lamda * (normalized V^2).

Lambda = eignevalue of the corresponding eigenvector.

When Qnet is compared to RMSF we notice that at N- and C- termini: Qnet >> RMSF.

Why?

Answer, because RMSF => **root** mean squared fluctuation.
To get agreement, we must take **sqrt**(Qnet).

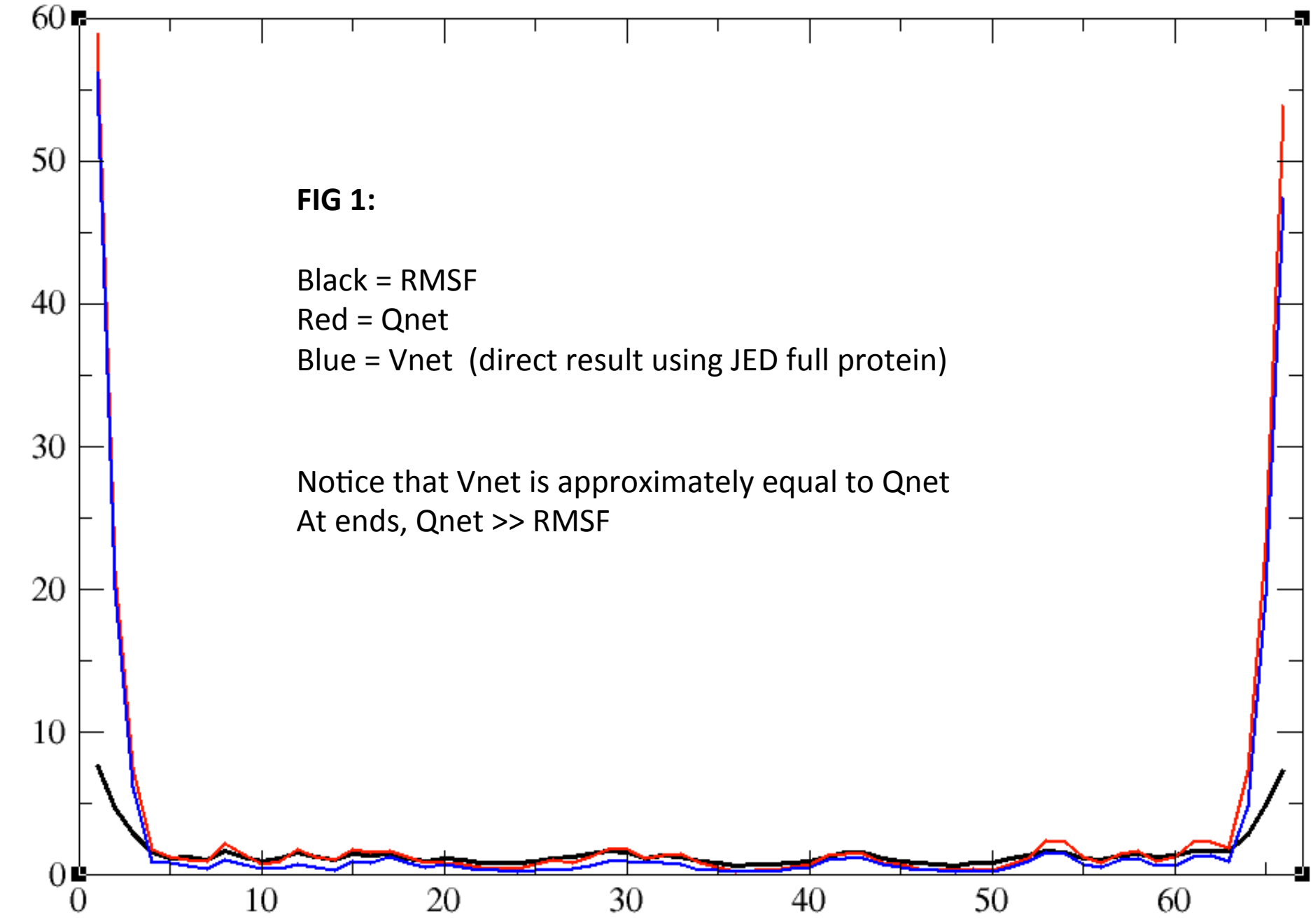

FIG 1:

Black = RMSF
Red = Qnet
Blue = Vnet (direct result using JED full protein)

Notice that Vnet is approximately equal to Qnet
At ends, Qnet >> RMSF

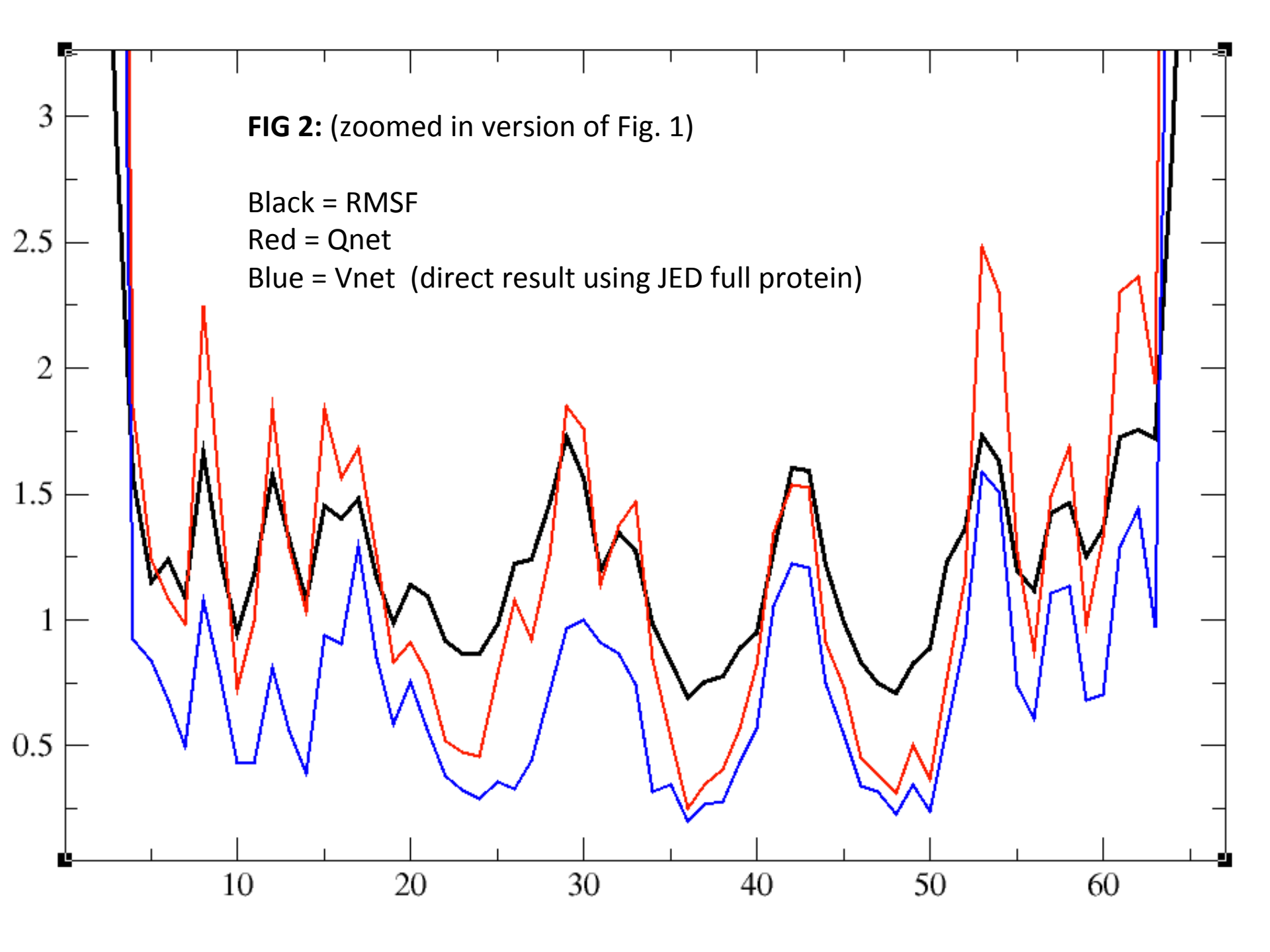
FIG 2: (zoomed in version of Fig. 1)
Black = RMSF
Red = Qnet
Blue = Vnet (direct result using JED full protein)
3
2.5
2
1.5
1
0.5
10
20
30
40
50
60

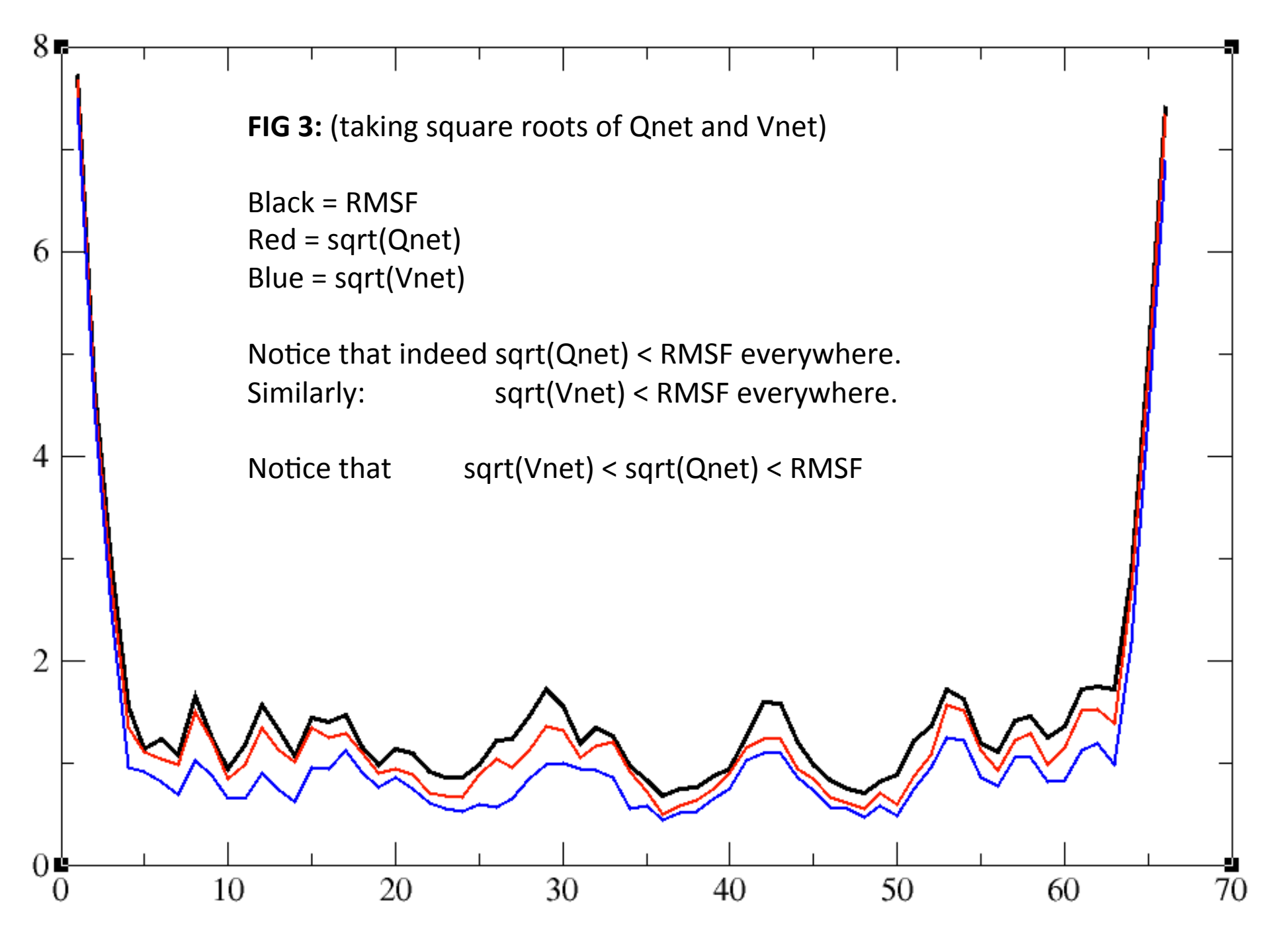

FIG 3: (taking square roots of Qnet and Vnet)

Black = RMSF
Red = sqrt(Qnet)
Blue = sqrt(Vnet)

Notice that indeed sqrt(Qnet) < RMSF everywhere.
Similarly: sqrt(Vnet) < RMSF everywhere.

Notice that sqrt(Vnet) < sqrt(Qnet) < RMSF

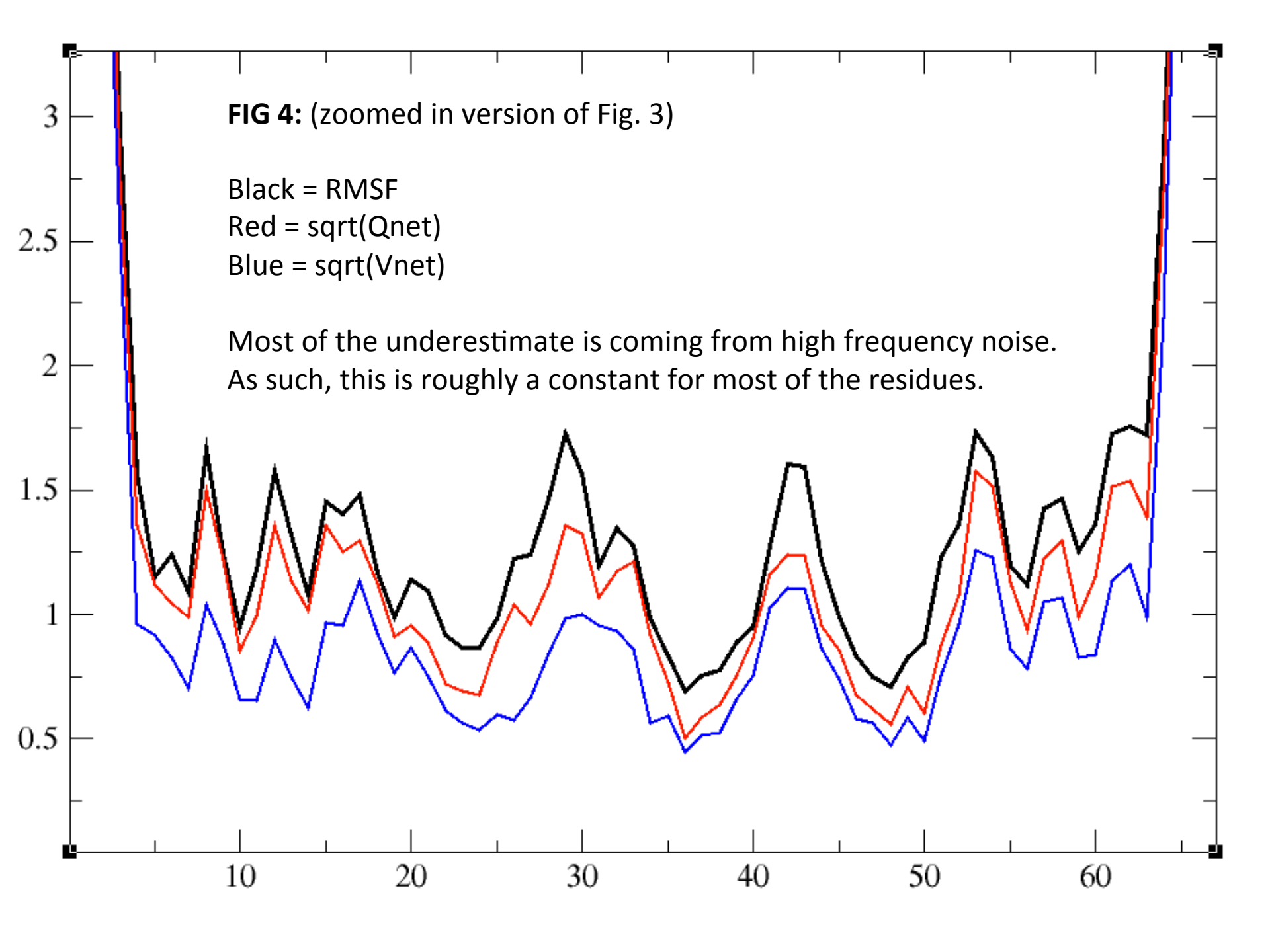
FIG 4: (zoomed in version of Fig. 3)
Black = RMSF
Red = sqrt(Qnet)
Blue = sqrt(Vnet)
Most of the underestimate is coming from high frequency noise.
As such, this is roughly a constant for most of the residues.
3
2.5
2
1.5
1
0.5
10
20
30
40
50
60

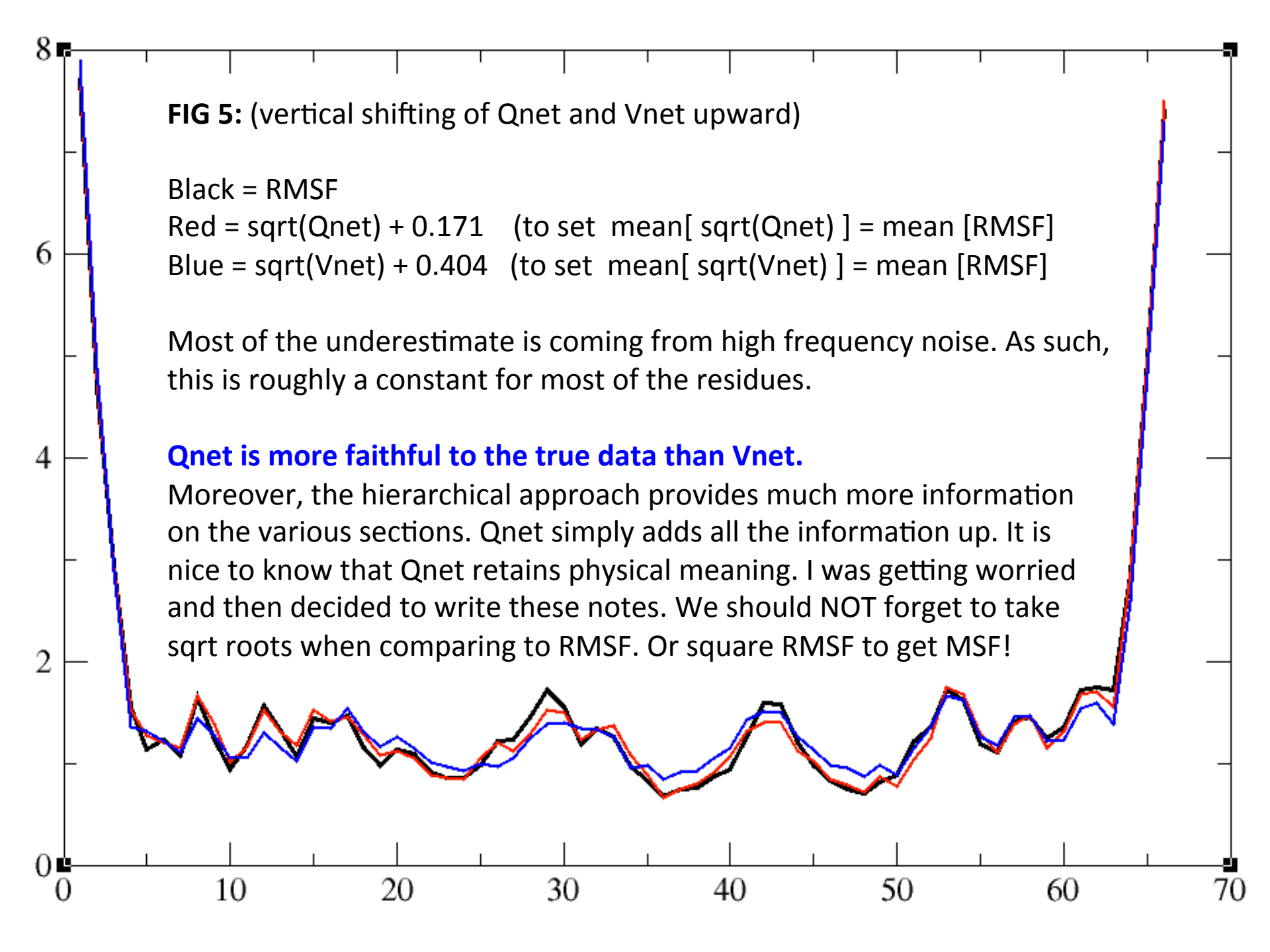

FIG 5: (vertical shifting of Qnet and Vnet upward)

Black = RMSF
Red = sqrt(Qnet) + 0.171 (to set mean[sqrt(Qnet)] = mean [RMSF]
Blue = sqrt(Vnet) + 0.404 (to set mean[sqrt(Vnet)] = mean [RMSF]

Most of the underestimate is coming from high frequency noise. As such, this is roughly a constant for most of the residues.

Qnet is more faithful to the true data than Vnet.
Moreover, the hierarchical approach provides much more information on the various sections. Qnet simply adds all the information up. It is nice to know that Qnet retains physical meaning. I was getting worried and then decided to write these notes. We should NOT forget to take sqrt roots when comparing to RMSF. Or square RMSF to get MSF!