Supplemental Information

Geometrical Description of Protein Structural Motifs

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Content:

Figure S1. Illustration of the geometrical approach developed here. A selected residue i is considered here. For n=3, a triangle (blue) connecting residue i+1 and i-1 with the Cu ion is drawn. The angle with the Cu ion is termed β (labeled $\beta_{n=3}$). For the case of n=5, a triangle (red) connecting residue i+2 and i-2 with the Cu ion is drawn. The angle with the Cu ion is here termed $\beta_{n=5}$. Δβ for residue i for the case of n=5 corresponds to the value of $\beta_{n=5}$ - $\beta_{n=3}$.

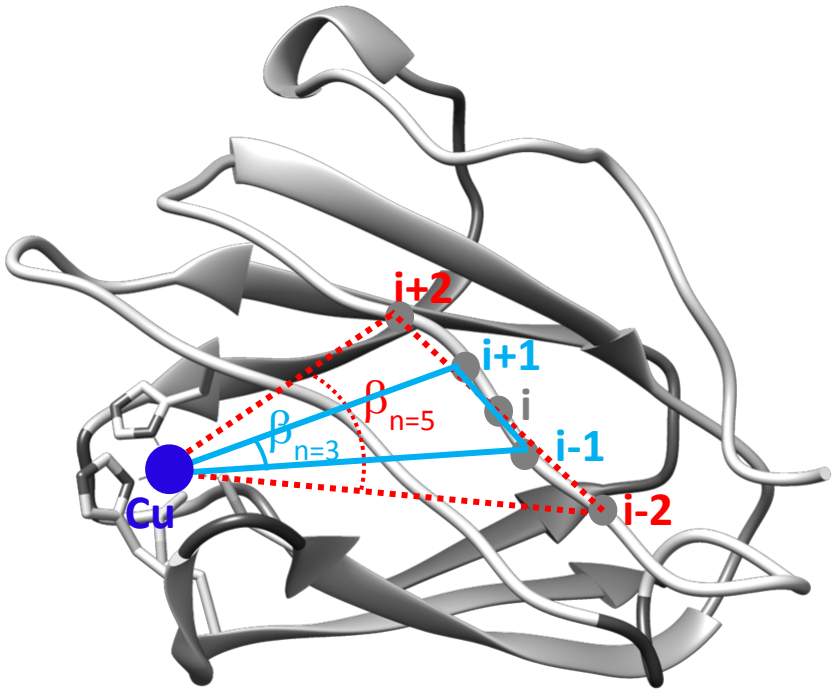


Figure S2. Plot of β for amicyanin (1AAC, chain A) for all residues, and for each extension (for n=3 to 15). Color conventions same as Fig. 1.

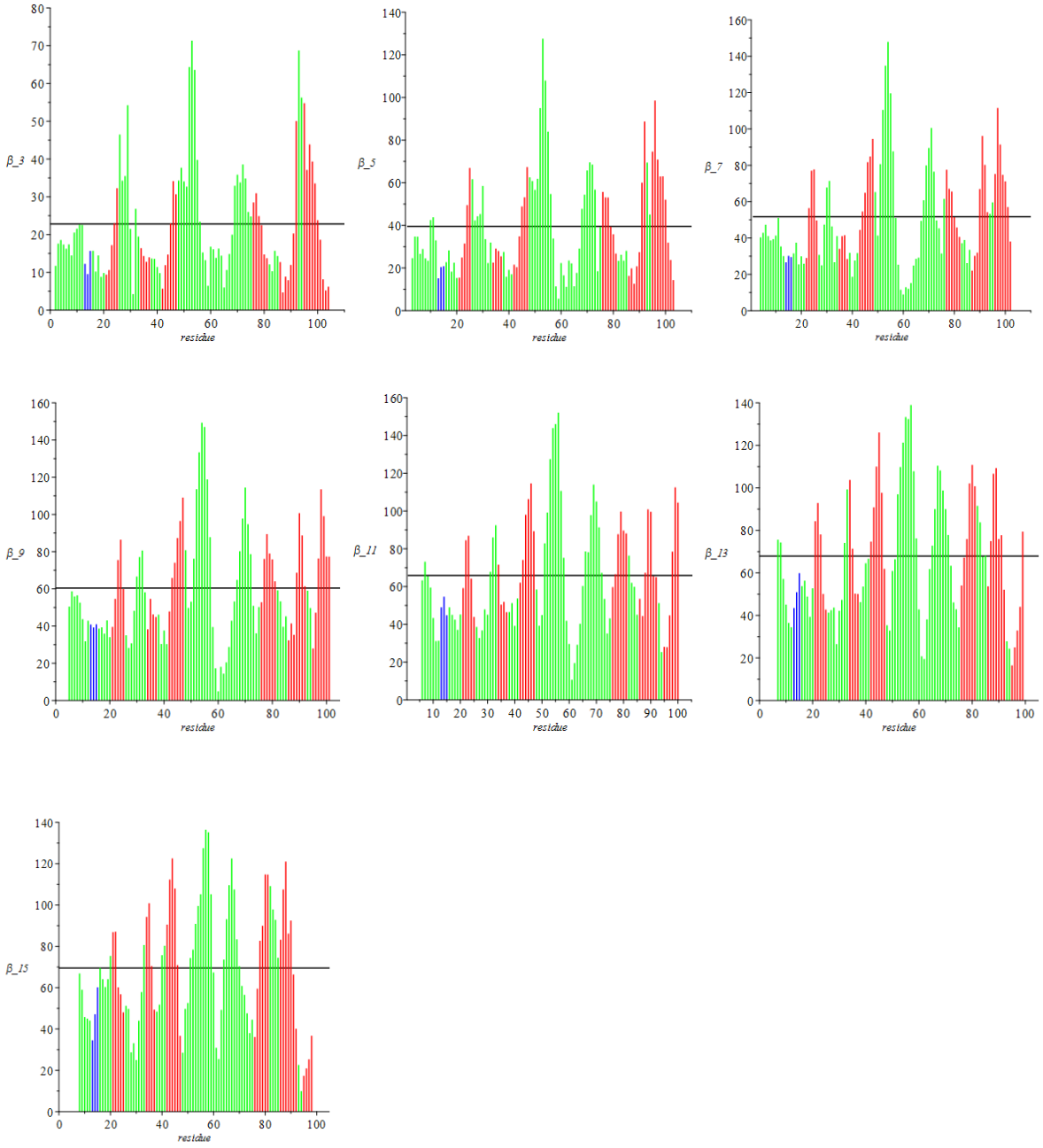


Figure S3. Δβ for amicyanin for extensions n=5, 7, 9, 11, 13 and 15. Color code as in Fig. 1.

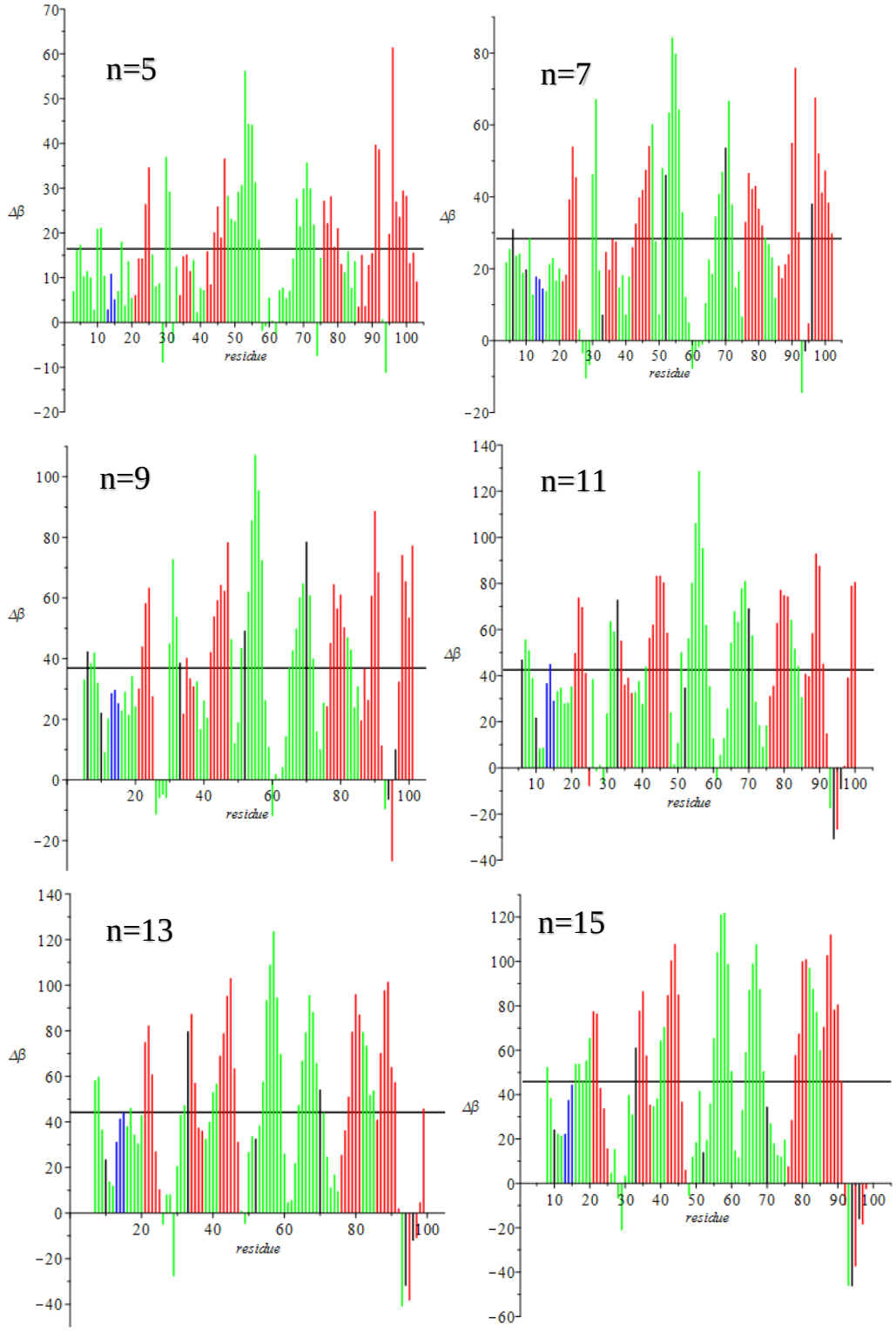


Figure S4. Δβ for the blue copper protein azurin (1JZF, chain A). Displayed are the profiles for n=5, n=7, n=9, n=11, n=13 and n=15. Color conventions as in Fig. 1, except for one place of adjacent α-helical regions; here the first helix is in blue and the second in cyan. In addition, the cysteine residues participating in the disulfide bond are yellow.

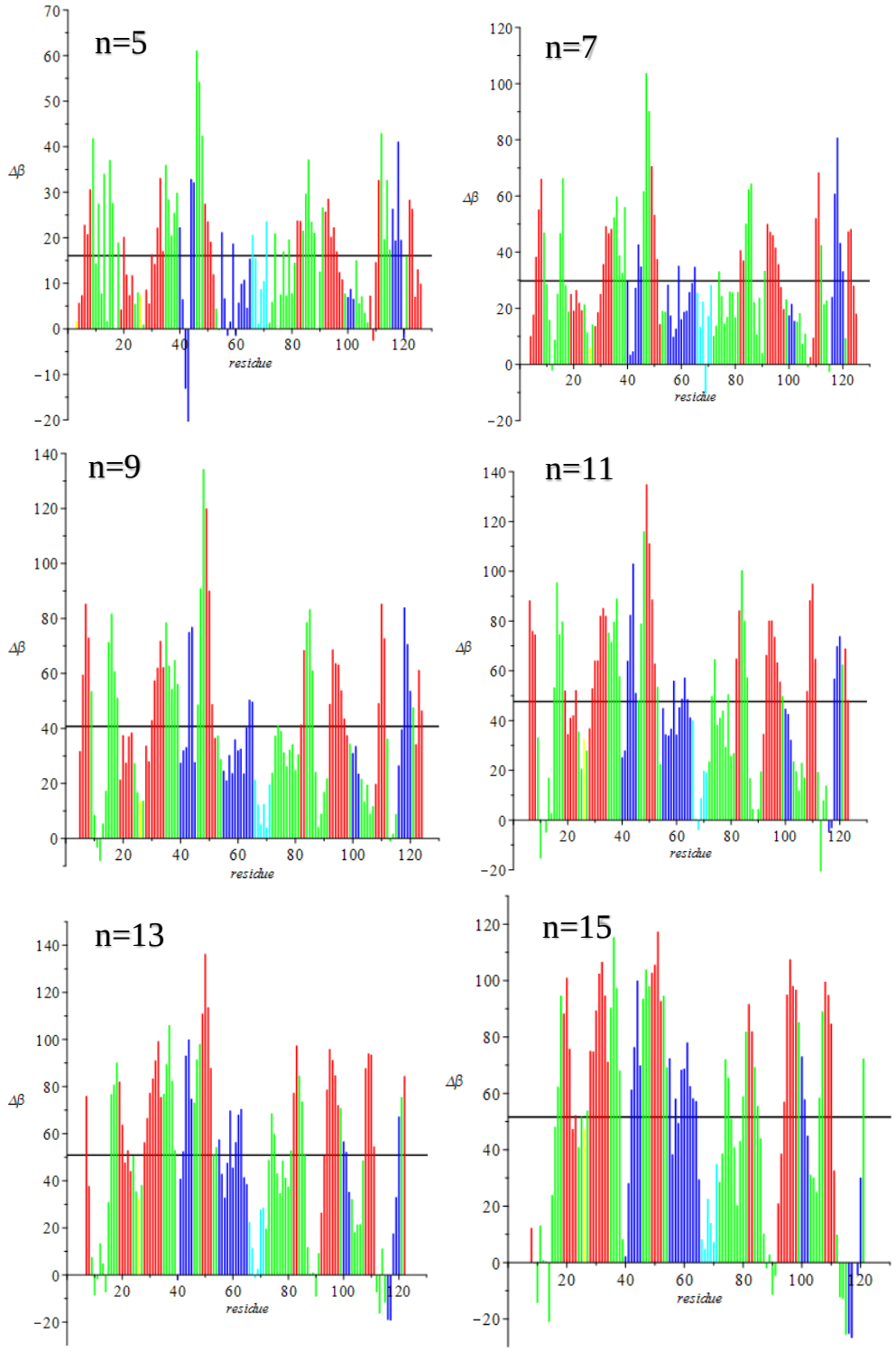


Figure S5. Overlay of amicyanin (1AAC, grey) and azurin (1JZF, gold) with turn regions highlighted in color as described in Fig. 4. In purple are the three turns in each protein with zero or negative Δβ (residues 27-28, 59-61 and 93-94 in amicyanin; residues 10-13, 89-90 and 114-116 in azurin). The copper is shown in blue along with side chains of coordinating residues.

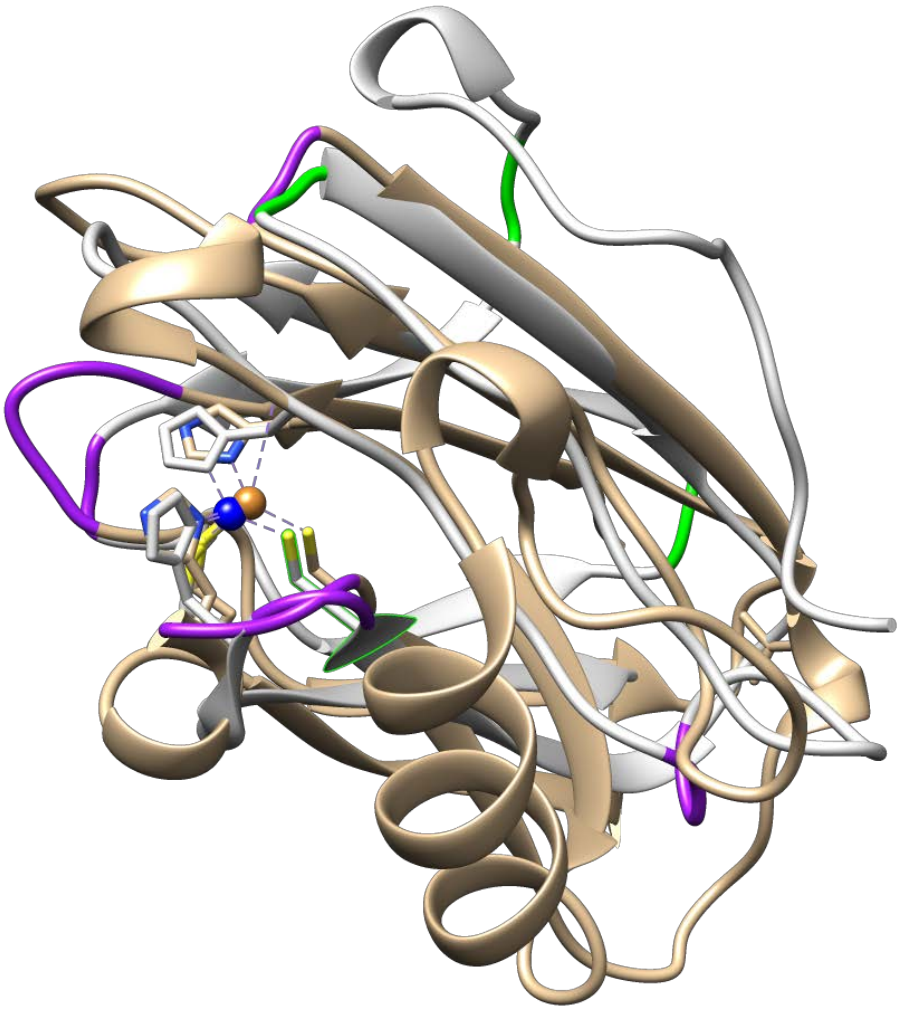
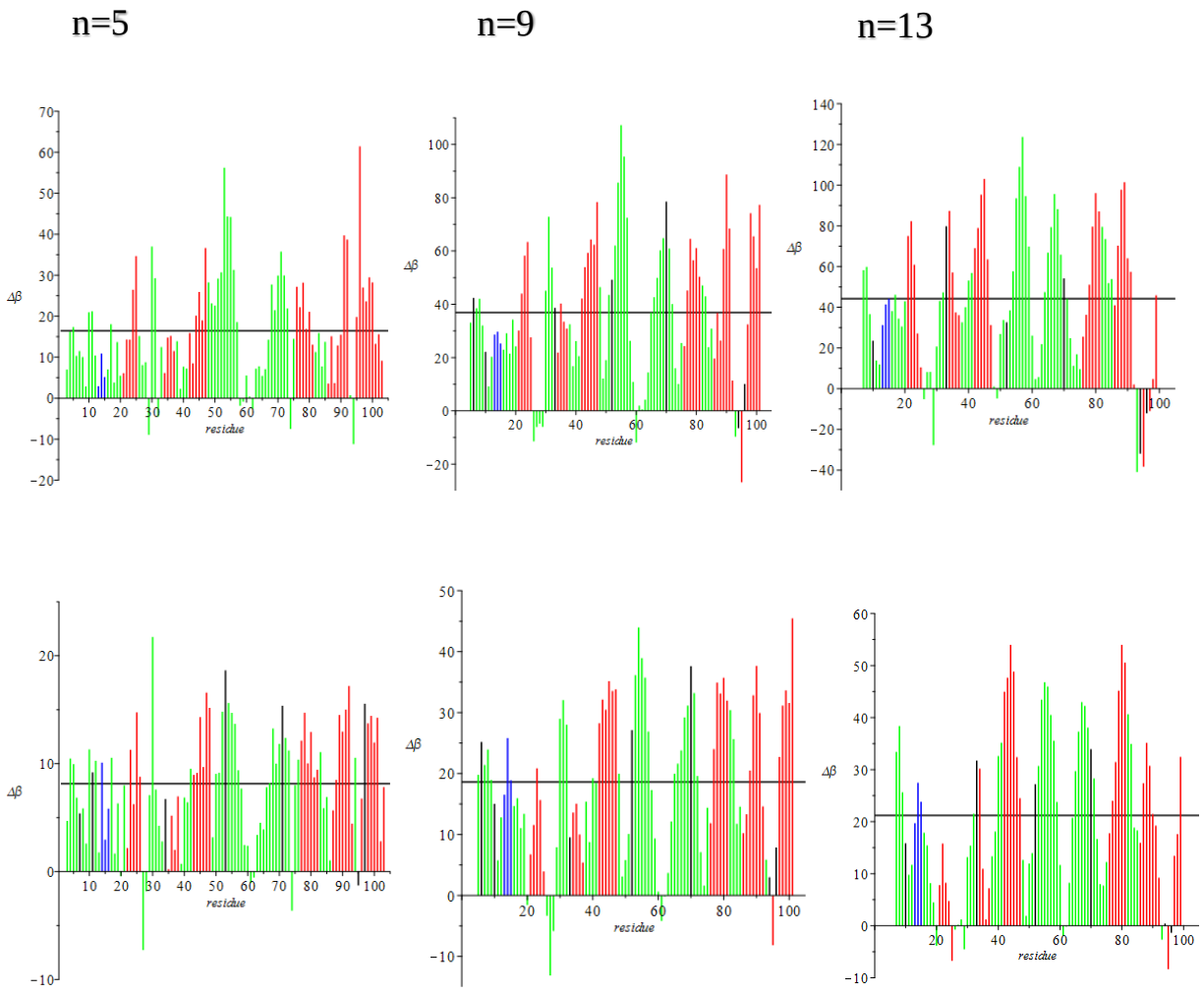


Figure S6. Δβ for amicyanin for extensions n=5, 9 and 13 (we also calculated n=7, 11 and 15; data not shown). For each n there are two companion plots. The top plot gives the results using Cu as the center of the coordinate system, and the bottom plot gives the results when the crystallographic origin is taken as the reference point of the coordinate system. Color code is the same as Fig. 1.



Appendix. Demonstration of the internal consistency of our approach.

Consider a sequence of five residues to be fully extended in a linear array. For the residue i=3,

T03:= R01to03 + R03to05 = 12.498 Å.

We use the crystallographic data to calculate new angles consistent with the above value of T03. The new angles are

arccos [β(01 to 05)] = (R01^2 + R05^2 – T03^2)*(2*R01*R05)^(-1)

β(01 to 05) = RAD * arccos [β(01 to 05)] = 30.403°

arccos [α(01 to 05)] = (R05^2 + T03^2 - R01^2)*(2*R05*T03)^(-1)

α(01 to 05)] = RAD * arccos [α(01 to 05)] = 96.497°

arccos [γ(01to05)] = (R01^2 + T03^2 - R05^2)*(2*R01*T03)^(-1)

γ(01to05) = RAD * arccos [γ(01to05)] = 53.100°

The sum of the angles is 180°

An independent calculation of these angles can be made. Whereas the above results were obtained by using the calculated distances R03, R02to04, R01to05 and the linear distance, T03 = R01to03 + R03to05, we calculate from the crystallographic data the angle for *each* triplet in the native state.

For a maximally-extended sequence of five residues, the following linear sum of two triplets is constructed using the native-state data:

B(01 to 05) = β(01 to 03) + β(03 to 05) = 30.281°.

The angles β(01 to 05) (30.4°) and B(01 to 05) (30.3°) are in nearly exact agreement. This correspondence reflects the relative unimportance of "end effects."