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Supporting Material

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Lars V. Bock[†], Brian Hutchings[‡], Helmut Grubmüller[†,*] and Dixon J. Woodbury[‡,*]

[†]Department of Theoretical and Computational Biophysics, Max-Planck-Institute for Biophysical Chemistry,Göttingen, Germany

[‡]Department of Physiology & Development Biology, Brigham Young University, Provo, Utah

Supporting Material

Name	Disulfide bond(s)	Length decrease [nm]	Shortening [#bonds]
1-2	C85-C88	0.38	4
1-3	C85-C90	1.16	10
1-4	C85-C92	1.98	16
2-3	C88-C90	0.092	1
2-4	C88-C92	0.76	7
3-4	C90-C92	0.109	1
1-2, 3-4	C85-C88 & C90-C92	0.50	5
1-3, 2-4	C85-C90 & C88-C92	1.22	10*
1-4, 2-3	C85-C92 & C88-C90	1.99	16

Table 1: Length decrease for the nine disulfide linkages with respect to the reduced state. Length decrease was estimated from the offset of the fitted semi-harmonic function for each data set. For each disulfide bond formed, the net number of bonds removed from the total segment is shown. As expected, there is a fairly linear relationship between the end-to-end distance and the number of bonds in the fully extended test segment. On average, the atom-atom distance is 0.128 nm or 0.38 nm per amino acid, which gives a simple way to estimate the maximum length of a peptide. *The shorting is not clear for this system because the 2-4 disulfide interacts with the loop of the 1-3 disulfide.

*Correspondence: hrgubmu@gwdg.de, dixon_woodbury@byu.edu

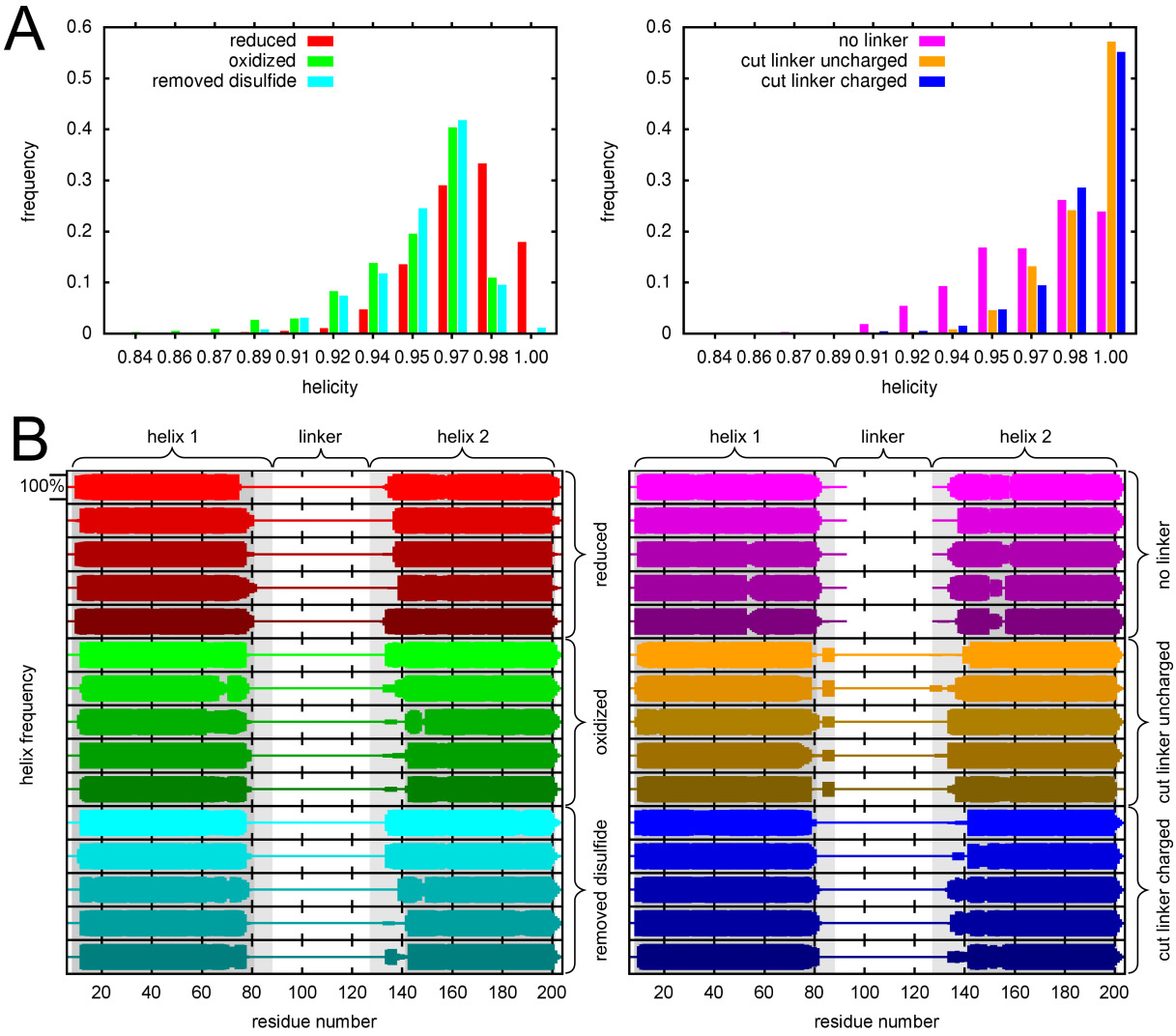

Figure 1: Helicity of SNAP-25B. Remaining helix content of the SNAP-25B helix regions; from the residues which are helical in the crystal structure (except for the first and the last two residues), the fraction of residues which are in an α-helical secondary structure was calculated for each frame of the final 40 ns of the respective set of simulations. Shown is the histogram of these fractions for the six different setups, considered (A). The frequency of each SNAP-25B residue of being in an α-helical structure calculated from the final 40 ns of each trajectory (B).