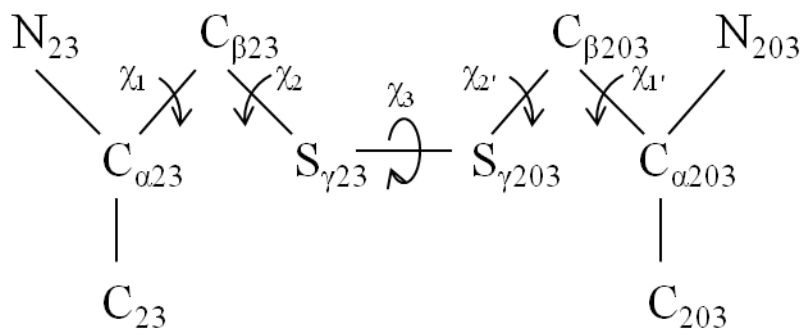
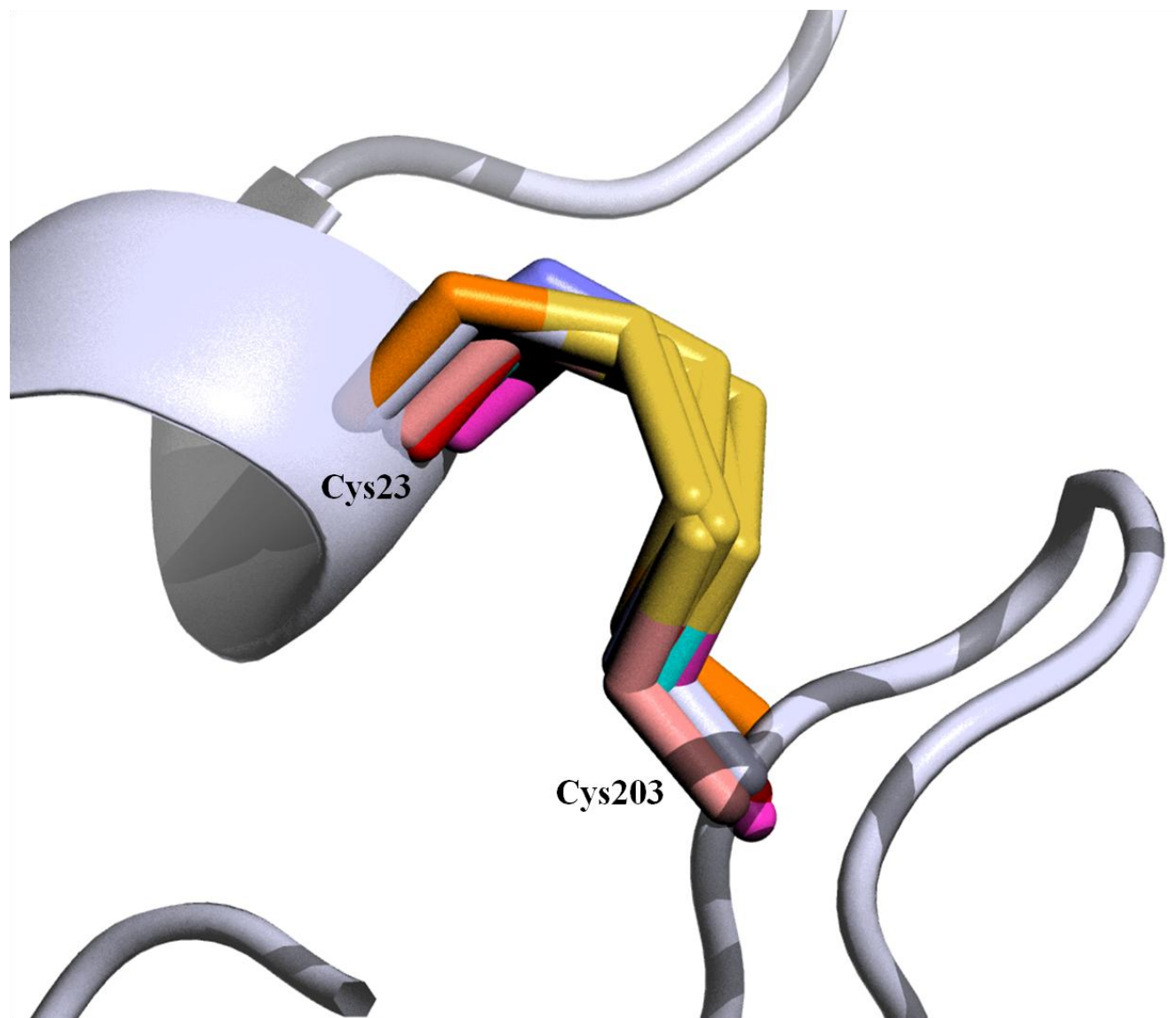


Supplementary Material

Supplementary Figure S1. Schematic of the five χ angles of the disulfide bond.



Supplementary Figure S2. Overlay of the disulfide linkage of dsHCAII with other CAs where this linkage is conserved. The C_α backbone for dsHCAII is represented by a blue-white cartoon and the disulfide linkage is shown in stick view. The carbons of the disulfide bond are color-coded according to CA isoforms as: HCAIV – orange; HCAVI – dark blue; HCAIX – red; HCAXII – cyan; mCAXIV – magenta; *N. gonorrhoeae* – pink). The various isoforms were aligned to the dsHCAII structure in Coot (Emsley & Cowtan, 2004). The residues for the disulfide linkage are numbered according to their positions in dsHCAII.



Supplementary Table S1. Geometric comparison and strain energy of the conserved disulfide linkage between residues 23 and 203 in various CAs.

	dsHCAII	HCAIV ^a	HCAVI ^b	HCAIX ^c	HCAXII ^d	mCAXIV ^e	NGCA ^f
χ_1 (°)	162.25	-55.86	-53.73	-175.16	172.73	-71.99	-63.26
χ_2 (°)	-54.34	-56.34	119.82	111.37	-60.43	-54.06	-63.42
χ_3 (°)	79.80	78.68	82.77	87.00	87.07	86.64	94.47
χ_2' (°)	139.05	105.53	-61.88	-60.08	113.75	117.29	109.79
χ_1' (°)	172.40	-45.06	-59.87	167.88	179.92	-64.09	-53.30
S-S Bond (Å)	2.1	2.3	2.1	2.1	2.0	2.0	2.0
C _α Distance (Å)	5.2	4.9	5.0	4.9	4.9	4.8	5.1
DSE (kJ mol ⁻¹) ^g	21.5	41.9	16.5	33.9	36.5	20.8	47.4
Classification ^h	(+) RHHook	(-) RHHook	(-) RHHook	(+/-) RHHook	(+) RHHook	(-) RHHook	(-) RHHook

^a (Stams et al., 1998).

^b (Pilka et al., 2008).

^c (Alterio et al., 2009).

^d (Whittington et al., 2001).

^e (Whittington et al., 2004).

^f (Huang et al., 1998).

^g DSE calculated according to Eq. 10 in main text and torsion angles described in Fig. S1.

^h Classification of the disulfide linkage at residues 23 and 203 (HCAII numbering). Symbols in parenthesis represent the magnitude of gauche values for χ_1 and χ_1' . RH: Right-Handed.

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