

$n \rightarrow \pi^*$ Interactions Modulate the Properties of Cysteine Residues and Disulfide Bonds in Proteins

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Table S1. Matrix Elements and Data from Second-Order Perturbation Theory Calculations on $n \rightarrow \pi^*$ Interactions in CXXC Motifs

CXXC Sequence	PDB Entry	$E_{n \rightarrow \pi^*}$	$E_{n \rightarrow \pi^*}$	$E_{n \rightarrow \pi^*}$	r
		$S_i^{\gamma} \rightarrow C_i=O$ (kcal/mol)	$C_i=O \rightarrow C_{i+1}=O$ (kcal/mol)	$C_{i+1}=O \rightarrow C_{i+2}=O$ (kcal/mol)	$S_i^{\gamma} \cdots C_i=O$ (Å)
CGTC	2o85	0.73	0.58	1.07	3.18
CGSC	2o87	0.84	0.45	0.60	3.17
CGPC	2o7k	0.93	0.28	0.95	3.16
CPHC	1a2j	0.41	1.2	0.48	3.15

Table S2. Matrix Elements and Data from Second-Order Perturbation Theory Calculations on $n \rightarrow \pi^*$ Interactions in the CXXC Motif of Thioredoxins

PDB Entry	<i>S</i> ^γ State	$E_{n \rightarrow \pi^*}$	$E_{n \rightarrow \pi^*}$	$E_{n \rightarrow \pi^*}$	r
		$S_i^{\gamma} \rightarrow C_i=O$ (kcal/mol)	$C_i=O \rightarrow C_{i+1}=O$ (kcal/mol)	$C_{i+1}=O \rightarrow C_{i+2}=O$ (kcal/mol)	$S_i^{\gamma} \cdots C_i=O$ (Å)
1xwa	<i>Drosophila melanogaster</i> thioredoxin disulfide	1.58	1.21	0.46	3.13
1xwc	<i>Drosophila melanogaster</i> thioredoxin thiol	0.75	1.98	0.63	3.23
1xwc	<i>Drosophila melanogaster</i> thioredoxin thiolate	2.75	0.10	1.48	3.09
1eru	<i>Homo sapiens</i> thioredoxin disulfide	1.24	0.75	0.12	3.12
1ert	<i>Homo sapiens</i> thioredoxin thiol	1.06	1.66	0.10	3.17
1ert	<i>Homo sapiens</i> thioredoxin thiolate	3.24	0.43	0.23	3.09
1w4v	<i>Homo sapiens</i> thioredoxin 2 disulfide	1.06	0.88	0.41	3.09
1w89	<i>Homo sapiens</i> thioredoxin 2 thiol	0.90	0.13	0.42	3.21
1w89	<i>Homo sapiens</i> thioredoxin 2 thiolate	2.16	0.10	1.24	3.16

Table S3. Data Used to Generate Figure 5D

Dihedral Angle, ξ (°)	$E_{n \rightarrow \sigma^*}$ (kcal/mol)	$E_{n \rightarrow \pi^*}$ (kcal/mol)
161.2	0.5	1.65
151.2	0.74	1.65
141.2	1.01	1.65
131.2	1.01	1.65
121.2	0.71	1.65
111.2	0.45	1.65
101.2	0.16	1.65
91.2	0	1.65
81.2	0	1.65
71.2	0	1.65
61.2	0	1.65

Table S4. Data Used to Generate Figure 5E

Dihedral Angle, ξ (°)	$E_{n \rightarrow \sigma^*}$ (kcal/mol)	$E_{n \rightarrow \pi^*}$ (kcal/mol)
161.2	0.62	0
151.2	0.71	0
141.2	0.62	0
131.2	0.5	0
121.2	0.33	0
111.2	0.17	0
101.2	0	0
91.2	0	0
81.2	0	0
71.2	0	0
61.2	0	0

Table S5. Atomic Coordinates of the Cys36–Cys55 Disulfide Bond in PDB Entry 4gn2 (*Pseudomonas aeruginosa* Class D β -Lactamase)

C	4.208600	3.490800	-0.894800
C	3.362200	2.431400	-0.194300
O	2.829700	2.679800	0.885100
N	3.228900	1.265500	-0.822000
C	2.565500	0.125500	-0.194300
C	3.419100	-1.129500	-0.290500
O	3.943500	-1.442200	-1.356800
C	1.198000	-0.144000	-0.833600
S	0.525500	-1.794300	-0.486100
N	3.566800	-1.825000	0.834800
C	4.008300	-3.217400	0.831900
C	-1.772100	2.971800	1.668100
C	-1.874300	1.915600	0.574000
O	-1.304300	2.073500	-0.507200
N	-2.599100	0.837900	0.865400
C	-2.666500	-0.322200	-0.022100
C	-4.043900	-0.545000	-0.651900
O	-4.236000	-1.499300	-1.413700
C	-2.231300	-1.580800	0.730600
S	-0.503400	-1.543700	1.248700
N	-4.988300	0.338700	-0.332800
C	-6.369300	0.229900	-0.810800
H	4.757000	3.038000	-1.694200
H	3.694900	-3.689100	-0.075900
H	-2.021200	2.533100	2.611700
H	-6.673700	-0.795700	-0.791600
H	2.425500	0.375400	0.836600
H	0.522000	0.547500	-0.375700
H	1.360400	-0.113100	-1.890700
H	-1.996900	-0.116400	-0.830900
H	-2.807900	-1.598300	1.631800
H	-2.310500	-2.384800	0.029100
H	-7.012300	0.804800	-0.177500
H	-6.430400	0.601400	-1.812400
H	-4.744700	1.108200	0.257600
H	-3.115800	0.821100	1.721400
H	-0.772600	3.352200	1.704300
H	-2.450600	3.771500	1.456200
H	3.369500	-1.380700	1.708700
H	3.578000	-3.729700	1.667000
H	5.075300	-3.253400	0.902700
H	3.592600	1.167300	-1.748300
H	4.891600	3.922700	-0.193500
H	3.570500	4.254600	-1.287800

Table S6. Atomic coordinates of CXXC Motif in PDB Entry 1a2j (*Escheria coli* DsbA, Oxidized)

N	-4.45786600	-2.39956100	-0.51846600
C	-3.79262500	-1.39737900	0.29383100
C	-2.57632200	-0.87918500	-0.50355000
O	-1.50425000	-1.47047200	-0.42621200
C	-3.37517600	-1.98290800	1.63385800
S	-2.55758700	-0.69469900	2.64066700
N	-2.73417300	0.19549900	-1.30234600
C	-1.62222600	0.64101900	-2.17332100
C	-0.37769300	1.02066000	-1.38487700
O	0.72720700	0.65400500	-1.73672900
C	-2.23990200	1.80661300	-2.95499400
C	-3.72366900	1.43964200	-3.01919400
C	-3.99977800	0.87526900	-1.62810700
N	-0.56857200	1.78176700	-0.28376200
C	0.57564100	2.18819100	0.51148700
C	1.28566600	0.96006100	1.09265300
O	2.49247300	0.93719400	1.23543700
C	0.12201000	3.09875400	1.65670500
C	-0.66153100	4.26979300	1.16231200
C	-1.91165500	4.67549600	1.54064400
N	-0.16758100	5.10920700	0.19169000
C	-1.09257300	6.01052400	-0.00238100
N	-2.17468700	5.79681400	0.78942800
N	0.48259000	-0.06394800	1.47220200
C	1.06491000	-1.29302800	1.96832500
C	1.99008900	-1.95119600	0.92967600
O	3.02087700	-2.50465500	1.27038700
C	0.00946300	-2.31145700	2.36479100
S	-1.15195700	-1.80542100	3.67605300
N	1.54348300	-1.91264800	-0.33832300
C	2.29297700	-2.50895400	-1.42411800
C	3.58773600	-1.76906400	-1.76982400
O	4.43419000	-2.32824200	-2.44131600
C	1.41467100	-2.60265400	-2.66552900
N	3.69334700	-0.50790300	-1.31035300
C	4.88198300	0.28787900	-1.50899800
C	5.95344500	0.06242800	-0.43391300
O	7.02043300	0.64999100	-0.51036600
C	4.51929800	1.76730500	-1.56091900
N	5.66204900	-0.78820300	0.56525300
C	6.63775000	-1.03154200	1.60473700
H	-1.77243800	1.92616700	-3.92997100
H	-2.10633000	2.73942600	-2.39989100
H	-3.88588300	0.66265400	-3.76892200
H	-4.36482800	2.28613700	-3.25798500

H	-4.84088800	0.18511200	-1.60014400
H	-4.19080900	1.68029600	-0.91065100
H	-1.32128500	-0.17982900	-2.82760100
H	-0.48306900	2.52317800	2.36314800
H	1.01863400	3.43145500	2.18345700
H	-2.60095700	4.29409400	2.27495500
H	-3.00539600	6.36344500	0.83024300
H	-1.03724800	6.83569100	-0.69492600
H	1.30330100	2.70299800	-0.11728200
H	0.53110600	-3.20904600	-2.45935900
H	1.09784700	-1.60326400	-2.97142600
H	2.62005900	-3.50356700	-1.11432400
H	4.02106400	2.05981100	-0.63326700
H	5.42704500	2.35716200	-1.67213800
H	5.34197500	-0.02693100	-2.44751700
H	6.89715200	-0.10528700	2.12067000
H	-3.94085200	-3.23407400	-0.75055300
H	-4.52246000	-0.60207600	0.44671700
H	-4.25289100	-2.36323500	2.15414000
H	-2.66254700	-2.79143400	1.48074100
H	1.70879900	-1.06396000	2.81915800
H	-0.56392800	-2.62669800	1.49230100
H	0.51475300	-3.18827600	2.77470300
H	6.21594500	-1.74014300	2.31356400
H	7.55416300	-1.44157500	1.17785900
H	4.75644900	-1.23053500	0.62114500
H	3.84861200	1.96129300	-2.39854800
H	2.92485900	-0.09664100	-0.79937900
H	0.68189000	-1.42672400	-0.55404700
H	-0.49551200	-0.05137500	1.22148000
H	-1.48478800	2.14200900	-0.05930100
H	1.98382900	-3.05808900	-3.47400800
C	-5.77570800	-2.30456100	-0.87225300
O	-6.44374100	-1.32472300	-0.60938800
C	-6.34531500	-3.50500200	-1.58534500
H	-5.58292500	-4.17658200	-1.97725800
H	-6.96673000	-4.05306500	-0.87480000
H	-6.98944700	-3.15876700	-2.39041600

Table S7. Atomic Coordinates of CXXC Motif in PDB Entry 1ert (*Homo sapiens* Thioredoxin, Thiol)

C	4.15420414	3.36414545	-0.01328355
C	2.81530740	2.68046827	0.17388256
O	1.89983949	2.79642402	-0.61707629
H	3.98645744	4.35160482	-0.43645789
N	2.71460217	1.86692302	1.26636364

C	1.55068052	1.03099474	1.49834495
C	0.55884684	1.73191269	2.41391745
O	0.80515396	1.90750920	3.59754262
C	2.01057600	-0.27990800	2.12876300
S	0.64752900	-1.43659100	2.47084000
H	3.42690634	1.89739659	1.97952612
H	1.09697316	0.83970466	0.52527338
H	2.53895598	-0.08045456	3.06024175
H	2.69512843	-0.77861441	1.44434269
N	-0.59674748	2.11644058	1.84334557
C	-1.57860952	2.88080332	2.58313255
C	-2.01533508	2.28879003	3.92652755
O	-2.04210872	3.02157758	4.90358262
H	-2.45973097	2.99746235	1.94873931
H	-0.66433994	2.07374103	0.83756285
H	-1.19726072	3.87180459	2.83171596
N	-2.35056992	0.98040065	4.00625265
C	-2.75587773	0.42092591	5.30579428
C	-1.57747387	0.14032669	6.25055526
O	-1.78495588	-0.40211529	7.32008395
C	-3.52643699	-0.84759434	4.93691787
C	-2.90005031	-1.26070706	3.60488138
C	-2.67691036	0.07176943	2.89397249
H	-1.86860593	0.02276791	2.16972789
H	-3.37348741	1.14318558	5.84201540
H	-4.58236448	-0.60722320	4.80030263
H	-3.52184122	-1.93861192	3.02288296
H	-3.59417043	0.40629678	2.39744923
H	-3.44032498	-1.59619739	5.72152396
H	-1.93653025	-1.74579905	3.78069088
N	-0.36588269	0.56910852	5.83963024
C	0.78027844	0.67530298	6.71491884
C	1.33470520	2.10744679	6.70996229
O	2.52447359	2.32494717	6.85041055
C	1.88203896	-0.32079930	6.38003795
S	1.27466185	-2.04572033	6.34350160
H	0.28474414	-1.87445164	7.23250931
H	-0.26996417	1.00299023	4.93146246
H	0.41783863	0.47113708	7.72725806
H	2.68994404	-0.21772180	7.09889227
H	2.28753619	-0.10725655	5.38934767
N	0.40578514	3.07298209	6.59277415
H	-0.52426621	2.83095890	6.28226106
H	4.73401667	2.77829701	-0.72790113
H	4.71830856	3.44620338	0.91490568
C	0.81221635	4.44908119	6.43672724
H	1.39448807	4.77173666	7.29955289

H	1.42999245	4.57452909	5.54384094
H	-0.07981928	5.06516502	6.34915496
H	0.76208906	-2.16579632	1.34900010

Table S8. Atomic Coordinates of CXXC Motif in PDB Entry 1ert (*Homo sapiens* Thioredoxin, Thiolate)

C	5.98368500	1.36601800	-0.15266200
C	5.06381400	0.19569200	0.11988800
O	5.44343600	-0.95562500	-0.01206700
H	6.38717400	1.26088500	-1.15917900
N	3.82987800	0.53688500	0.54426800
C	2.75998700	-0.40917500	0.82600500
C	1.84831600	-0.44539600	-0.39654700
O	1.29490600	0.55584100	-0.81728200
C	1.96752700	0.05836400	2.04032000
S	0.48121200	-0.94608000	2.29834300
H	3.55080800	1.50497400	0.50204900
H	3.21453600	-1.38177100	1.00863100
H	1.70172300	1.10837700	1.86782100
H	2.63030300	0.02889900	2.90807600
N	1.75710700	-1.63520400	-1.03896000
C	0.89737100	-1.76927700	-2.18615800
C	-0.60227000	-1.53271100	-1.94803400
O	-1.21054100	-0.84502600	-2.76255800
H	1.03127200	-2.76931000	-2.60477500
H	2.14357800	-2.44810400	-0.59012200
H	1.16913600	-1.03557900	-2.94390500
N	-1.22747700	-2.07476200	-0.88079300
C	-2.65112400	-1.77379700	-0.68344900
C	-2.93075300	-0.30315600	-0.35039300
O	-4.05985800	0.12726000	-0.51816600
C	-3.11097000	-2.77171200	0.38575800
C	-1.82255600	-3.16577000	1.10888600
C	-0.75227000	-3.13542100	0.01982700
H	0.20972100	-2.87895900	0.45607800
H	-3.18647200	-1.91920100	-1.62310400
H	-3.56057300	-3.63895400	-0.10277400
H	-1.88525400	-4.14073700	1.59162000
H	-0.70216400	-4.08777300	-0.52267200
H	-3.85720400	-2.32826900	1.04342900
H	-1.56848900	-2.42083600	1.86378600
N	-1.87996000	0.43426500	0.05555400
C	-1.98200200	1.85882300	0.27350200
C	-1.40423700	2.69269300	-0.87624500
O	-1.21649000	3.89518700	-0.74146000
C	-1.31754500	2.24296300	1.59134500

S	-2.18692000	1.58246800	3.05226800
H	-3.21156600	2.44710400	2.98408600
H	-1.03879300	-0.03708000	0.40188400
H	-3.04626300	2.10758900	0.30971400
H	-1.23342000	3.32372500	1.65955500
H	-0.32125300	1.80272800	1.64200300
N	-1.20092300	2.03352200	-2.02209400
H	-1.23763200	1.02329300	-2.02498200
H	6.81838500	1.31478200	0.54688600
H	5.49300200	2.33335900	-0.05535000
C	-0.59128100	2.69028100	-3.14628500
H	-1.13149000	3.60710700	-3.38480200
H	0.44889100	2.95255000	-2.93276700
H	-0.62277000	2.01445700	-3.9990710

Table S9. Atomic Coordinates of CXXC Motif in PDB Entry 1eru (*Homo sapiens* Thioredoxin, Oxidized)

C	6.15227200	-1.00700600	0.79733700
C	4.96865900	-0.11925400	0.52040100
O	4.98213800	1.09213900	0.63531100
H	5.85549000	-2.01514000	1.08395000
N	3.86906400	-0.77680700	0.06842800
C	2.74756700	-0.06654500	-0.50094700
C	1.69769100	0.26408300	0.56684000
O	0.83417200	-0.53161900	0.89429600
C	2.14178100	-0.96794900	-1.57837400
S	0.65382200	-0.23213800	-2.33983800
H	1.82778100	-1.90288300	-1.11361000
H	3.87623500	-1.78293600	0.01488900
H	3.13094000	0.86046000	-0.93335700
H	2.88957200	-1.17497600	-2.34285400
N	1.77293300	1.50732400	1.08211100
C	0.79743000	1.94944400	2.05893300
C	-0.67213000	1.80576400	1.61345900
O	-1.46766300	1.32842000	2.40845900
H	0.99549900	2.99815700	2.28701700
H	2.61653800	2.04020700	0.91748700
H	0.86149300	1.36836000	2.97848000
N	-1.06903800	2.20586500	0.37909400
C	-2.49608200	2.09208000	0.00843300
C	-2.93450000	0.63815800	-0.33725300
O	-4.10986500	0.42232700	-0.54736800
C	-2.64074300	3.03998700	-1.17999800
C	-1.25169400	3.01372000	-1.81693800
C	-0.30979600	2.98262500	-0.61404200
H	0.63761500	2.50600300	-0.85066300

H	-3.12156200	2.37090200	0.85560700
H	-2.87484400	4.04341700	-0.81897300
H	-1.05550500	3.86249400	-2.46990300
H	-0.11530500	3.99197200	-0.23599100
H	-3.44015900	2.71684400	-1.84375500
H	-1.12494700	2.09511200	-2.39404900
N	-1.96832300	-0.31495600	-0.37847700
C	-2.21739200	-1.75604900	-0.41964600
C	-2.35706600	-2.36129600	1.01313000
O	-2.53670400	-3.56168800	1.12889800
C	-1.02911500	-2.47197600	-1.05526400
S	-0.51194900	-1.90626700	-2.71033000
H	-1.27545100	-3.52658100	-1.18123500
H	-1.02086500	-0.04023800	-0.15458300
H	-3.14541900	-1.93497700	-0.96152400
H	-0.16658600	-2.40999100	-0.38947100
N	-2.19604400	-1.51398200	2.04538300
C	-2.13562600	-1.92788400	3.44201800
H	-2.03347900	-0.53481100	1.86676200
H	-1.57161000	-2.85677600	3.52355600
H	6.75566700	-1.06432100	-0.11040900
H	6.75846500	-0.56259400	1.58292600
H	-3.13385800	-2.09242700	3.85114100
H	-1.63996500	-1.13696300	4.00018200

Table S10. Atomic Coordinates of CXXC Motif in PDB Entry 1w4v (*Homo sapiens* Thioredoxin 2, Oxidized)

C	6.12706000	-1.23503400	1.05820300
C	5.02032400	-0.26662300	0.63558200
O	5.09413200	0.93236000	0.82284300
N	3.94805200	-0.81239500	-0.01439800
C	2.84727000	-0.01945100	-0.56574200
C	1.77978200	0.25104600	0.50467100
O	0.98154500	-0.60640200	0.83810000
C	2.23811300	-0.84997100	-1.69806100
S	0.70200500	-0.11749100	-2.37191000
N	1.75213300	1.50103400	1.01717100
C	0.78999700	1.82617300	2.05623600
C	-0.67272900	1.69961200	1.62158500
O	-1.47326700	1.15980000	2.36811600
N	-1.03930700	2.17677300	0.41002000
C	-2.44378100	2.04947300	-0.01722300
C	-2.91156600	0.62101100	-0.24458400
O	-4.09612700	0.37356000	-0.33318200
C	-2.48582200	2.85527400	-1.32284400
C	-1.40236200	3.91374400	-1.11805100

C	-0.29103400	3.12384000	-0.42929200
N	-1.92832000	-0.29085400	-0.39573900
C	-2.19986200	-1.69782900	-0.52437100
C	-2.49639900	-2.39429800	0.82267700
O	-2.80588400	-3.57396500	0.82909500
C	-0.98758800	-2.40161000	-1.12854300
S	-0.44136100	-1.80114900	-2.76592900
N	-2.34005100	-1.64697200	1.92494200
C	-2.56373700	-2.17738800	3.25330200
H	6.50768100	-0.91445500	2.02483200
H	0.89098600	1.15331500	2.90763200
H	0.97826000	2.84778600	2.39043700
H	-3.47718700	3.26161200	-1.50808600
H	-2.21842700	2.20422600	-2.15978300
H	-1.76482800	4.70104300	-0.45341100
H	-1.06631100	4.37117100	-2.04730900
H	0.31757400	2.58469000	-1.15938600
H	0.36246200	3.75024900	0.17787600
H	-3.10319700	2.47242400	0.74354000
H	-2.03808900	-3.12510100	3.37181500
H	3.26705700	0.91967500	-0.92978600
H	1.95472400	-1.82324500	-1.29686000
H	2.97120400	-0.98483500	-2.49158100
H	-3.08282300	-1.83192500	-1.15097600
H	-1.22944900	-3.45306400	-1.28716100
H	-0.14044100	-2.34688900	-0.44220100
H	5.78589200	-2.26778900	1.11139700
H	6.93290500	-1.16164600	0.32727300
H	3.85186100	-1.81561700	-0.03982100
H	2.56289500	2.08697800	0.87625300
H	-2.08294900	-0.67364700	1.85041400
H	-0.97093600	-0.01180700	-0.23322700
H	-3.62603300	-2.35348600	3.43305700
H	-2.18985400	-1.45516600	3.97549500

Table S11. Atomic Coordinates of CXXC Motif in PDB Entry 1w89 (*Homo sapiens* Thioredoxin 2, Thiol)

C	-3.44520712	-2.90144375	-2.11559308
C	-2.34300077	-2.20063264	-1.36082821
O	-1.41475084	-1.65022902	-1.91684094
N	-2.48008647	-2.17873511	0.00208419
C	-1.73682120	-1.22430137	0.79667802
C	-0.67984857	-1.91095838	1.66609327
O	-0.98037526	-2.49265674	2.69724589
C	-2.68187300	-0.41156000	1.67746500
S	-1.83278400	0.95331900	2.53640300

N	0.59300715	-1.82205620	1.22730412
C	1.66491261	-2.58671473	1.84150011
C	1.83594604	-2.41385115	3.35307709
O	2.02044807	-3.40931686	4.03751243
N	1.79019283	-1.17755804	3.88948675
C	1.96305523	-1.01035395	5.34323616
C	0.84678606	-1.63832677	6.19879012
O	1.03019709	-1.75628772	7.39275870
C	1.99691065	0.51320426	5.51310648
C	2.59003155	1.00235877	4.19164905
C	1.92002209	0.09383854	3.16102568
N	-0.31666143	-1.98238025	5.58309955
C	-1.34915038	-2.73469502	6.28398071
C	-1.00163027	-4.25590864	6.44242661
O	-1.73756622	-4.95005230	7.12171268
C	-2.68116052	-2.67985695	5.54960057
S	-3.38280704	-1.01335906	5.35124697
N	0.06220822	-4.73257377	5.76607820
C	0.47541748	-6.13773529	5.80667931
H	-3.93199971	-3.67681166	-1.52470100
H	-3.15861694	-1.04715992	2.42442093
H	-3.45461196	0.03299671	1.05152153
H	-1.46489494	1.62294551	1.43195626
H	-1.24209630	-0.55864685	0.08884496
H	1.50724163	-3.65686496	1.70338261
H	2.59970082	-2.31023354	1.35024881
H	2.56677448	0.80375441	6.39225641
H	0.97569859	0.88738641	5.62758629
H	3.67048540	0.84212746	4.18321545
H	2.39534538	2.05587255	3.99729596
H	0.93832986	0.47319684	2.87108188
H	2.51911064	-0.03896453	2.25966251
H	2.89108864	-1.48399720	5.66881270
H	-3.38855856	-3.32262187	6.06675739
H	-2.55470620	-3.04806056	4.52925981
H	-3.49962202	-0.72426739	6.65260292
H	-1.43957908	-2.34354649	7.29766874
H	-0.35725311	-6.78131004	5.52292497
H	-4.19021032	-2.15387485	-2.39396603
H	-3.03268687	-3.32991272	-3.02545038
H	1.29689689	-6.26031613	5.10518461
H	0.80098025	-6.41701538	6.80964486
H	0.65714458	-4.09742910	5.25290433
H	-0.36346889	-1.97804156	4.57026034
H	-3.28019795	-2.62610226	0.42252328
H	0.74601527	-1.41649545	0.31597312

Table S12. Atomic Coordinates of CXXC Motif in PDB Entry 1w89 (*Homo sapiens* Thioredoxin 2, Thiolate)

C	-0.91701605	-9.95228978	0.87210097
C	-1.81844925	-8.82618431	1.31223560
O	-2.93495083	-9.03324927	1.75203812
N	-1.27863385	-7.59466266	1.15988116
C	-2.06227612	-6.38079467	1.25302633
C	-2.10460206	-5.76840053	-0.14752050
O	-1.11865835	-5.76897644	-0.86172376
C	-1.44340636	-5.38904031	2.24321438
S	-2.36038890	-3.81610323	2.32993028
N	-3.31347734	-5.29005649	-0.55218217
C	-3.41908149	-4.54695865	-1.78916295
C	-2.94557313	-3.09426506	-1.72855824
O	-2.12023263	-2.67625267	-2.53189590
N	-3.48052352	-2.30564019	-0.77704584
C	-3.04733829	-0.91712451	-0.64024943
C	-1.53301415	-0.68425207	-0.48066792
O	-1.06616413	0.36022534	-0.90301554
C	-3.82468593	-0.44005555	0.59014731
C	-5.13724031	-1.21534602	0.48057109
C	-4.66339119	-2.60188734	0.04472789
N	-0.79245170	-1.63090970	0.13832299
C	0.65124552	-1.45691800	0.28631537
C	1.40520926	-1.48760388	-1.08507570
O	2.57032023	-1.11923171	-1.11394848
C	1.24032800	-2.53503800	1.18319500
S	0.89371000	-2.32315000	2.95986500
N	0.75949922	-1.95397272	-2.17324157
C	1.36274427	-1.93846688	-3.50839258
H	-1.16199023	-10.20510484	-0.16148569
H	-0.40456262	-5.21218332	1.94481799
H	-1.42469550	-5.87642094	3.21965460
H	-3.06143230	-6.65857610	1.58574397
H	-2.79121182	-5.03148069	-2.53326955
H	-4.45632855	-4.57563989	-2.13157836
H	-3.94165653	0.64180038	0.59804089
H	-3.28803901	-0.74799084	1.49209298
H	-5.77616614	-0.76831247	-0.28567829
H	-5.69078505	-1.25583778	1.41773908
H	-4.36825669	-3.19045674	0.91663400
H	-5.41540457	-3.13771455	-0.53890022
H	-3.31579624	-0.34661490	-1.53340293
H	2.32353144	-2.49772037	1.07992141
H	0.89609372	-3.51998695	0.85940435
H	1.91036073	-1.44751267	3.21180017
H	0.86587735	-0.46835051	0.69520471

H	2.29343417	-2.50658385	-3.50731834
H	0.13871657	-9.68769269	0.92495155
H	-1.11204755	-10.82478954	1.49186027
H	0.65261886	-2.39000433	-4.19724413
H	1.58278700	-0.91530254	-3.81919351
H	-0.22207919	-2.19378260	-2.10401110
H	-1.25916594	-2.40973688	0.61793781
H	-0.42785309	-7.50559302	0.62194094
H	-3.95674454	-5.08648158	0.19961377

Table S13. Atomic Coordinates of CXXC Motif in PDB Entry 1xwa (*Drosophila melanogaster* Thioredoxin, Oxidized)

C	-6.06485300	-1.18103900	-0.87553500
C	-5.03779400	-0.14042200	-0.47409700
O	-5.24385000	1.05488200	-0.52730500
N	-3.86627600	-0.64668600	0.01358900
C	-2.80384500	0.18605100	0.54623200
C	-1.72920600	0.41826700	-0.51417000
O	-0.99238000	-0.48092800	-0.87757200
C	-2.19996800	-0.56149800	1.74308200
S	-0.63458200	0.18415300	2.33054200
N	-1.63444300	1.67669100	-0.99675300
C	-0.70046700	1.96427800	-2.06885000
C	0.74783400	1.62916200	-1.72220700
O	1.41737700	0.94064300	-2.47317800
N	1.24432900	2.11689200	-0.56283200
C	2.65119700	1.86368700	-0.23759400
C	3.00023700	0.40674900	0.04735200
O	4.16028300	0.05202700	0.06099000
C	2.88469700	2.72677800	1.01080000
C	1.90013700	3.88158600	0.82985800
C	0.66403100	3.18074500	0.26771600
N	1.95547300	-0.39507300	0.34864400
C	2.10439900	-1.80761200	0.60116300
C	2.16579000	-2.66106200	-0.68262700
O	2.38412000	-3.85773900	-0.59532200
C	0.87613500	-2.32156700	1.35407800
S	0.44514100	-1.48591800	2.91860400
N	1.87245400	-2.03248200	-1.83039100
C	1.75271300	-2.76163400	-3.07615000
H	-6.71850000	-0.75300500	-1.63087900
H	-0.93105200	1.37381800	-2.95588900
H	-0.78173700	3.02246100	-2.32140400
H	3.92385400	3.03529200	1.09417500
H	2.62469100	2.15002200	1.90275400
H	2.28638100	4.59557800	0.09908900

H	1.68659800	4.41422200	1.75516700
H	0.03502300	3.84200000	-0.32790500
H	0.05897300	2.74843000	1.06855400
H	3.28656400	2.17162200	-1.07081600
H	1.01794900	-3.56200800	-2.97808000
H	-3.25709300	1.12953100	0.85219900
H	-1.95296400	-1.57526300	1.42760300
H	-2.92561400	-0.60834000	2.55315300
H	3.02326300	-1.97857100	1.16184700
H	0.00427300	-2.27800600	0.69695900
H	1.03769400	-3.36479700	1.62633500
H	-5.60388800	-2.09316200	-1.25343600
H	-6.66291900	-1.43069400	0.00231700
H	-3.67756700	-1.63217700	-0.08620200
H	-2.37712400	2.32742700	-0.79029300
H	1.70189100	-1.03675600	-1.83976200
H	1.01768400	-0.03535800	0.23439900
H	1.43661400	-2.06543100	-3.84944900
H	2.70666400	-3.20988800	-3.35778200

Table S14. Atomic Coordinates of CXXC Motif in PDB Entry 1xwc (*Drosophila melanogaster* Thioredoxin, Thiol)

C	-3.01979054	-3.50867456	-1.30429270
C	-2.19921555	-2.40054787	-0.68855305
O	-1.49821418	-1.67192690	-1.35931386
N	-2.29151807	-2.26274628	0.67113738
C	-1.65115605	-1.15144261	1.35039155
C	-1.03145980	-1.68135118	2.63106535
O	-1.72373236	-1.99354400	3.58815537
C	-2.63518700	-0.02064500	1.63341900
S	-1.79801500	1.44906500	2.32093700
N	0.30752087	-1.82990922	2.61995400
C	0.99728567	-2.53677971	3.67811224
C	0.67897852	-2.03597314	5.09473882
O	0.41153991	-2.84614502	5.96833152
N	0.70084140	-0.70659391	5.33128253
C	0.43025680	-0.19985253	6.68823236
C	-0.96749435	-0.48406853	7.22888115
O	-1.17901756	-0.34525378	8.41520475
C	0.66426391	1.30826914	6.54498548
C	1.73936738	1.39255885	5.46213575
C	1.29616838	0.32349255	4.46404135
N	-1.92199742	-0.80895193	6.32070196
C	-3.26431847	-1.16667402	6.72919527
C	-3.46847195	-2.66237376	6.99544032
O	-4.58125749	-3.07774438	7.27515129

C	-4.27527467	-0.74527942	5.67060516
S	-4.14083852	1.05861094	5.40153269
N	-2.39001775	-3.44772372	6.88603792
C	-2.51453679	-4.86766182	7.11229114
H	-2.37440341	-4.08525216	-1.96443208
H	-3.40021613	-0.34401584	2.33939627
H	-3.11184911	0.26719546	0.69773539
H	-1.67281804	2.10115844	1.15337328
H	-0.87933443	-0.78660541	0.67171516
H	0.72746328	-3.59314006	3.68528259
H	2.07104828	-2.45215484	3.50316325
H	-0.25684363	1.78517225	6.19737018
H	0.94767592	1.75938612	7.49278417
H	1.81161722	2.37707119	5.00289581
H	2.71421337	1.13278570	5.88087500
H	0.55243648	0.71585315	3.76754501
H	2.12725726	-0.08873412	3.89057972
H	1.12465879	-0.65288329	7.39929798
H	-5.27060496	-0.99450493	6.02649806
H	-4.07233927	-1.27492206	4.73837395
H	-5.29365573	1.20001556	4.73784725
H	-3.46931230	-0.65065067	7.66919232
H	-3.26949333	-5.29399531	6.45029810
H	-3.47712120	-4.16776110	-0.56786770
H	-3.80007605	-3.05316598	-1.91442559
H	-2.94171144	-2.82994490	1.19409434
H	0.80925291	-1.58077494	1.78290655
H	-1.48610498	-3.06737930	6.64148301
H	-1.65158785	-1.03869147	5.37086408
H	-1.55160553	-5.33479746	6.91781864
H	-2.81628366	-5.07226170	8.14078998

Table S15. Atomic Coordinates of CXXC Motif in PDB Entry 1xwc (*Drosophila melanogaster* Thioredoxin, Thiolate)

C	-0.29509271	-9.66233661	2.11156958
C	-1.29250856	-8.62542007	2.58666663
O	-2.33693359	-8.95170420	3.12255326
N	-0.92626523	-7.34222370	2.36481764
C	-1.80256751	-6.19750902	2.56034117
C	-2.10311752	-5.63027512	1.17860324
O	-1.21770243	-5.45504060	0.36115614
C	-1.11506919	-5.12427366	3.41036117
S	-2.07808500	-3.57999444	3.49366784
N	-3.41305157	-5.40610529	0.89664808
C	-3.76760959	-4.78774467	-0.35543957
C	-3.39233762	-3.30702397	-0.51890754

O	-2.79093353	-2.94385016	-1.52271497
N	-3.75616287	-2.44506991	0.45066861
C	-3.35315217	-1.03314036	0.40300781
C	-1.86507923	-0.78846906	0.13843755
O	-1.53023185	0.19320677	-0.50078954
C	-3.79959418	-0.51998711	1.77416208
C	-5.08635646	-1.30772023	2.02374694
C	-4.73091130	-2.70861903	1.52051156
N	-0.99126467	-1.67097863	0.66765920
C	0.43857697	-1.48128552	0.49452098
C	0.96044415	-1.84252775	-0.89854825
O	2.11035990	-1.55468356	-1.20460390
C	1.20657400	-2.33096800	1.50453400
S	1.08983200	-1.76775400	3.23263100
N	0.13418019	-2.51567666	-1.70618389
C	0.57383058	-2.89476606	-3.02523250
H	-0.69678809	-10.13416476	1.21360864
H	-0.13005278	-4.93119350	2.97204817
H	-0.95425438	-5.54031545	4.40657368
H	-2.70843990	-6.55379145	3.04847668
H	-3.24488964	-5.29995050	-1.16045713
H	-4.84337092	-4.90123159	-0.50949501
H	-3.04749235	-0.79167393	2.52026379
H	-3.93217908	0.56036691	1.77634040
H	-5.37794813	-1.32420752	3.07306615
H	-5.90615325	-0.88312763	1.43826412
H	-4.25667070	-3.28241217	2.31878762
H	-5.60039901	-3.24024103	1.12517990
H	-3.87261423	-0.51703644	-0.40887283
H	2.26135506	-2.29309578	1.23945133
H	0.87169369	-3.36925737	1.43910427
H	2.20519163	-0.98095649	3.22160960
H	0.68254120	-0.42691573	0.63776520
H	1.42325037	-3.57836372	-2.96839735
H	0.68368371	-9.24167896	1.88485045
H	-0.19839787	-10.42811804	2.87916042
H	-0.12089356	-7.16209732	1.78298971
H	-4.02923060	-5.31963353	1.69026392
H	-0.82709280	-2.68319179	-1.43640591
H	-1.32930390	-2.38393085	1.32158173
H	-0.25306377	-3.38458101	-3.53580864
H	0.88725106	-2.01771022	-3.59552635

Table S16. Atomic coordinates of CXXC Motif in PDB Entry 2o7k (*Staphylococcus aureus* Thioredoxin, Oxidized)

N	-4.48735800	-1.41010600	0.26675500
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C	-3.63142700	-0.24014100	0.31289500
C	-2.33326600	-0.50214100	-0.47538600
O	-1.34121700	-0.97269300	0.05295800
C	-3.29533200	0.14001400	1.74673600
S	-2.30930400	1.68492200	1.70860500
H	-2.68269000	-0.63686600	2.20331300
H	-4.39775000	-2.11006500	0.98689000
H	-4.17925600	0.56914000	-0.17611200
H	-4.20354500	0.29248100	2.32751500
N	-2.36191200	-0.16198700	-1.78801100
C	-1.23544100	-0.54545100	-2.62521100
C	0.06141000	0.15635300	-2.24969300
O	1.12541600	-0.42112400	-2.30962300
H	-1.47425700	-0.29958000	-3.66015200
H	-3.28070800	-0.04780600	-2.20267400
H	-1.03112100	-1.61448400	-2.55123800
N	-0.03662700	1.46848000	-1.89668400
C	1.15871300	2.17070900	-1.44850700
C	1.75378300	1.56033300	-0.18014700
O	2.95548400	1.53005900	0.00874700
C	0.82079400	3.65441700	-1.26400500
C	1.96913100	4.44764000	-0.67904700
O	0.50482500	4.23695100	-2.51567000
H	-0.09080800	3.65703800	-3.00045300
H	-0.94861000	1.81806900	-1.63062600
H	1.92913700	2.07519100	-2.21510700
H	-0.04828200	3.72220500	-0.59005300
H	1.69942400	5.50309200	-0.67243400
H	2.86516300	4.31517600	-1.28634800
H	2.19064900	4.12900400	0.33896000
N	0.85770100	1.10553300	0.72188700
C	1.29498400	0.52347800	1.96773300
C	2.10511100	-0.77139200	1.80804700
O	2.82644800	-1.14073500	2.71265800
C	0.10060500	0.14236800	2.83843300
S	-1.04380000	1.47458100	3.33255500
H	0.48067500	-0.24841100	3.78362800
H	-0.11967000	1.04179600	0.47655000
H	1.94712000	1.22480900	2.49080200
H	-0.47707300	-0.64591200	2.35270000
N	1.87827800	-1.46662900	0.67703800
C	2.54950500	-2.71829900	0.39893400
C	3.95957300	-2.54450500	-0.18324300
O	4.63724700	-3.53210400	-0.41287600
C	1.70800700	-3.55224800	-0.55895900
H	0.74383000	-3.78789000	-0.10666300
H	1.26832300	-1.08520700	-0.03415800

H	2.68867300	-3.24173300	1.34642300
H	2.23832400	-4.47262900	-0.79446200
H	1.53852400	-2.99661800	-1.48503400
N	4.37761000	-1.29232900	-0.43318800
C	5.70788600	-1.06428200	-0.95661900
H	3.79742200	-0.49780200	-0.20662000
H	5.83043600	-1.56115000	-1.91978000
H	5.85251400	0.00693900	-1.07812200
H	6.46155900	-1.45961500	-0.27395800
C	-5.23048500	-1.67304700	-0.84529700
O	-5.21847400	-0.92135200	-1.80520600
C	-6.06630600	-2.92515000	-0.81599000
H	-7.09979600	-2.64980900	-1.02242400
H	-5.73099000	-3.58122100	-1.61890500
H	-6.01270000	-3.45487400	0.13345000

Table S17. Atomic coordinates of CXXC Motif in PDB Entry 2o85 (*Staphylococcus aureus* Thioredoxin P31T, Oxidized)

N	-4.48735800	-1.41010600	0.26675500
C	-3.63142700	-0.24014100	0.31289500
C	-2.33326600	-0.50214100	-0.47538600
O	-1.34121700	-0.97269300	0.05295800
C	-3.29533200	0.14001400	1.74673600
S	-2.30930400	1.68492200	1.70860500
H	-2.68269000	-0.63686600	2.20331300
H	-4.39775000	-2.11006500	0.98689000
H	-4.17925600	0.56914000	-0.17611200
H	-4.20354500	0.29248100	2.32751500
N	-2.36191200	-0.16198700	-1.78801100
C	-1.23544100	-0.54545100	-2.62521100
C	0.06141000	0.15635300	-2.24969300
O	1.12541600	-0.42112400	-2.30962300
H	-1.47425700	-0.29958000	-3.66015200
H	-3.28070800	-0.04780600	-2.20267400
H	-1.03112100	-1.61448400	-2.55123800
N	-0.03662700	1.46848000	-1.89668400
C	1.15871300	2.17070900	-1.44850700
C	1.75378300	1.56033300	-0.18014700
O	2.95548400	1.53005900	0.00874700
C	0.82079400	3.65441700	-1.26400500
C	1.96913100	4.44764000	-0.67904700
O	0.50482500	4.23695100	-2.51567000
H	-0.09080800	3.65703800	-3.00045300
H	-0.94861000	1.81806900	-1.63062600
H	1.92913700	2.07519100	-2.21510700
H	-0.04828200	3.72220500	-0.59005300

H	1.69942400	5.50309200	-0.67243400
H	2.86516300	4.31517600	-1.28634800
H	2.19064900	4.12900400	0.33896000
N	0.85770100	1.10553300	0.72188700
C	1.29498400	0.52347800	1.96773300
C	2.10511100	-0.77139200	1.80804700
O	2.82644800	-1.14073500	2.71265800
C	0.10060500	0.14236800	2.83843300
S	-1.04380000	1.47458100	3.33255500
H	0.48067500	-0.24841100	3.78362800
H	-0.11967000	1.04179600	0.47655000
H	1.94712000	1.22480900	2.49080200
H	-0.47707300	-0.64591200	2.35270000
N	1.87827800	-1.46662900	0.67703800
C	2.54950500	-2.71829900	0.39893400
C	3.95957300	-2.54450500	-0.18324300
O	4.63724700	-3.53210400	-0.41287600
C	1.70800700	-3.55224800	-0.55895900
H	0.74383000	-3.78789000	-0.10666300
H	1.26832300	-1.08520700	-0.03415800
H	2.68867300	-3.24173300	1.34642300
H	2.23832400	-4.47262900	-0.79446200
H	1.53852400	-2.99661800	-1.48503400
N	4.37761000	-1.29232900	-0.43318800
C	5.70788600	-1.06428200	-0.95661900
H	3.79742200	-0.49780200	-0.20662000
H	5.83043600	-1.56115000	-1.91978000
H	5.85251400	0.00693900	-1.07812200
H	6.46155900	-1.45961500	-0.27395800
C	-5.23048500	-1.67304700	-0.84529700
O	-5.21847400	-0.92135200	-1.80520600
C	-6.06630600	-2.92515000	-0.81599000
H	-7.09979600	-2.64980900	-1.02242400
H	-5.73099000	-3.58122100	-1.61890500
H	-6.01270000	-3.45487400	0.13345000

Table S18. Atomic coordinates of CXXC Motif in PDB Entry 2o87 (*Staphylococcus aureus* Thioredoxin P31S, Oxidized)

N	-4.48735800	-1.41010600	0.26675500
C	-3.63142700	-0.24014100	0.31289500
C	-2.33326600	-0.50214100	-0.47538600
O	-1.34121700	-0.97269300	0.05295800
C	-3.29533200	0.14001400	1.74673600
S	-2.30930400	1.68492200	1.70860500
H	-2.68269000	-0.63686600	2.20331300
H	-4.39775000	-2.11006500	0.98689000

H	-4.17925600	0.56914000	-0.17611200
H	-4.20354500	0.29248100	2.32751500
N	-2.36191200	-0.16198700	-1.78801100
C	-1.23544100	-0.54545100	-2.62521100
C	0.06141000	0.15635300	-2.24969300
O	1.12541600	-0.42112400	-2.30962300
H	-1.47425700	-0.29958000	-3.66015200
H	-3.28070800	-0.04780600	-2.20267400
H	-1.03112100	-1.61448400	-2.55123800
N	-0.03662700	1.46848000	-1.89668400
C	1.15871300	2.17070900	-1.44850700
C	1.75378300	1.56033300	-0.18014700
O	2.95548400	1.53005900	0.00874700
C	0.82079400	3.65441700	-1.26400500
C	1.96913100	4.44764000	-0.67904700
O	0.50482500	4.23695100	-2.51567000
H	-0.09080800	3.65703800	-3.00045300
H	-0.94861000	1.81806900	-1.63062600
H	1.92913700	2.07519100	-2.21510700
H	-0.04828200	3.72220500	-0.59005300
H	1.69942400	5.50309200	-0.67243400
H	2.86516300	4.31517600	-1.28634800
H	2.19064900	4.12900400	0.33896000
N	0.85770100	1.10553300	0.72188700
C	1.29498400	0.52347800	1.96773300
C	2.10511100	-0.77139200	1.80804700
O	2.82644800	-1.14073500	2.71265800
C	0.10060500	0.14236800	2.83843300
S	-1.04380000	1.47458100	3.33255500
H	0.48067500	-0.24841100	3.78362800
H	-0.11967000	1.04179600	0.47655000
H	1.94712000	1.22480900	2.49080200
H	-0.47707300	-0.64591200	2.35270000
N	1.87827800	-1.46662900	0.67703800
C	2.54950500	-2.71829900	0.39893400
C	3.95957300	-2.54450500	-0.18324300
O	4.63724700	-3.53210400	-0.41287600
C	1.70800700	-3.55224800	-0.55895900
H	0.74383000	-3.78789000	-0.10666300
H	1.26832300	-1.08520700	-0.03415800
H	2.68867300	-3.24173300	1.34642300
H	2.23832400	-4.47262900	-0.79446200
H	1.53852400	-2.99661800	-1.48503400
N	4.37761000	-1.29232900	-0.43318800
C	5.70788600	-1.06428200	-0.95661900
H	3.79742200	-0.49780200	-0.20662000
H	5.83043600	-1.56115000	-1.91978000

H	5.85251400	0.00693900	-1.07812200
H	6.46155900	-1.45961500	-0.27395800
C	-5.23048500	-1.67304700	-0.84529700
O	-5.21847400	-0.92135200	-1.80520600
C	-6.06630600	-2.92515000	-0.81599000
H	-7.09979600	-2.64980900	-1.02242400
H	-5.73099000	-3.58122100	-1.61890500
H	-6.01270000	-3.45487400	0.13345000

Table S19. Atomic Coordinates of the Vicinal Disulfide Bond in PDB Entry 1qlw (*Alcaligenes sp.* Carboxylic Esterase)

C	-3.271700	0.738100	-0.007300
O	-2.882100	1.638600	0.703200
N	-2.643400	-0.476500	-0.003000
C	-1.446400	-0.615400	0.778700
C	-0.349200	0.286400	0.225100
O	-0.325400	0.666000	-0.921000
C	-0.912600	-2.062700	0.784300
S	0.217400	-2.529800	-0.590500
N	0.695100	0.491900	1.076400
C	2.001400	0.748400	0.521700
C	2.221600	2.138900	-0.105200
O	3.230400	2.325300	-0.729500
C	2.425900	-0.335800	-0.488300
S	2.104000	-2.041600	0.093500
N	1.287800	3.143300	0.132800
H	0.441700	2.855800	0.613200
H	-1.652000	-0.321600	1.816600
H	-1.741500	-2.775100	0.721200
H	-0.396900	-2.280700	1.719600
H	2.713300	0.730000	1.353000
H	1.980400	-0.177600	-1.469300
H	3.508300	-0.305900	-0.628800
H	0.594300	0.281300	2.055500
H	-2.926800	-1.203900	-0.638500
C	-4.447800	0.853600	-0.940300
H	-5.215100	0.115400	-0.689800
H	-4.863000	1.855700	-0.852100
H	-4.131600	0.679600	-1.972900
H	1.658600	4.029300	0.449300

Table S20. Atomic Coordinates of the Vicinal Disulfide Bond in PDB Entry 1uv4 (*Bacillus subtilis* Arabinanase)

C	-3.530400	1.579800	-1.561900
C	-2.856000	1.108800	-0.295000

O	-2.770700	1.789400	0.704500
N	-2.296200	-0.137100	-0.348700
C	-1.651500	-0.704000	0.816000
C	-0.371400	0.008900	1.240000
O	0.050000	-0.110300	2.363400
C	-1.268500	-2.163500	0.560800
S	-0.129600	-2.448800	-0.852200
N	0.286300	0.684000	0.240400
C	1.738900	0.663100	0.243700
C	2.333100	2.010300	-0.185200
O	3.379500	2.070800	-0.794000
C	2.266300	-0.460500	-0.642600
S	1.775700	-2.138800	-0.114800
N	1.621200	3.086000	0.213700
H	-4.049400	0.770800	-2.077600
H	-2.329600	-0.652000	1.671100
H	-0.816900	-2.581100	1.459100
H	-2.156700	-2.745900	0.305000
H	2.039000	0.496500	1.282300
H	3.356500	-0.475700	-0.613400
H	1.967100	-0.317700	-1.682100
H	-4.233700	2.367800	-1.305100
H	-2.776500	1.992100	-2.236500
H	-2.356300	-0.682000	-1.195500
H	-0.135900	0.569800	-0.673200
H	1.947700	4.002600	-0.046100
H	0.696400	2.970600	0.598800

**Table S21. Atomic Coordinates of the Vicinal Disulfide Bond in PDB Entry 1wd3
(*Aspergillus kawachi* Arabinofuranoside)**

N	34.498001	13.471000	5.438000
C	34.895000	13.193000	4.062000
C	35.583000	11.832000	3.971000
O	36.481998	11.546000	4.769000
C	35.847000	14.282000	3.571000
S	36.408001	14.069000	1.855000
H	36.723454	14.287459	4.218994
H	34.576466	14.461731	5.617986
H	34.002735	13.178955	3.436090
H	35.291119	15.219061	3.602824
H	35.099865	12.964488	6.071488
N	35.167999	10.971000	3.040000
C	34.075001	11.198000	2.083000
C	33.611000	9.816000	1.642000
O	34.442001	8.983000	1.287000
C	34.562000	11.915000	0.819000

S	34.674999	13.731000	0.855000
H	33.880207	11.648213	0.011484
H	35.647682	10.083703	2.987958
H	33.302673	11.804413	2.556154
H	32.549694	9.567547	1.641242
H	35.592567	11.581334	0.697755

Table S22. Atomic Coordinates of the Vicinal Disulfide Bond in PDB Entry 3cu9 (*Geobacillus stearothermophilus* 1,5- α -L-Arabinanase)

N	-25.409000	6.530000	5.604000
C	-25.611000	7.909000	5.995000
C	-25.469000	8.835000	4.795000
O	-25.131001	8.426000	3.672000
C	-24.546000	8.272000	7.047000
S	-22.908001	8.520000	6.302000
H	-24.482517	7.465109	7.777066
H	-25.450294	6.455341	4.597610
H	-26.614927	8.027121	6.402771
H	-24.845436	9.207802	7.518925
H	-26.129852	5.953995	6.014720
N	-25.649000	10.119000	5.071000
C	-25.004999	11.177000	4.321000
C	-25.532000	11.323000	2.911000
O	-24.802999	11.847000	2.036000
C	-23.462999	10.894000	4.313000
S	-22.792000	10.598000	5.958000
H	-22.953671	11.754553	3.879259
H	-26.259993	10.369410	5.835254
H	-25.226675	12.125827	4.809557
H	-26.534159	10.976609	2.658432
H	-23.301470	9.988565	3.728024

Table S23. Atomic Coordinates of the Vicinal Disulfide Bond in PDB Entry 4aah (*Methylophilus methylotrophus* Methanol Dehydrogenase)

N	-45.119999	24.903000	-11.344000
C	-46.349998	24.658001	-10.623000
C	-46.313000	23.507000	-9.647000
O	-46.917000	23.583000	-8.578000
C	-47.549000	24.350000	-11.582000
S	-47.396999	22.728001	-12.413000
H	-47.595230	25.128664	-12.343344
H	-44.887650	25.884464	-11.290694
H	-46.478863	25.591091	-10.074516
H	-48.454163	24.322899	-10.975331
H	-45.237148	24.636251	-12.311069

N	-45.731998	22.419001	-10.148000
C	-45.891998	21.156000	-9.393000
C	-44.674999	20.414000	-8.918000
O	-44.558998	19.200001	-9.172000
C	-46.799999	20.370001	-10.411000
S	-48.152000	21.363001	-11.124000
H	-47.237751	19.517132	-9.892264
H	-45.203659	22.453974	-11.008078
H	-46.297363	21.322029	-8.394895
H	-43.899548	20.933939	-8.355472
H	-46.157619	20.073425	-11.240150

Table S24. Atomic Coordinates of the Vicinal Disulfide Bond in PDB Entry 4mge (*Bacillus anthracis* Cellobiose Specific Transporter)

N	-16.281000	2.630000	31.055000
C	-16.756001	1.640000	32.042999
C	-15.490000	1.171000	32.744999
O	-14.435000	1.138000	32.095001
C	-17.483000	0.461000	31.358000
S	-18.534000	-0.506000	32.488998
H	-16.733505	-0.204523	30.929707
H	-16.280411	3.549615	31.472622
H	-17.482277	2.066331	32.735001
H	-18.139380	0.888357	30.599955
H	-16.892992	2.624919	30.251545
N	-15.541000	0.747000	34.014999
C	-16.764999	0.576000	34.792000
C	-16.747000	1.280000	36.172001
O	-17.445999	0.891000	37.095001
C	-17.020000	-0.896000	34.999001
S	-17.254999	-1.740000	33.411999
H	-17.915720	-1.021861	35.607231
H	-14.665755	0.529047	34.469471
H	-17.559399	1.047826	34.213718
H	-16.096241	2.141372	36.322502

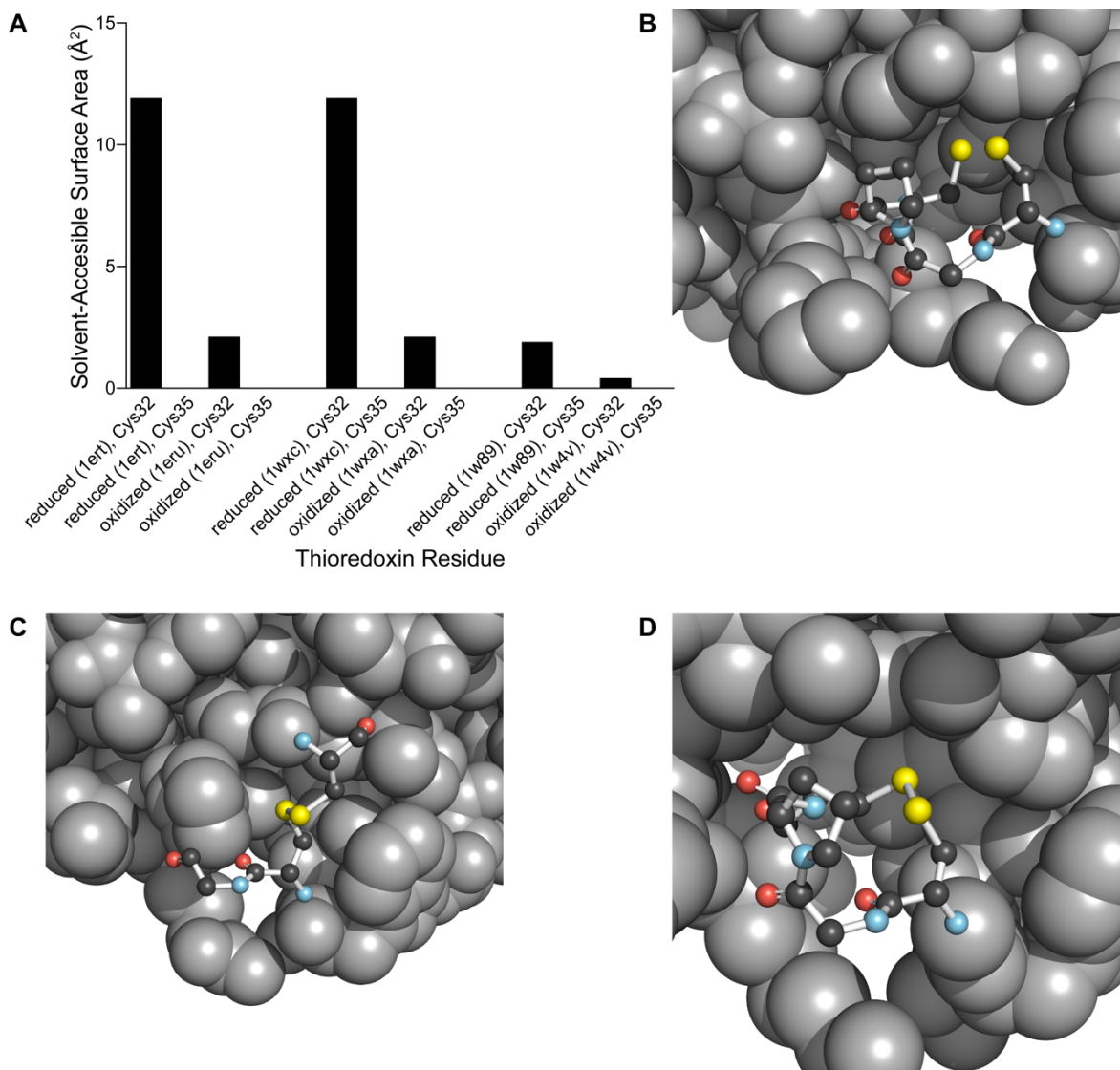


Figure S1. Solvent-accessibility of cysteine residues in a CXXC motif. (A) Bar graph of solvent-accessible surface area of the side chain of cysteine residues in the CXXC motif of oxidized and reduced *Homo sapiens* and *Hordeum vulgare* thioredoxins. Calculations were performed with the Get area server.² Space-filling model of enzymic residues near the CXXC motif (ball-and-stick) of reduced *Homo sapiens* thioredoxin (B; PDB entry 1ert), a *Hordeum vulgare* thioredoxin mixed disulfide (C; 2iwt), and oxidized *Homo sapiens* thioredoxin (D; 1eru).

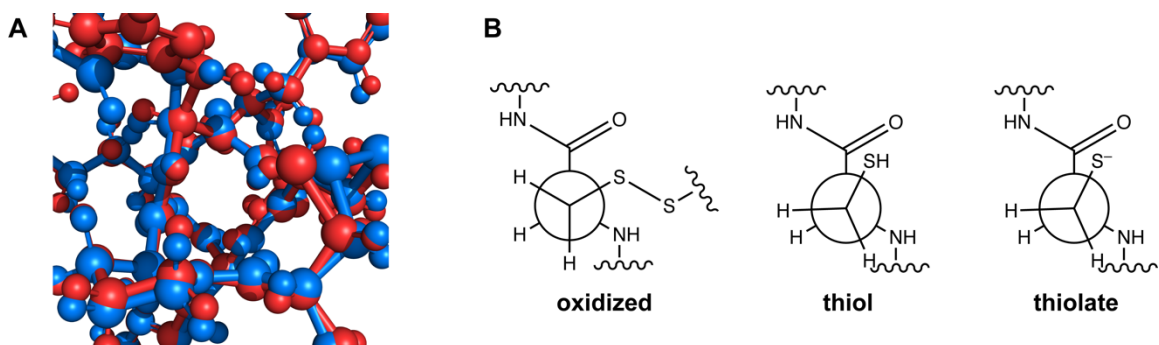


Figure S2. Conformational change upon reduction of a CXXC motif. (A) Image of reduced (red) and oxidized (blue) conformers of wild-type *Homo sapiens* thioredoxin (PDB entries 1ert and 1eru) with C^α atoms aligned. (B) Newman projection depicting changes in the χ_1 dihedral angle upon reduction and deprotonation of the CXXC disulfide.

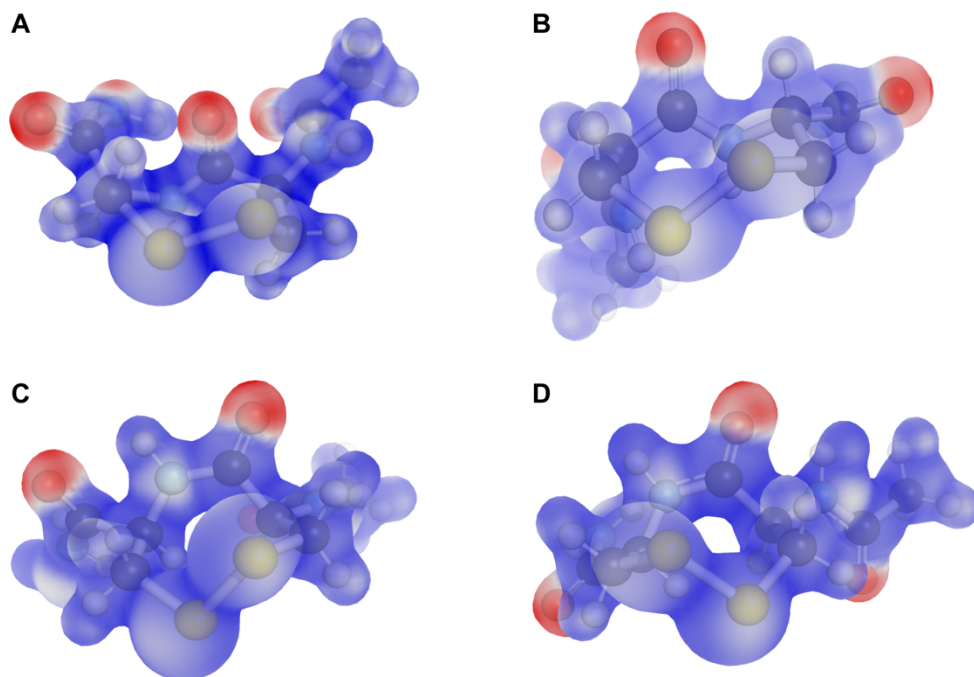


Figure S3. Electrostatic surface potential maps of representative vicinal disulfide bonds. Surfaces were calculated with the Gaussian cubegen utility and visualized with the program Chimera.¹ Red indicates an electronically enriched surface. (A) trans-up conformation (PDB entry 1qlw). (B) trans-down conformation (1uv4). (C) cis-up conformation (1wd3). (D) cis-down conformation (4mge). Herein, “trans” (*Z*) and “cis” (*E*) refer to the intervening peptide bond, and “up” and “down” refer to the sulfur being proximal or distal, respectively, to its cysteinyl carbonyl group.

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