Cysteine pK_a Depression by a Protonated Glutamic Acid in Human DJ-1

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SUPPORTING INFORMATION

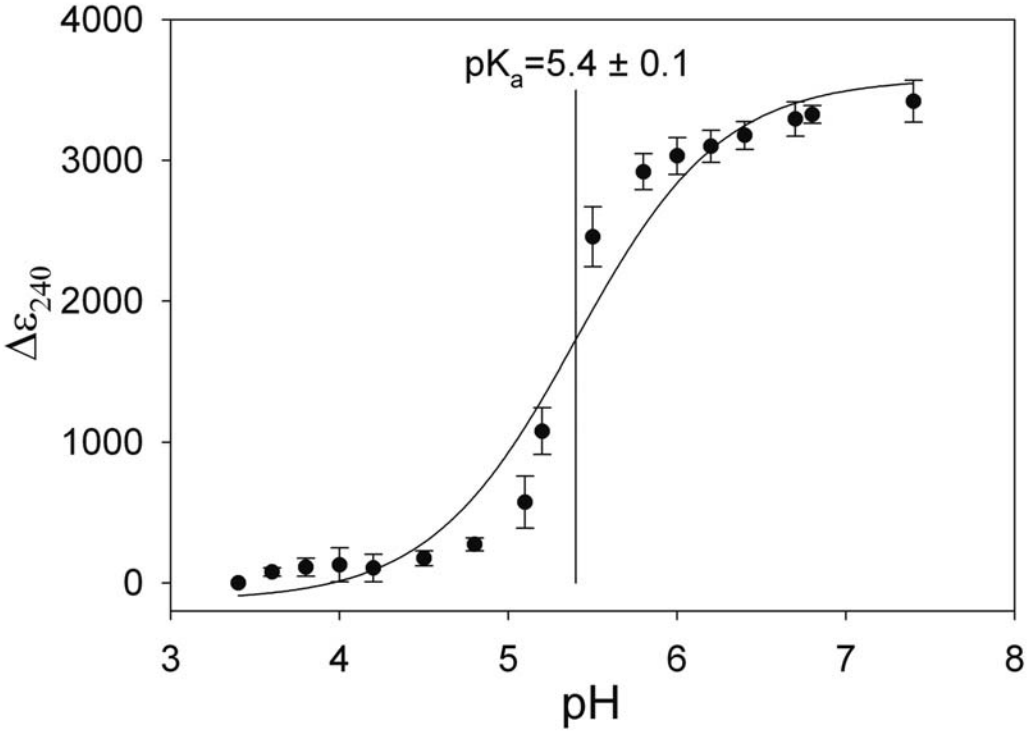

Figure S1: C106 pK_a is unchanged by elevation of ionic strength in the double buffer. The pK_a of C106 in human DJ-1 was determined by measuring the change in the extinction coefficient at 240 nm ($\Delta\varepsilon_{240}$) as a function of pH in 10 mM sodium citrate-sodium phosphate buffer supplemented by 100 mM NaCl. The $\Delta\varepsilon_{240}$ value is calculated by subtraction of the ε_{240} measured at the lowest pH from all other measured ε_{240} values. C106 has a pK_a=5.4±0.1 in this buffer, which is identical to the pK_a measured in the double buffer alone (Figure 2A). Data were measured in triplicate and the standard deviation about the mean values is indicated with error bars.

PDB code	atom 1	res. 1 name	chain	res. 1 no.	atom 2	res. 2 name	chain	res. 2 no.	atom1-atom2 dist. (Å)	H bond angle	dihedral angle
1A4M	SG	CYS	A	153	OD2	ASP	A	181	3.52	117.40	-161.30
1A4M	SG	CYS	B	653	OD2	ASP	B	681	3.45	120.30	-164.70
1A4M	SG	CYS	C	1153	OD2	ASP	C	1181	3.30	123.30	-171.20
1ABR	SG	CYS	A	247	OE2	GLU	A	207	3.85	103.40	-172.50
1AHO	SG	BCYS	A	12	OD1	ASP	A	8	3.64	105.30	17.60
1AJ8	SG	CYS	A	21	OE2	GLU	A	187	3.71	110.30	-160.80
1AJ8	SG	CYS	B	21	OE2	GLU	B	187	3.82	108.90	-168.80
1B5L	SG	CYS	A	29	OE1	GLU	A	142	3.95	109.20	167.90
1B7B	SG	CYS	B	235	OE2	GLU	B	243	3.54	95.10	170.40
1BX7	SG	CYS	A	44	OD1	ASP	A	40	3.97	105.60	20.00
1C6V	SG	CYS	A	65	OE1	GLU	A	92	3.30	106.10	-163.70
1D2E	SG	CYS	A	222	OD2	ASP	A	228	3.41	117.10	-170.90
1D2E	SG	CYS	C	222	OD2	ASP	C	228	3.49	118.30	172.00
1DYO	SG	CYS	A	89	OE2	GLU	A	138	3.96	124.10	176.50
1DYO	SG	CYS	B	89	OE2	GLU	B	138	3.99	123.30	179.90
1E5Q	SG	CYS	A	155	OD2	ASP	A	126	3.95	104.70	163.30
1E5Q	SG	CYS	C	155	OD2	ASP	C	126	3.98	105.00	170.00
1E5Q	SG	CYS	D	155	OD2	ASP	D	126	3.96	104.10	163.20
1E5Q	SG	CYS	F	155	OD2	ASP	F	126	3.91	106.50	167.90
1E5Q	SG	CYS	G	155	OD2	ASP	G	126	3.93	105.30	165.00
1E89	SG	CYS	A	162	OD2	ASP	A	235	3.27	122.80	5.00
1EDZ	SG	CYS	A	115	OE1	GLU	A	117	3.44	108.40	-168.40
1FE0	SG	CYS	A	41	OD1	ASP	A	32	3.87	104.70	-17.60
1FX4	SG	CYS	A	959	OE1	GLU	A	955	3.85	101.60	-161.00
1FXZ	SG	CYS	A	12	OE1	GLU	A	11	3.98	117.40	-179.20
1G2I	SG	CYS	B	300	OE1	GLU	B	215	3.82	104.80	6.70
1G2I	SG	CYS	C	500	OE1	GLU	C	415	3.90	101.90	7.60
1G2I	SG	CYS	A	100	OE2	GLU	A	15	3.97	102.90	-8.80
1G2I	SG	CYS	B	300	OE2	GLU	B	215	3.93	99.10	-6.30
1G2I	SG	CYS	C	500	OE2	GLU	C	415	3.89	102.00	-7.60
1G8M	SG	CYS	A	288	OE2	GLU	A	284	3.77	118.00	169.00
1G8M	SG	CYS	B	288	OE2	GLU	B	284	3.85	116.90	169.80
1GG4	SG	CYS	B	871	OE2	GLU	B	867	3.42	94.80	-178.90
1GXC	SG	CYS	G	124	OD2	ASP	G	126	2.92	119.90	-163.60
1GYC	SG	CYS	A	117	OD1	ASP	A	456	3.71	110.20	163.20
1H2B	SG	CYS	A	112	OD1	ASP	A	109	3.85	120.00	7.60
1H2B	SG	CYS	B	112	OD1	ASP	B	109	3.97	122.40	12.70
1HCN	SG	CYS	B	26	OE2	GLU	B	19	3.42	100.30	-169.80
1HZ4	SG	CYS	A	174	OE2	GLU	A	133	3.41	115.00	169.00
1IZN	SG	CYS	C	157	OE2	GLU	C	176	3.96	108.10	178.60
1JVB	SG	CYS	A	112	OE2	GLU	A	98	3.49	99.00	174.60
1JVN	SG	CYS	B	470	OD2	ASP	B	481	3.63	108.80	179.60
1KHU	SG	CYS	C	310	OD1	ASP	C	297	3.14	122.60	18.40
1KHU	SG	CYS	D	310	OD1	ASP	D	297	3.15	120.20	15.80
1KNW	SG	CYS	A	26	OD2	ASP	A	299	3.50	109.90	0.20
1KYA	SG	CYS	A	117	OD1	ASP	A	456	3.66	105.80	163.40
1KYA	SG	CYS	B	117	OD1	ASP	B	456	3.66	105.50	162.70
1KYA	SG	CYS	C	117	OD1	ASP	C	456	3.67	106.00	164.00
1KYA	SG	CYS	D	117	OD1	ASP	D	456	3.57	107.90	162.90
1L6J	SG	CYS	A	99	OE1	GLU	A	402	2.95	121.10	17.40

1LP3	SG	CYS	A	224	OD2	ASP	A	146	2.80	104.10	17.90
1MKM	SG	CYS	B	196	OD2	ASP	B	186	3.73	116.00	-164.90
1N82	SG	CYS	A	182	OE2	GLU	A	181	3.27	120.60	165.90
1N82	SG	BCYS	B	1182	OE2	GLU	B	1181	2.97	124.40	167.30
1NEK	SG	CYS	B	75	OD2	ASP	B	63	3.17	122.70	-14.80
1NFG	SG	CYS	A	240	OE2	GLU	A	242	3.91	97.50	-165.10
1NFG	SG	CYS	B	240	OE2	GLU	B	242	3.91	97.50	-165.10
1NFG	SG	CYS	C	240	OE2	GLU	C	242	3.91	97.50	-165.10
1NFG	SG	CYS	D	240	OE2	GLU	D	242	3.91	97.50	-165.00
1NOZ	SG	CYS	B	169	OE2	GLU	B	170	3.18	97.40	179.20
1NSC	SG	CYS	A	86	OD2	ASP	A	416	3.96	101.30	175.00
1NSC	SG	CYS	B	86	OD2	ASP	B	416	3.96	102.30	175.90
1O7F	SG	CYS	A	18	OD1	ASP	A	30	3.46	107.90	161.50
1OHF	SG	CYS	B	552	OD2	ASP	C	548	3.46	113.00	11.20
1OI4	SG	CYS	B	325	OE2	GLU	B	238	3.49	112.50	11.40
1OR8	SG	CYS	A	85	OD1	ASP	A	76	3.47	105.80	-170.40
1OUO	SG	CYS	A	93	OD1	ASP	A	106	3.43	105.10	-169.00
1P35	SG	CYS	B	266	OE2	GLU	B	79	3.89	96.50	170.00
1P35	SG	CYS	C	266	OE2	GLU	C	79	3.96	104.60	164.00
1PDU	SG	CYS	B	339	OD1	ASP	B	336	3.85	96.30	-19.80
1PGS	SG	CYS	A	231	OD1	ASP	A	247	3.66	123.90	-174.10
1QDM	SG	CYS	A	37S	OE1	GLU	A	73S	3.53	124.00	160.00
1QH4	SG	CYS	A	141	OE2	GLU	A	150	3.41	106.20	-6.00
1QH4	SG	CYS	B	141	OE2	GLU	B	150	3.47	102.10	-5.20
1QH4	SG	CYS	C	141	OE2	GLU	C	150	3.42	107.20	-4.30
1QH4	SG	CYS	D	141	OE2	GLU	D	150	3.40	105.90	-4.00
1QJ4	SG	CYS	A	161	OD2	ASP	A	234	3.36	116.10	8.30
1QUB	SG	CYS	A	306	OE2	GLU	A	292	3.41	103.60	160.90
1R9D	SG	CYS	A	26	OE2	GLU	A	28	3.85	108.00	-165.30
1R9D	SG	CYS	B	26	OE2	GLU	B	28	3.93	105.10	-166.90
1RQB	SG	CYS	A	216	OD2	ASP	A	185	3.77	113.80	179.50
1RW7	SG	CYS	A	138	OE2	GLU	A	30	3.23	116.50	17.70
1RZU	SG	CYS	A	57	OE1	GLU	A	72	3.40	116.50	-167.90
1S3G	SG	CYS	A	130	OD1	ASP	A	153	3.19	116.70	-6.40
1S4E	SG	CYS	A	282	OE2	GLU	A	284	3.60	112.40	-163.50
1S4E	SG	CYS	B	282	OE2	GLU	B	284	3.49	109.20	-170.80
1S4E	SG	CYS	E	282	OE2	GLU	E	284	3.38	113.50	-168.10
1S4E	SG	CYS	F	282	OE2	GLU	F	284	3.33	117.80	-166.50
1S4E	SG	CYS	H	282	OE2	GLU	H	284	3.54	111.80	-167.50
1S6Y	SG	CYS	A	172	OE2	GLU	A	358	3.85	119.80	2.50
1SI5	SG	CYS	H	561	OD1	ASP	H	558	3.98	113.90	173.40
1SVV	SG	CYS	B	51	OD1	ASP	B	48	3.33	120.10	-19.10
1SVV	SG	CYS	A	51	OD2	ASP	A	48	3.26	113.10	-16.50
1TJO	SG	CYS	C	30	OD1	ASP	C	145	3.64	116.90	-162.10
1TJO	SG	CYS	D	30	OD1	ASP	D	145	3.64	120.80	-160.90
1U1J	SG	CYS	A	636	OD2	ASP	A	409	3.79	116.70	-170.80
1U6K	SG	CYS	A	48	OD1	ASP	A	45	3.23	109.10	-17.20
1ULZ	SG	CYS	A	228	OE1	GLU	A	295	3.49	122.00	-167.80
1V10	SG	CYS	A	117	OD1	ASP	A	455	3.17	111.40	172.30
1VPR	SG	CYS	A	972	OE1	GLU	A	1141	3.82	106.40	-175.10
1VQ2	SG	CYS	A	19	OE1	GLU	A	102	3.73	97.70	15.10
1VQ2	SG	CYS	A	19	OE2	GLU	A	102	3.65	102.20	-15.70
1W07	SG	ACYS	B	376	OE2	GLU	B	372	3.56	123.10	172.60

1WN0	SG	CYS	A	105	OD1	ASP	A	76	3.73	112.70	-171.20
1XFK	SG	CYS	A	52	OE2	GLU	A	128	3.58	118.70	166.70
1XG2	SG	CYS	B	114	OD2	ASP	B	132	3.41	110.90	-15.80
1XKL	SG	CYS	A	164	OD2	ASP	A	237	3.13	112.20	5.90
1XKL	SG	CYS	B	164	OD2	ASP	B	237	3.18	116.20	-2.00
1XKL	SG	CYS	C	164	OD2	ASP	C	237	3.18	113.80	2.20
1XKL	SG	CYS	D	164	OD2	ASP	D	237	3.16	111.10	0.10
1Y1N	SG	CYS	A	104	OD1	ASP	A	78	3.49	110.60	170.30
1YM3	SG	CYS	A	107	OD1	ASP	A	53	3.87	108.00	11.50
1YO8	SG	CYS	A	799	OE2	GLU	A	795	3.96	104.80	166.70
1YOX	SG	CYS	A	179	OD2	ASP	A	176	3.44	118.30	-176.30
1YOX	SG	CYS	E	179	OD2	ASP	E	176	3.96	103.80	174.50
1YRL	SG	CYS	C	156	OE2	GLU	C	160	3.37	112.60	-178.60
1Z08	SG	CYS	A	29	OD1	ASP	A	100	3.52	110.70	-161.70
1Z08	SG	CYS	B	29	OD1	ASP	B	100	3.59	109.00	-162.10
1Z08	SG	CYS	D	29	OD1	ASP	D	100	3.60	112.30	-162.70
2A1F	SG	CYS	D	170	OD2	ASP	D	169	3.97	109.00	-179.60
2AB0	SG	BCYS	A	106	OE2	GLU	A	17	3.02	116.70	12.90
2AB0	SG	ACYS	B	106	OE2	GLU	B	17	3.01	116.10	13.50
2B34	SG	CYS	C	114	OE2	GLU	C	110	3.17	109.70	164.30
2B3H	SG	CYS	A	202	OD1	ASP	A	176	3.56	115.70	166.50
2C1X	SG	CYS	A	368	OE2	GLU	A	383	3.90	114.20	-163.50
2CMZ	SG	CYS	A	224	OE1	GLU	A	138	3.80	119.60	-160.00
2D0V	SG	CYS	A	103	OE2	GLU	A	177	3.77	123.50	-171.00
2D2M	SG	CYS	D	2	OE2	GLU	D	1	3.61	111.90	-174.60
2DJF	SG	CYS	C	424	OE2	GLU	C	423	3.65	122.00	-161.30
2DSC	SG	CYS	A	131	OD1	ASP	B	194	3.90	111.40	160.70
2E11	SG	CYS	A	130	OE2	GLU	A	159	3.23	123.00	-6.60
2E11	SG	CYS	B	130	OE2	GLU	B	159	3.20	124.10	-7.60
2E11	SG	CYS	D	130	OE2	GLU	D	159	3.44	118.30	-6.50
2EA9	SG	CYS	A	82	OE1	GLU	A	93	3.98	117.30	-167.70
2EER	SG	CYS	A	112	OE2	GLU	A	98	3.58	99.60	-166.00
2EER	SG	CYS	B	112	OE2	GLU	B	98	3.77	98.30	-171.60
2ETL	SG	CYS	B	152	OE2	GLU	B	7	3.08	107.40	-165.30
2EZ9	SG	CYS	A	475	OD1	ASP	A	499	3.90	103.80	174.50
2EZ9	SG	CYS	B	475	OD1	ASP	B	499	3.95	104.00	174.90
2FEX	SG	CYS	A	101	OE2	GLU	A	16	3.17	121.50	13.50
2FEX	SG	CYS	C	101	OE2	GLU	C	16	3.22	121.70	17.90
2FUV	SG	ACYS	B	519	OE2	GLU	B	532	3.85	95.30	170.20
2G50	SG	CYS	A	473	OD2	ASP	A	475	3.27	118.00	-161.80
2G50	SG	CYS	G	473	OD2	ASP	G	475	3.40	117.90	-169.70
2G50	SG	CYS	H	473	OD2	ASP	H	475	3.42	116.00	-165.00
2GE3	SG	CYS	C	86	OE2	GLU	C	123	3.96	116.10	19.10
2GEL	SG	CYS	G	13	OE1	GLU	G	28	3.73	106.30	174.30
2GJ2	SG	CYS	A	46	OE1	GLU	D	31	3.20	103.90	3.80
2GJ2	SG	CYS	B	46	OE1	GLU	C	31	3.55	114.00	4.10
2GJ2	SG	CYS	C	46	OE1	GLU	B	31	3.13	123.50	2.90
2GJ2	SG	CYS	D	46	OE1	GLU	A	31	2.90	104.40	-8.30
2GL6	SG	CYS	A	238	OD1	ASP	A	96	3.69	101.50	-169.60
2GL6	SG	CYS	B	238	OD1	ASP	B	96	3.46	104.80	-170.70
2GL6	SG	CYS	C	238	OD1	ASP	C	96	3.59	108.10	-166.90
2GL6	SG	CYS	D	238	OD1	ASP	D	96	3.41	112.60	-173.50
2GL6	SG	CYS	F	238	OD1	ASP	F	96	3.56	102.00	-163.10

2GL6	SG	CYS	G	238	OD1	ASP	G	96	3.57	106.40	-172.70
2GL6	SG	CYS	H	238	OD1	ASP	H	96	3.99	95.70	-163.50
2GYQ	SG	CYS	A	79	OE1	GLU	B	88	3.41	123.30	14.10
2GYQ	SG	CYS	B	79	OE1	AGLU	A	88	3.21	106.00	7.60
2GYQ	SG	CYS	B	79	OE2	AGLU	A	88	3.38	95.00	-7.00
2H0Q	SG	CYS	A	374	OE1	GLU	A	603	3.81	117.10	165.90
2H4C	SG	CYS	C	29	OD1	ASP	C	42	3.69	120.50	170.90
2H4C	SG	CYS	H	29	OD1	ASP	H	42	3.92	115.20	-174.70
2H5E	SG	CYS	B	175	OD1	ASP	B	147	3.99	118.90	167.90
2H5U	SG	CYS	A	117	OD1	ASP	A	456	3.48	107.20	172.60
2H63	SG	CYS	C	74	OE2	GLU	C	97	3.32	122.40	-163.60
2H63	SG	CYS	D	74	OE2	GLU	D	97	3.67	119.20	164.30
2HDY	SG	CYS	A	359	OE1	GLU	A	331	3.12	113.60	179.90
2HDY	SG	CYS	B	359	OE1	GLU	B	331	3.28	106.30	-172.00
2HFK	SG	CYS	B	48	OE1	GLU	B	50	3.98	106.00	-166.50
2HL0	SG	CYS	A	127	OE2	GLU	A	134	3.69	104.90	-162.20
2HR7	SG	CYS	B	8	OE2	GLU	B	6	3.44	111.90	-178.90
2HRC	SG	CYS	A	360	OE2	GLU	A	324	3.07	103.90	-176.10
2HRG	SG	BCYS	A	117	OD2	ASP	A	453	3.66	111.00	170.70
2HZH	SG	CYS	A	117	OD2	ASP	A	456	3.95	104.80	179.00
2IV2	SG	ACYS	X	588	OD2	ASP	X	404	3.49	120.60	169.00
2J1G	SG	CYS	A	232	OD1	ASP	A	226	3.36	108.30	178.90
2JDQ	SG	CYS	A	203	OD2	ASP	A	199	3.60	113.60	-167.40
2JFK	SG	CYS	C	593	OD2	ASP	C	591	3.32	122.60	171.90
2NPI	SG	CYS	A	87	OD1	ASP	A	89	3.83	104.00	-168.50
2NTE	SG	CYS	B	743	OE1	GLU	B	740	3.90	114.30	176.30
2NYT	SG	CYS	A	131	OE1	GLU	A	60	3.65	123.20	-11.60
2NYT	SG	CYS	C	131	OE1	GLU	C	60	3.68	121.60	-10.40
2O1S	SG	CYS	B	330	OE1	GLU	B	354	3.76	118.00	-163.60
2O2P	SG	ACYS	A	707	OE1	GLU	A	673	3.85	96.60	-0.60
2O2P	SG	ACYS	B	707	OE1	GLU	B	673	3.79	97.90	0.80
2O2P	SG	ACYS	C	707	OE1	GLU	C	673	3.93	96.50	2.80
2O2P	SG	ACYS	D	707	OE1	GLU	D	673	3.78	99.80	1.30
2O2P	SG	ACYS	A	707	OE2	GLU	A	673	3.64	106.80	0.70
2O2P	SG	ACYS	B	707	OE2	GLU	B	673	3.64	105.60	-0.90
2O2P	SG	ACYS	C	707	OE2	GLU	C	673	3.71	107.50	-3.10
2O2P	SG	ACYS	D	707	OE2	GLU	D	673	3.70	104.10	-1.40
2O55	SG	CYS	A	49	OE2	GLU	A	53	3.31	112.00	-164.90
2OME	SG	CYS	A	124	OE2	GLU	A	340	3.49	114.90	-166.30
2OME	SG	CYS	H	124	OE2	GLU	H	340	3.48	112.50	-174.70
2OO4	SG	CYS	A	1496	OD2	ASP	A	1492	3.93	118.90	163.00
2OO4	SG	CYS	A	1534	OD2	ASP	A	1530	3.83	118.20	169.70
2OO4	SG	CYS	B	1496	OE2	GLU	B	1482	3.35	114.80	160.80
2OO7	SG	CYS	A	130	OD1	ASP	A	153	3.28	116.20	-10.40
2OO7	SG	CYS	B	130	OD1	ASP	B	153	3.30	115.20	-15.00
2OY0	SG	CYS	B	88	OD1	ASP	B	79	3.67	110.00	-172.40
2OY9	SG	CYS	B	73	OE2	GLU	B	66	3.62	123.30	-168.80
2P0I	SG	CYS	A	190	OD2	ASP	A	192	3.61	107.40	-167.50
2P26	SG	CYS	A	398	OE2	GLU	A	16	3.54	106.80	167.20
2P2W	SG	CYS	A	17	OE2	GLU	A	175	3.75	112.10	-169.10
2PLW	SG	CYS	A	37	OD2	ASP	A	28	3.29	124.40	172.60
2POZ	SG	CYS	C	383	OE2	GLU	C	57	3.66	104.30	174.40
2POZ	SG	CYS	G	383	OE2	GLU	G	57	3.93	102.30	161.40

2QBX	SG	CYS	A	105	OE2	GLU	A	117	3.88	102.60	168.50
2QBX	SG	CYS	B	105	OE2	GLU	B	117	3.46	101.60	163.40
2QH9	SG	CYS	B	18	OD2	ASP	B	11	3.94	110.10	162.40
2QT3	SG	CYS	A	300	OE2	GLU	A	324	3.58	116.80	177.80
2QT3	SG	CYS	B	300	OE2	GLU	B	324	3.61	118.40	177.20
2QZU	SG	CYS	A	158	OD2	ASP	A	136	3.40	119.50	-18.60
2RDL	SG	CYS	A	22	OE2	GLU	A	157	3.24	103.20	165.00
2RK3	SG	CYS	A	106	OE2	GLU	A	18	3.28	110.30	15.00
2TOD	SG	CYS	A	135	OD2	ASP	A	137	3.41	118.90	-169.20
2TOD	SG	CYS	B	135	OD2	ASP	B	137	3.37	116.20	177.50
2TOD	SG	CYS	C	135	OD2	ASP	C	137	3.31	116.10	178.10
2TOD	SG	CYS	D	135	OD2	ASP	D	137	3.28	123.30	-176.20
2UX0	SG	CYS	D	518	OE2	GLU	D	500	3.52	123.00	-167.50
2UX0	SG	CYS	F	518	OE2	GLU	F	500	3.67	113.80	-169.40
2V3V	SG	CYS	A	350	OE1	GLU	A	156	3.54	106.30	11.40
2V3V	SG	CYS	A	350	OE2	GLU	A	156	3.75	95.90	-10.30
2V90	SG	CYS	B	323	OE2	GLU	B	253	3.79	103.60	-165.20
2ZBA	SG	CYS	A	298	OE1	GLU	A	296	3.75	109.60	-166.10
3B89	SG	CYS	A	20	OD2	ASP	A	22	3.88	103.20	174.40
3B98	SG	CYS	B	348	OE1	GLU	B	354	3.96	111.70	-164.90
3BGE	SG	BCYS	A	319	OE2	GLU	A	327	2.91	96.70	-178.10
3BRU	SG	CYS	A	125	OE2	GLU	A	187	3.12	113.90	-9.70
3BRU	SG	CYS	B	125	OE2	GLU	B	187	3.06	118.50	-2.10
3BV6	SG	CYS	D	45	OD2	ASP	D	121	3.54	119.10	171.80
3BV6	SG	CYS	F	45	OD2	ASP	F	121	3.61	116.60	163.40
3C8X	SG	CYS	A	105	OE2	GLU	A	117	3.86	97.40	-170.20

Table S2: Candidate D/E-C dyads in the 4/15/08 release of the PDB. A search for all potential D/E-C candidate dyads was performed on the 11,765 non-redundant crystal structures determined at 3.0 Å or better in the 4/15/08 release of the PDB. This search required that at least one carboxylic acid oxygen from aspartic or glutamic acid be within 4.0 Å of the sulfur atom of cysteine, that the C(δ/γ)-O(δ/ε;1/2)-Sγ hydrogen bond angle be 109.5±15°, and that the O(δ/ε;1/2)–C(δ/γ)-O(δ/ε;1/2)–Sγ dihedral angle be either 0±20° or 180±20°. Each identified interaction is tabulated above, including multiple instances of such interactions in the same set of coordinates.