

Table 1. ^{15}N chemical shifts of hyperfine signals from wild-type and mutant *Clostridium pasteurianum* rubredoxin (CpRd)

Oxidized (Fe^{III}) proteins									
CpRd variant	^{15}N chemical shifts, ppm								
	C6/C39	T7	C9/C42	G10/G43	Y11	P40	L41	V8	V44
Wild type	613/588	358	-34/-79	327/312	633	407	542	525	346
V44G	599/573	345	-53/-94	318/286	638	410	560	497	791
V44A	604/576	341	-61/-71	318/311	664	406	571	517	626
V44I	628/586	368	-12/-102	320/311	612	414	569	529	453
V44L	610/592	346	3/-147	316/304	610	409	534	451	451
V8G	627/596	402	-28/-28	333/306	818	430	627	766	327
V8A	626/592	360	44/-49	333/328	697	414	573	562	368
V8I	622/598	367	-35/-83	326/314	641	410	545	531	343
V8L	622/598	382	12/-75	333/317	647	410	551	511	348
V8G/V44G	625/575	338	-16/-64	321/263	733	421	625	703/526	

Reduced (Fe^{II}) proteins									
CpRd variant	^{15}N chemical shifts, ppm								
	C6/C39	T7	C9/C42	G10/G43	Y11	P40	L41	V8	V44
Wild type	322/294	279	-1/-25	223/222	394	278	437	498	270
V44G	297/289	272	-28/-62	228/214	425	279	446	450	482
V44A	298/277	266	-30/-30	214/214	397	277	466	484	386
V44I	324/288	288	4/-29	229/217	370	279	449	511	337
V44L	314/298	310	20/-45	220/218	377	281	459	493	327
V8G	325/297	256	-20/-48	205/204	393	293	516	547	248
V8A	320/288	260	48/11	214/211	382	282	462	482	243
V8I	321/296	283	0/-25	223/220	400	277	433	497	267
V8L	316/297	285	41/-17	221/216	397	277	437	487	256
V8G/V44G	304/286	243	-27/-42	207/195	406	290	521	448/384	

^{15}N chemical shifts are at the residue positions specified in the first line for wild-type CpRd.