

Cu,Zn-Superoxide Dismutase without Zn is Folded but Catalytically Inactive

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Supporting Information

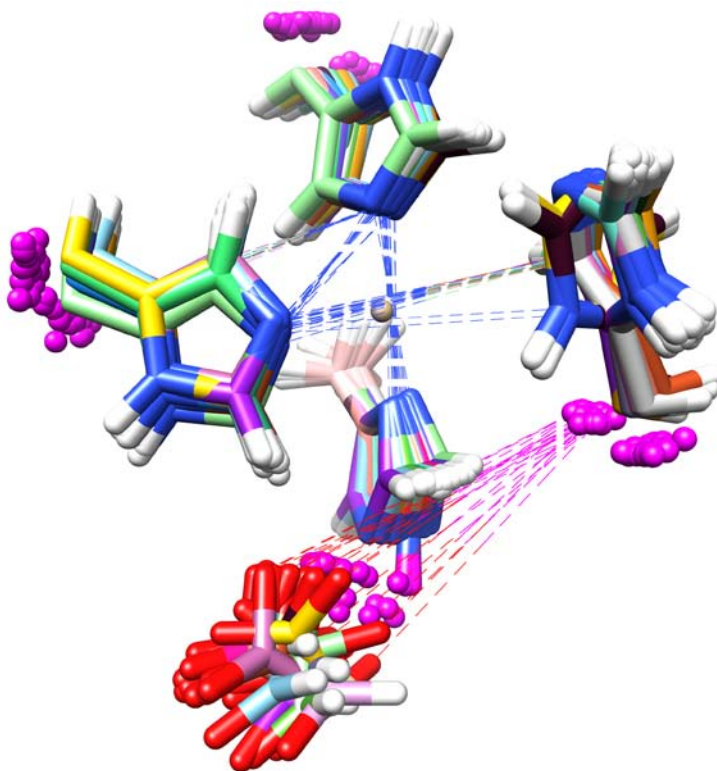


Figure S1. Overlaid structures of the active site of Zn-less WT-SOD1 from the QM/DMD iterations 20-50. The center atom is Cu, and clockwise from the bottom the residues are D124, H63, H48, H120, and H46. The purple atoms are added hydrogens added during the QM phases of QM/DMD. The dashed lines represent the position of the residues along the backbone of the SOD1 variant.

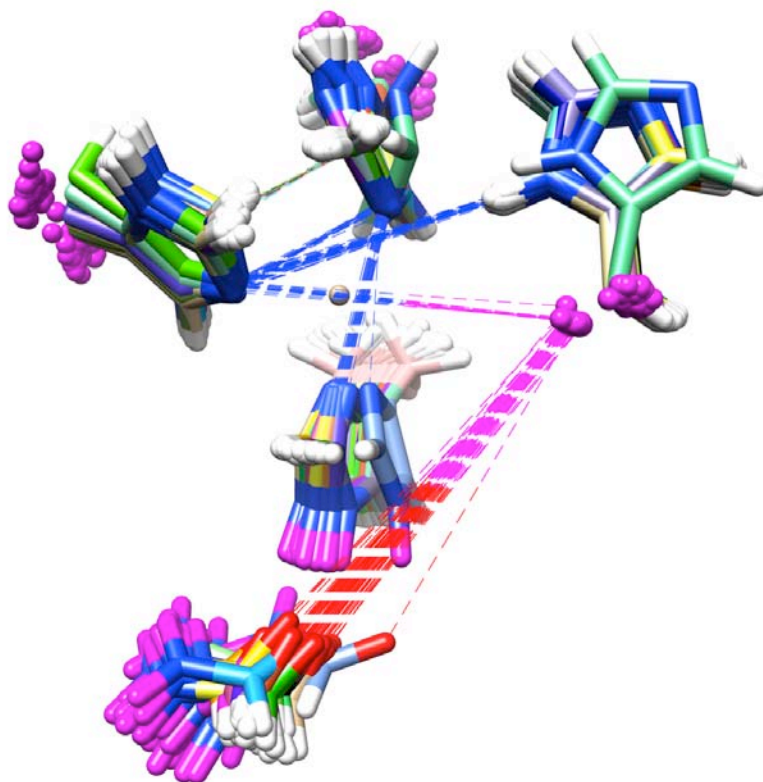


Figure S2. Overlaid structures of the active site of Zn-less D124N-SOD1 from the QM/DMD iterations 50-100. The center atom is Cu, and clockwise from the bottom the residues are D124, H63, H48, H120, and H46. The purple atoms are added hydrogens added during the QM phases of QM/DMD. The dashed lines represent the position of the residues along the backbone of the SOD1 variant.

XYZ coordinates for SOD1 structures with Natural Bond Order partial charges in the 5th column.

Structures were obtained from RI-TPSS/def2-SVP (def2-TZVPP for Cu and Zn), and charges were obtained from single point energy calculations using RI-TPSSH. A suggested viewing option is to save the xyz coordinates in a .xyz file and open using the Jmol program.

The SOD1 variants are wildtype-SOD1 (WT-SOD1), Zn-deficient WT-SOD1, and the Zn-deficient D124N-SOD1.

WT-SOD1

H	98.0259725	98.4159724	99.6329720	0.26494
C	97.3719727	97.4519726	99.1939721	-0.66369
C	96.0391908	97.9926152	98.7737200	0.12448
N	95.2415207	97.3230981	97.8542726	-0.65140
C	95.3866574	99.1694234	99.1031499	-0.02611
C	94.1422296	98.0550484	97.6505442	0.26422
N	94.2016416	99.1748244	98.3933426	-0.55652
H	97.9244745	97.0533101	98.3275296	0.21781
H	97.3028694	96.6825285	99.9814162	0.23847
H	95.6821775	99.9936128	99.7504739	0.24783
H	93.3198946	97.8300472	96.9731178	0.23895
H	93.4499436	99.8949448	98.2709739	0.48220
H	100.1879719	92.5429740	100.1579719	0.25023
C	100.0399719	92.4159741	99.0909722	-0.64346
C	98.6955641	92.8260838	98.5416905	0.14444
N	97.6387983	91.9359142	98.3694461	-0.56061
C	98.2121145	94.0191648	98.0233500	-0.04164
C	96.5926395	92.5804049	97.7869275	0.25894
N	96.9063980	93.8585748	97.5678518	-0.65691
H	97.6424524	90.9543809	98.6485653	0.44534
H	100.2369077	91.3552714	98.8578574	0.23234
H	100.8247136	93.0113686	98.5954823	0.24594
H	98.7288506	94.9742463	97.9496825	0.23229
H	95.6279140	92.1143040	97.5872007	0.23292
H	95.6809731	93.0629739	102.3949712	0.23120
C	94.9769733	93.8629736	102.5239712	-0.64491
C	94.5885012	94.4809435	101.2528855	0.16701
N	93.4777318	95.3033774	101.0571961	-0.73562
C	95.2406203	94.3139778	100.0549495	-0.05692
C	93.5140050	95.5924853	99.7323296	0.27465
N	94.5567681	94.9899636	99.0774228	-0.65523
H	94.0999404	93.4545562	103.0579420	0.23975
H	95.4313146	94.6027184	103.2138281	0.23934
H	96.1416711	93.7376800	99.8720819	0.20977
H	92.7799098	96.2145000	99.2226844	0.21013
H	88.5719751	96.6369729	103.9939708	0.23432

C	88.3389752	96.8259728	102.9569711	-0.63580
C	89.3798973	97.4646534	102.0742236	0.15453
N	90.7007066	97.0548488	101.8321289	-0.74402
C	89.1068898	98.5169200	101.2101246	-0.00536
C	91.1729205	97.8699798	100.8665157	0.25616
N	90.2379399	98.7527174	100.4642794	-0.55711
H	87.4426118	97.4656764	102.9429508	0.24570
H	88.0361413	95.8530922	102.5216691	0.22730
H	88.1924969	99.0903507	101.0653991	0.24877
H	92.1926142	97.8682297	100.4857722	0.20209
H	90.3233675	99.4469427	99.6833934	0.47128
H	93.4499738	95.6629731	107.1719699	0.25183
C	93.6609737	95.1289733	106.2529702	-0.62953
C	92.4090273	94.5143929	105.6505287	0.16929
N	91.9577356	94.5413336	104.3078842	-0.73463
C	91.5258286	93.7172523	106.3574414	-0.01477
C	90.8530667	93.7839443	104.2553886	0.26764
N	90.5661011	93.2748095	105.4719539	-0.55071
H	94.1351099	95.8305764	105.5561519	0.23008
H	94.3848236	94.3271625	106.4848193	0.23184
H	91.5186795	93.4318331	107.4083259	0.24886
H	90.2435427	93.6087605	103.3686533	0.22077
H	89.7729955	92.6742437	105.6969465	0.44951
H	95.3269732	98.8289722	103.4169710	0.23935
C	94.2749735	98.6479723	103.1949710	-0.70971
C	93.5377123	98.0804326	104.3815015	0.82868
O	93.7695438	98.4829199	105.5314763	-0.46441
O	92.6470111	97.1711688	104.1574228	-0.87262
H	93.8173124	99.6170182	102.9267987	0.24735
H	94.1958516	97.9694872	102.3279228	0.19821
H	96.3219730	98.7659723	92.1559741	0.24301
C	95.4649732	98.4989723	92.7429740	-0.64070
C	95.6049656	97.3089202	93.6457999	0.15623
N	95.2115937	96.0215619	93.2951025	-0.55581
C	95.9555837	97.2058014	94.9784623	-0.03470
C	95.3105800	95.2089424	94.3795151	0.25992
N	95.7552380	95.9069758	95.4277526	-0.64726
H	95.2174315	99.3791339	93.3587515	0.24957
H	94.6223843	98.3468477	92.0464323	0.23780
H	96.3038447	97.9904558	95.6459298	0.23918
H	94.8493093	95.7466369	92.3816459	0.44408
H	95.0335180	94.1553732	94.3803433	0.21929
H	90.1079747	102.0409713	95.6749731	0.24577
C	90.8569745	102.1209713	96.4419729	-0.71591
C	91.0348497	100.9372784	97.3685091	0.84956
O	90.1970982	100.6212063	98.2609921	-0.59206

O	92.1229144	100.2674042	97.2896994	-0.66230
H	91.8255784	102.3258745	95.9561716	0.23302
H	90.5814800	102.9962196	97.0581423	0.25147
H	98.8329722	93.3129738	91.6399743	0.22031
C	99.2459721	93.2949738	92.6389740	-0.61643
C	99.0247763	91.9081658	93.2580954	-0.20327
N	99.3743713	90.7945834	92.3484911	-0.62864
C	100.4605230	90.0031994	92.4044103	0.72844
N	101.5315809	90.3604589	93.1382683	-0.78962
N	100.4628680	88.8277825	91.7534681	-0.77559
H	98.7060148	90.5896561	91.6050503	0.42659
H	102.2903783	89.7012629	93.3040294	0.43733
H	101.7279179	91.3401788	93.3317008	0.43133
H	101.3285546	88.3249998	91.5620342	0.43964
H	99.6062362	88.4265201	91.3758106	0.43462
H	100.3193471	93.5401795	92.5614990	0.21909
H	98.7575236	94.0691553	93.2534704	0.23051
H	99.5958280	91.7701848	94.1919008	0.21907
H	97.9603046	91.7682390	93.5167117	0.22613
Cu	95.5522874	95.4350414	97.3948809	1.14415
Zn	92.2075757	95.9158783	102.7332388	1.57112

WT-SOD with superoxide

H	98.0259725	98.4159724	99.6329720	0.24609
C	97.3719727	97.4519726	99.1939721	-0.64841
C	96.0381808	97.9489404	98.7367974	0.12903
N	95.2580846	97.2555626	97.8219801	-0.67579
C	95.3683785	99.1160035	99.0737576	-0.04100
C	94.1527076	97.9820900	97.6229354	0.25888
N	94.1863531	99.1072817	98.3647062	-0.56614
H	97.9438804	97.0219154	98.3556350	0.21939
H	97.2922779	96.6989262	99.9973522	0.23435
H	95.6512934	99.9389348	99.7279003	0.23776
H	93.3287308	97.7392543	96.9531497	0.23015
H	93.4277772	99.8146888	98.2626429	0.47463
H	100.1879719	92.5429740	100.1579719	0.24365
C	100.0399719	92.4159741	99.0909722	-0.64411
C	98.6739564	92.7677535	98.5699693	0.12467
N	97.5686177	91.9276089	98.6884172	-0.57944
C	98.1870812	93.8596169	97.8598247	-0.05214
C	96.4951658	92.5266372	98.0879306	0.20257
N	96.8393262	93.7031682	97.5723063	-0.63111
H	97.5478531	91.0458169	99.2015671	0.44152
H	100.2888649	91.3666958	98.8501498	0.23151
H	100.7877246	93.0526627	98.5909555	0.24428
H	98.7324402	94.7536463	97.5569985	0.23008

H	95.4865561	92.1112527	98.0988307	0.24096
H	95.6809731	93.0629739	102.3949712	0.22217
C	94.9769733	93.8629736	102.5239712	-0.63909
C	94.5089700	94.4778205	101.2716141	0.13307
N	93.3457335	95.2279435	101.1204908	-0.77790
C	95.1196780	94.3688814	100.0509758	-0.06979
C	93.2978125	95.5021062	99.7801083	0.24811
N	94.3476890	94.9925419	99.0996064	-0.66728
H	94.1248978	93.4498677	103.0950890	0.23199
H	95.4498633	94.6052472	103.1993005	0.22546
H	96.0772713	93.9094168	99.8395449	0.19861
H	92.4845323	96.0476309	99.3033276	0.20592
H	88.5719751	96.6369729	103.9939708	0.22930
C	88.3389752	96.8259728	102.9569711	-0.63210
C	89.3693600	97.4881181	102.0791276	0.14179
N	90.6971775	97.0946256	101.8485057	-0.73840
C	89.0880842	98.5350003	101.2172316	-0.02608
C	91.1669402	97.9126688	100.8874032	0.25132
N	90.2232346	98.7851266	100.4793362	-0.55960
H	87.4288569	97.4465865	102.9420378	0.23858
H	88.0571208	95.8477668	102.5188424	0.22175
H	88.1709807	99.1024946	101.0686914	0.24119
H	92.1843092	97.9090678	100.4993283	0.20917
H	90.2994070	99.4765358	99.6965465	0.46716
H	93.4499738	95.6629731	107.1719699	0.24436
C	93.6609737	95.1289733	106.2529702	-0.62743
C	92.4046855	94.5075855	105.6654619	0.16332
N	91.9417704	94.5536909	104.3299729	-0.72097
C	91.5296175	93.7039842	106.3712473	-0.03336
C	90.8385726	93.8002659	104.2747560	0.26069
N	90.5590309	93.2750475	105.4876200	-0.55555
H	94.1172573	95.8355250	105.5495965	0.23313
H	94.3948135	94.3341457	106.4761917	0.22579
H	91.5286376	93.4060584	107.4183822	0.24115
H	90.2253648	93.6361179	103.3884857	0.21837
H	89.7675152	92.6731638	105.7098449	0.44210
H	95.3269732	98.8289722	103.4169710	0.23443
C	94.2749735	98.6479723	103.1949710	-0.70635
C	93.5321596	98.0923869	104.3913208	0.82744
O	93.7855810	98.5243800	105.5289849	-0.48284
O	92.6397141	97.1869265	104.1762683	-0.88166
H	93.8170311	99.6128251	102.9131522	0.24189
H	94.1981609	97.9587502	102.3358204	0.20291
H	96.3219730	98.7659723	92.1559741	0.23606
C	95.4649732	98.4989723	92.7429740	-0.63977
C	95.5390250	97.2587754	93.5787602	0.14278

N	95.0982196	96.0096681	93.1541092	-0.56219
C	95.8150109	97.0837910	94.9202537	-0.03248
C	95.0892759	95.1575367	94.2143669	0.26348
N	95.5145483	95.7864084	95.3099404	-0.65243
H	95.2662290	99.3537924	93.4103965	0.24584
H	94.6060147	98.4327517	92.0514243	0.23250
H	96.1682031	97.8208015	95.6366518	0.23820
H	94.7611402	95.7921957	92.2170299	0.43527
H	94.7348247	94.1297185	94.1673128	0.21172
H	90.1079747	102.0409713	95.6749731	0.23905
C	90.8569745	102.1209713	96.4419729	-0.71430
C	90.9782083	100.9390914	97.3911557	0.84294
O	90.1065380	100.6802577	98.2708074	-0.59100
O	92.0281550	100.2143749	97.3361346	-0.65715
H	91.8343599	102.2802480	95.9578809	0.22783
H	90.6042546	103.0155927	97.0386530	0.24373
H	98.8329722	93.3129738	91.6399743	0.21498
C	99.2459721	93.2949738	92.6389740	-0.63861
C	99.2304018	91.8818719	93.2666482	-0.21720
N	98.2707216	91.7413265	94.3763397	-0.61908
C	96.9489503	91.5502322	94.2610160	0.73011
N	96.3339728	91.6420147	93.0648551	-0.79538
N	96.2120298	91.2276673	95.3398693	-0.80607
H	98.6109776	91.9483004	95.3164509	0.42545
H	95.4303385	91.1911750	92.9328713	0.43599
H	96.8278961	91.9581202	92.2345316	0.42686
H	95.2951614	91.6989185	95.4884471	0.44052
H	96.7242587	91.0886057	96.2094819	0.40703
H	100.2807836	93.6645549	92.5518875	0.24448
H	98.6929955	94.0118848	93.2701145	0.22033
H	99.0035873	91.0979091	92.5232719	0.22792
H	100.2130064	91.6256065	93.6908038	0.24423
Cu	95.1495216	95.2789747	97.2635943	1.16451
Zn	92.2027446	95.9255726	102.7422364	1.57352
O	93.7283279	93.8125345	96.5592738	-0.19484
O	93.8884312	92.6637638	96.0247935	-0.22898

Zn-deficient WT-SOD1

H	98.2329724	98.8829722	98.8599722	0.22888
C	97.5949726	98.1169724	98.4249724	-0.63428
C	96.7213864	98.8360620	97.4227107	0.10451
N	96.2947117	98.2820308	96.2268948	-0.75001
C	96.1842989	100.1242489	97.4824899	-0.01808
C	95.5141865	99.2438739	95.6438935	0.23656
N	95.4308447	100.3660516	96.3592551	-0.60062
H	98.2324354	97.3650710	97.9278813	0.20761

H	97.0096650	97.6220290	99.2217803	0.21708
H	96.3010393	100.8752976	98.2663025	0.21131
H	94.9921273	99.0892923	94.6967092	0.18495
H	94.1059183	101.2783440	96.1294280	0.50319
H	99.5549720	93.2789738	99.5349721	0.24171
C	99.8049720	92.9989739	98.5319723	-0.63526
C	99.0286227	93.7113763	97.4835957	0.13803
N	99.3306878	93.5945564	96.1317291	-0.56063
C	97.9370221	94.5467254	97.5279311	-0.04019
C	98.4481300	94.3480124	95.4157829	0.25553
N	97.5865238	94.9351630	96.2401255	-0.66258
H	100.0991945	93.0503885	95.7457185	0.42251
H	100.8883578	93.1864373	98.4077196	0.22923
H	99.6595009	91.9040073	98.4539791	0.22868
H	97.3796768	94.8957088	98.3956046	0.24033
H	98.4744637	94.4567552	94.3321355	0.20988
H	94.8539734	93.2939738	100.5529718	0.22372
C	93.9909736	93.9119736	100.3509718	-0.63243
C	94.1850768	94.8469972	99.1923691	0.11746
N	93.7976101	96.1861711	99.1641005	-0.56762
C	94.7187455	94.6134913	97.9393076	-0.06840
C	94.1106872	96.7031135	97.9539838	0.27925
N	94.6871211	95.7733397	97.1785800	-0.70617
H	93.4213684	96.8257812	99.8972394	0.47076
H	93.1296844	93.2395893	100.1807274	0.22990
H	93.7709533	94.4780566	101.2723014	0.23051
H	95.1380927	93.6872183	97.5466683	0.21296
H	93.9244769	97.7484336	97.6947027	0.25002
H	87.3029755	97.3189727	102.5829712	0.23461
C	87.5759754	97.2079727	101.5499715	-0.63061
C	87.7339110	98.4860144	100.7935195	0.16751
N	88.8735695	99.2595714	100.7569825	-0.58230
C	86.8381728	99.1531074	99.9288212	-0.00946
C	88.6288316	100.3088211	99.9126397	0.28044
N	87.4003792	100.2717368	99.3949453	-0.52611
H	89.8057528	99.1273421	101.1976838	0.45857
H	88.5097268	96.6199672	101.5324613	0.22350
H	86.7857576	96.6032447	101.0745006	0.22961
H	85.8170844	98.8458436	99.6890228	0.20946
H	89.3920340	101.0628559	99.7116409	0.20915
H	92.2349741	97.7739725	104.4129707	0.23015
C	92.3029741	97.2599727	103.4549710	-0.64632
C	91.2695969	96.2010837	103.2719493	0.12868
N	90.9994348	95.6794807	102.0144395	-0.59210
C	90.4332782	95.4871506	104.1220558	-0.04902
C	90.0337148	94.7069203	102.1627956	0.20216

N	89.6767683	94.5679653	103.4268187	-0.51769
H	91.3666729	96.0609031	101.1426609	0.41615
H	92.1912618	98.0316508	102.6740847	0.24381
H	93.3253599	96.8424544	103.3671721	0.21356
H	90.3474711	95.5966709	105.2049123	0.21242
H	89.6394335	94.1416230	101.3153266	0.19956
H	94.4109735	100.7369717	100.6889717	0.21264
C	93.3959738	100.9249717	100.3879718	-0.70246
C	92.5919348	99.6552322	100.7066258	0.83269
O	91.5173949	99.7731515	101.3784043	-0.64838
O	93.0198409	98.5181660	100.3370342	-0.71730
H	93.3774116	101.0780079	99.2951423	0.24050
H	92.9791352	101.7978540	100.9116592	0.21915
H	97.9119725	98.1829724	91.6959743	0.23737
C	97.0639727	97.8419725	92.2879741	-0.64491
C	96.9435190	96.3545740	92.2752914	0.14921
N	96.0111376	95.6731497	93.0456186	-0.55749
C	97.6143028	95.3574584	91.5904422	-0.05919
C	96.1444423	94.3378949	92.8210675	0.24757
N	97.1136500	94.1103571	91.9382101	-0.62892
H	95.3582643	96.1025456	93.7077510	0.44148
H	97.1928981	98.2125534	93.3218402	0.24758
H	96.1526030	98.3155835	91.8793111	0.23848
H	98.4150542	95.4750780	90.8607330	0.21676
H	95.5352747	93.5872658	93.3254171	0.21721
H	90.7749745	101.8069714	95.0079733	0.22204
C	90.8569745	101.7149714	96.0879730	-0.69931
C	92.1928100	101.0820138	96.4465660	0.81560
O	92.3103563	100.0887777	97.1596299	-0.64816
O	93.2110919	101.7427112	95.8940724	-0.72958
H	90.8125622	102.7356652	96.5066315	0.22984
H	90.0298232	101.1131717	96.4917510	0.22292
H	99.4778630	93.4651197	89.1873105	0.21781
C	100.3803819	93.4329706	89.8211096	-0.62385
C	100.1101993	92.6719557	91.1224049	-0.20224
N	99.7298807	91.2658567	90.9004355	-0.62351
C	98.4739162	90.8041427	90.7264010	0.70500
N	97.4107918	91.5799057	90.9275094	-0.80403
N	98.3163764	89.5046713	90.3715066	-0.78740
H	100.4870393	90.6199389	90.6837560	0.40930
H	96.4905315	91.1809825	90.7543896	0.40546
H	97.4108290	92.5952717	91.3020175	0.45687
H	97.3912473	89.1052019	90.2418457	0.42014
H	99.1048353	88.9328518	90.0816239	0.41688
H	101.1959678	92.9613401	89.2464649	0.21947
H	100.6831872	94.4691447	90.0480923	0.23051

H	99.3094459	93.1511357	91.7072059	0.22179
H	101.0076913	92.6566870	91.7632795	0.22440
Cu	96.2977323	96.3831517	96.1169011	0.85406

Zn-deficient WT-SOD1 with superoxide

H	98.2329724	98.8829722	98.8599722	0.21767
C	97.5949726	98.1169724	98.4249724	-0.62459
C	96.7439143	98.7642481	97.3598761	0.09665
N	96.3214065	98.1406981	96.1858795	-0.75569
C	96.1728943	100.0311334	97.3669948	-0.05119
C	95.5127133	99.0520149	95.5737742	0.21463
N	95.4011228	100.2035722	96.2399947	-0.60929
H	98.2375893	97.3294968	98.0025824	0.20283
H	96.9806282	97.6622670	99.2246346	0.21950
H	96.2607207	100.8131079	98.1239936	0.20960
H	94.9924391	98.8467641	94.6345932	0.17726
H	94.0917834	101.1105238	96.0186538	0.51025
H	99.5549720	93.2789738	99.5349721	0.23567
C	99.8049720	92.9989739	98.5319723	-0.63182
C	99.3096620	94.0275045	97.5669022	0.12991
N	100.0954338	94.6859520	96.6263146	-0.58042
C	98.0433887	94.5361468	97.3800849	-0.02369
C	99.2982812	95.5569930	95.9304014	0.23752
N	98.0504572	95.4710332	96.3665643	-0.63802
H	101.1055581	94.5936268	96.5329580	0.42712
H	100.9008236	92.8846237	98.4748273	0.21934
H	99.3539362	92.0118374	98.3271844	0.23602
H	97.1269046	94.2975029	97.9163661	0.23929
H	99.6614346	96.2287401	95.1525286	0.21713
H	94.8539734	93.2939738	100.5529718	0.21785
C	93.9909736	93.9119736	100.3509718	-0.63392
C	94.2082307	94.8753836	99.2171115	0.12425
N	93.9195868	96.2368681	99.2612378	-0.57433
C	94.7003828	94.6618564	97.9404909	-0.08376
C	94.2511708	96.7927820	98.0743096	0.29378
N	94.7419351	95.8622682	97.2494645	-0.69622
H	93.5472259	96.8650141	100.0102000	0.48112
H	93.1358797	93.2418930	100.1468703	0.23129
H	93.7470758	94.4591881	101.2769857	0.23509
H	95.0138281	93.7328802	97.4614190	0.22669
H	94.1213714	97.8554319	97.8607460	0.25232
H	87.3029755	97.3189727	102.5829712	0.22043
C	87.5759754	97.2079727	101.5499715	-0.62783
C	87.6497380	98.4917037	100.7794374	0.13145
N	88.7941615	99.2378541	100.5990692	-0.59171
C	86.6684507	99.1840596	100.0537355	-0.04358

C	88.4668960	100.3034763	99.8042945	0.25475
N	87.1828970	100.3036936	99.4561153	-0.55292
H	89.7676522	99.1068798	100.9495045	0.46457
H	88.5414802	96.6787037	101.5277728	0.22183
H	86.8222721	96.5459709	101.0895439	0.22140
H	85.6178828	98.9022133	99.9432410	0.19918
H	89.2219479	101.0335375	99.5068141	0.20356
H	92.2349741	97.7739725	104.4129707	0.22403
C	92.3029741	97.2599727	103.4549710	-0.65177
C	91.3366171	96.1736004	103.1283756	0.11818
N	91.0522860	95.9341978	101.7900728	-0.60119
C	90.6747727	95.1614846	103.8056718	-0.06855
C	90.2490649	94.8205966	101.7264568	0.19820
N	90.0027071	94.3301873	102.9295940	-0.53806
H	91.3429613	96.5616212	101.0346242	0.43097
H	92.2121926	98.0519685	102.6920137	0.25047
H	93.3425559	96.8806552	103.3805429	0.21189
H	90.6529404	94.9900798	104.8840326	0.20495
H	89.8720763	94.4253751	100.7804529	0.19784
H	94.4109735	100.7369717	100.6889717	0.20333
C	93.3959738	100.9249717	100.3879718	-0.70430
C	92.5864038	99.6363022	100.6637850	0.85876
O	91.4099734	99.7498828	101.1204429	-0.73497
O	93.1417244	98.5100033	100.4488437	-0.79251
H	93.3767176	101.1093984	99.3000811	0.23542
H	92.9623701	101.7816848	100.9257259	0.21036
H	97.9119725	98.1829724	91.6959743	0.22869
C	97.0639727	97.8419725	92.2879741	-0.64418
C	96.4992875	96.5678079	91.7425061	0.13003
N	95.2781985	96.0612957	92.1520536	-0.56613
C	96.9593696	95.6357253	90.8237017	-0.08621
C	95.0625363	94.8810109	91.5015324	0.23615
N	96.0660086	94.5860175	90.6848412	-0.59545
H	94.6896719	96.4480906	92.8891442	0.43579
H	97.3858276	97.7260127	93.3411848	0.22985
H	96.3098955	98.6491675	92.2778961	0.23631
H	97.8747963	95.6919925	90.2314343	0.20258
H	94.1690133	94.2781390	91.6734675	0.20903
H	90.7749745	101.8069714	95.0079733	0.21744
C	90.8569745	101.7149714	96.0879730	-0.70311
C	92.1788938	101.0363654	96.4332315	0.83567
O	92.2755887	100.0858234	97.2023055	-0.65140
O	93.2026114	101.6094863	95.7981463	-0.75370
H	90.8499735	102.7357954	96.5092680	0.22697
H	90.0156624	101.1403662	96.5020106	0.22588
H	99.4782721	93.4649738	89.1870750	0.21186

C	100.3806718	93.4328738	89.8210748	-0.61394
C	99.9406715	93.6399908	91.2798853	-0.20306
N	98.7053047	92.8813444	91.5231620	-0.64806
C	98.0194338	92.8560200	92.6913099	0.74145
N	98.5889181	93.1743682	93.8639840	-0.81223
N	96.7460122	92.4239001	92.6957859	-0.80972
H	98.1019335	92.7783135	90.7036959	0.42084
H	97.9244682	93.3474299	94.6516489	0.44890
H	99.5311084	93.5450538	93.9086905	0.40349
H	96.2409003	92.6276820	93.5906266	0.44212
H	96.2290321	92.6113739	91.8318226	0.41771
H	100.8544315	92.4473354	89.6807096	0.22159
H	101.0801582	94.2195718	89.5004680	0.22977
H	99.7615294	94.7146926	91.4843682	0.20677
H	100.7264641	93.2886068	91.9740656	0.20655
Cu	96.1605326	96.2224443	95.8655148	1.16170
O	95.7759552	94.6957893	94.7902498	-0.36352
O	96.1820762	93.4726504	95.1564796	-0.38047

Zn-deficient D124N-SOD1

H	98.2269724	99.4019721	97.8119725	0.24377
C	97.7139726	99.0449722	96.9299728	-0.64338
C	96.5199510	99.8931618	96.5586397	0.12408
N	95.6844725	99.4998419	95.5032084	-0.71701
C	96.0192539	101.0817961	97.0555244	-0.00810
C	94.7292868	100.4364215	95.3834663	0.28179
N	94.9064060	101.4021604	96.3004352	-0.55727
H	97.3991257	98.0024732	97.1250110	0.22338
H	98.4450378	99.0269151	96.0986309	0.21314
H	96.3363937	101.6972842	97.8942213	0.24425
H	93.9189173	100.4323544	94.6559652	0.22306
H	94.2564098	102.2430475	96.3602228	0.47547
H	99.3489721	93.6689737	96.4639729	0.24324
C	99.4629721	93.8539736	95.3979732	-0.63960
C	98.2637918	94.5873846	94.8924430	0.15082
N	97.0518751	93.9841124	94.5795750	-0.55716
C	98.0248458	95.9364764	94.7551096	-0.05323
C	96.1330394	94.9403086	94.2856652	0.28908
N	96.6968875	96.1462620	94.3881756	-0.68301
H	96.8736624	92.9802265	94.5818695	0.44235
H	99.6086030	92.8878998	94.8857811	0.23512
H	100.3679400	94.4635925	95.2540130	0.24238
H	98.7086954	96.7653336	94.9294060	0.23059
H	95.0893615	94.7395569	94.0470100	0.22805
H	94.5719734	92.4389740	96.9919728	0.20970
C	93.5879737	92.8439739	97.1979727	-0.64680

C	93.1730710	94.0801152	96.4608544	0.11880
N	92.7442667	94.0820078	95.1352279	-0.59695
C	92.9542674	95.3832384	96.8830863	-0.04955
C	92.2814733	95.3400217	94.8341192	0.21532
N	92.3997133	96.1535843	95.8739892	-0.58950
H	92.6572064	93.2569338	94.5429742	0.42611
H	92.8608647	92.0327035	97.0156089	0.23742
H	93.5358388	93.0448335	98.2794093	0.26112
H	93.1336977	95.7887325	97.8793500	0.22471
H	91.8649665	95.5949024	93.8573740	0.20970
H	87.2269755	98.1709724	98.2939724	0.23987
C	87.9269753	98.0869725	97.4819726	-0.63072
C	89.2642730	98.6615353	97.8474096	0.11495
N	90.4615586	98.3397175	97.2046267	-0.57540
C	89.6259009	99.5899493	98.8122212	-0.04448
C	91.4662998	99.0484532	97.7895554	0.25219
N	90.9766124	99.8314455	98.7403407	-0.44725
H	90.6451737	97.6236093	96.4926377	0.44481
H	88.0148865	97.0138695	97.2287170	0.21268
H	87.4923702	98.5925285	96.5995064	0.23432
H	88.9873657	100.0903861	99.5406204	0.22996
H	92.5173584	98.9588025	97.5165063	0.22211
H	90.5259746	96.5349729	101.0659716	0.23852
C	90.7349745	96.3349729	100.0239719	-0.63227
C	90.7891146	94.8712247	99.7148847	0.10861
N	90.1944570	94.3317197	98.5828716	-0.58292
C	91.3774622	93.7786749	100.3367137	-0.06397
C	90.4406406	92.9805621	98.5761350	0.20642
N	91.1575752	92.6170434	99.6236011	-0.53041
H	89.6585999	94.8540590	97.8934150	0.41046
H	89.9385570	96.8293752	99.4456530	0.21154
H	91.6797675	96.8556314	99.7809181	0.22145
H	91.9362011	93.7732909	101.2747635	0.21514
H	90.0578078	92.3209842	97.7941456	0.19783
H	95.0579733	99.6309720	101.6499715	0.22678
C	94.1499736	100.2139719	101.7299714	-0.68492
C	93.3374371	100.2165689	100.4067778	0.80474
O	92.1590412	99.7171937	100.6340289	-0.37253
O	93.7828413	100.6637461	99.3447110	-0.68890
H	94.4290980	101.2635227	101.9266963	0.23902
H	93.5504694	99.8373509	102.5717317	0.23167
H	99.4059721	101.6819714	91.7499742	0.24097
C	98.7729723	100.8119717	91.7629742	-0.63798
C	99.5130372	99.6249642	91.2323869	0.13926
N	99.1424089	98.3122870	91.4953007	-0.57008
C	100.6098288	99.5092705	90.3970407	-0.04353

C	99.9948576	97.4779414	90.8318968	0.25196
N	100.8973146	98.1780682	90.1558979	-0.61646
H	98.3551100	98.0232122	92.0763998	0.42699
H	98.4424222	100.6472848	92.8045290	0.22518
H	97.8736884	101.0301947	91.1574975	0.23730
H	101.2000965	100.3130136	89.9553953	0.22437
H	99.9181380	96.3905430	90.8716052	0.21009
H	90.8929745	104.9439705	95.2949732	0.23899
C	90.9419745	104.6169706	96.3259730	-0.68804
C	91.9651880	103.5155644	96.6282361	0.71933
O	93.0502479	103.4117167	96.0203484	-0.69410
N	91.6451603	102.6962326	97.6590278	-0.80814
H	92.3007557	101.9944386	98.0220169	0.42667
H	90.7588695	102.7709169	98.1513869	0.40394
H	91.2297493	105.4981160	96.9296053	0.24600
H	89.9304649	104.3165006	96.6478885	0.21744
H	106.2576469	98.0257615	90.9526467	0.21887
C	105.4435509	97.3045899	91.1455537	-0.62337
C	104.2378441	97.5782764	90.2497224	-0.20068
N	104.6155587	97.4479772	88.8309880	-0.63247
C	103.7549846	97.3462602	87.8009740	0.72723
N	102.4371672	97.4009740	87.9999971	-0.81538
N	104.2529198	97.1690732	86.5541021	-0.79688
H	105.6021785	97.5676512	88.6046726	0.41615
H	101.8224436	97.2206205	87.2091746	0.40889
H	101.9468125	97.6835028	88.9107901	0.46080
H	103.6509840	97.2039075	85.7363388	0.42388
H	105.2396822	96.9856285	86.3939163	0.42340
H	105.8310713	96.2824244	90.9954128	0.22145
H	105.1516324	97.4114492	92.2026093	0.23764
H	103.8316390	98.5903909	90.4342952	0.21751
H	103.4241903	96.8611591	90.4531584	0.22011
Cu	95.9658399	97.8352005	94.7228107	0.68150

Zn-deficient D124N-SOD1 with superoxide

H	98.2269724	99.4019721	97.8119725	0.22955
C	97.7139726	99.0449722	96.9299728	-0.63405
C	96.6425677	100.0071213	96.4701159	0.12456
N	96.0890795	99.8771550	95.1927158	-0.73378
C	96.0151402	101.0740349	97.0908723	-0.02303
C	95.1684644	100.8456684	95.0631814	0.28136
N	95.0990261	101.5857942	96.1861239	-0.56553
H	97.2830731	98.0512035	97.1516110	0.22432
H	98.4597155	98.9104694	96.1255247	0.21209
H	96.0890678	101.4699419	98.1020743	0.24551
H	94.5558042	101.0221310	94.1800259	0.22226

H	94.4464403	102.4147794	96.2892989	0.47128
H	99.3489721	93.6689737	96.4639729	0.23438
C	99.4629721	93.8539736	95.3979732	-0.63575
C	98.3590559	94.7637459	94.9462346	0.13031
N	97.0213156	94.3853379	94.9581102	-0.56644
C	98.3393384	96.0911103	94.5634152	-0.04131
C	96.2543038	95.4505980	94.6021971	0.28384
N	97.0301160	96.5056753	94.3571298	-0.67789
H	96.6619320	93.4713854	95.2288096	0.43275
H	99.4505314	92.8849024	94.8684873	0.22519
H	100.4395045	94.3336178	95.2329776	0.23509
H	99.1761679	96.7767366	94.4381165	0.23020
H	95.1655283	95.4275759	94.5529351	0.22631
H	94.5719734	92.4389740	96.9919728	0.20000
C	93.5879737	92.8439739	97.1979727	-0.64501
C	93.2389074	94.1931293	96.6429666	0.10189
N	92.8169505	94.3992253	95.3300101	-0.60011
C	93.0487553	95.4266861	97.2506720	-0.04313
C	92.3820791	95.6995008	95.2206657	0.21361
N	92.5122680	96.3461125	96.3680790	-0.56247
H	92.7354017	93.6795949	94.6136326	0.41942
H	92.8574017	92.0931118	96.8451805	0.22670
H	93.4709760	92.8722935	98.2927195	0.26267
H	93.2410836	95.6837722	98.2924481	0.22778
H	91.9860071	96.1095255	94.2889785	0.20910
H	87.2269755	98.1709724	98.2939724	0.22885
C	87.9269753	98.0869725	97.4819726	-0.62494
C	88.9932596	99.1260503	97.6624443	0.10288
N	90.3439330	98.9563410	97.3823238	-0.58292
C	88.8962668	100.4328527	98.1177489	-0.04205
C	90.9815508	100.1271004	97.6818213	0.26141
N	90.1282772	101.0436897	98.1227959	-0.59329
H	90.8264017	98.1041734	97.0767879	0.43932
H	88.3475317	97.0652677	97.4980019	0.19898
H	87.3780331	98.2032691	96.5285423	0.22427
H	87.9939193	100.9556788	98.4410467	0.20973
H	92.0641316	100.2354066	97.6217088	0.21391
H	90.5259746	96.5349729	101.0659716	0.23225
C	90.7349745	96.3349729	100.0239719	-0.63793
C	90.8401577	94.8660099	99.7561633	0.11692
N	90.1698637	94.2469058	98.7135454	-0.57834
C	91.5507269	93.8348258	100.3555053	-0.07093
C	90.4950689	92.9133945	98.7278980	0.20568
N	91.3322025	92.6329704	99.7112619	-0.54179
H	89.5496070	94.7145438	98.0559366	0.41416
H	89.9178309	96.7882958	99.4389133	0.21161

H	91.6559264	96.8902589	99.7683969	0.24535
H	92.2033765	93.9029717	101.2282555	0.21142
H	90.0837877	92.2039141	98.0065815	0.19552
H	95.0579733	99.6309720	101.6499715	0.21948
C	94.1499736	100.2139719	101.7299714	-0.71218
C	93.5408739	100.2327361	100.3226825	0.81641
O	92.7783976	99.2801853	99.9796096	-0.55842
O	93.8512780	101.1444209	99.4951906	-0.66298
H	94.4013161	101.2351506	102.0584182	0.22397
H	93.4699868	99.7248233	102.4451140	0.22350
H	99.4059721	101.6819714	91.7499742	0.23074
C	98.7729723	100.8119717	91.7629742	-0.64039
C	99.4960540	99.5336546	91.4786964	0.13401
N	98.8237601	98.3240814	91.4603951	-0.59301
C	100.8160855	99.2086350	91.1948398	-0.07285
C	99.7300432	97.3524204	91.1630700	0.20083
N	100.9555683	97.8441597	90.9984176	-0.61667
H	97.7789281	98.1868096	91.4980234	0.44969
H	98.2846514	100.7665626	92.7556173	0.23255
H	97.9653395	100.9708744	91.0243879	0.23260
H	101.6677226	99.8892456	91.1310752	0.20774
H	99.4395646	96.3015909	91.0939739	0.18396
H	90.8929745	104.9439705	95.2949732	0.22355
C	90.9419745	104.6169706	96.3259730	-0.68673
C	92.1662470	103.7517648	96.6944358	0.71640
O	93.2087979	103.7033669	96.0048715	-0.70081
N	92.0552168	103.1211668	97.8881104	-0.83961
H	92.8293051	102.5314177	98.2191901	0.41326
H	91.1359414	102.7756573	98.2136749	0.43395
H	90.9635793	105.5145920	96.9700167	0.23397
H	90.0170919	104.0663034	96.5738509	0.22371
H	106.2573702	98.0257725	90.9527745	0.24120
C	105.4432704	97.3045727	91.1455744	-0.61900
C	104.5028668	97.3411563	89.9404508	-0.21038
N	103.5735442	96.1999021	89.9484190	-0.60851
C	102.4073565	96.1542298	89.3004277	0.75403
N	101.5539448	95.1313447	89.5406698	-0.79030
N	102.1303098	97.0169910	88.3017532	-0.78183
H	103.8206503	95.3966825	90.5249040	0.41875
H	100.6919299	95.0789312	89.0033533	0.42069
H	101.5096641	94.7485387	90.4824547	0.41872
H	101.1568313	97.2979872	88.1853821	0.42731
H	102.8039320	97.7490147	88.0894509	0.42187
H	105.9135860	96.3104912	91.2527648	0.21414
H	104.9236077	97.5653853	92.0811738	0.22564
H	105.0911672	97.3199088	89.0030167	0.21651

H	103.8987895	98.2659330	89.9555534	0.22483
Cu	96.3364120	98.3163281	94.1026794	0.88332
O	95.4388986	98.3160144	92.3435737	-0.31638
O	96.1108376	97.9325276	91.2958109	-0.23905