BIOLOGICAL
CRYSTALLOGRAPHY

Volume 70 (2014)

Supporting information for article:

The high-resolution structures of cholesterol oxidase in the reduced state provide insights into redox stabilization

Emily Golden, Amir Karton and Alice Vrielink

Table S1 B3LYP-D3/Def2-TZVPP optimized geometries (Å) for all the species considered in the present work (shown in Fig. 5 of the main text).

HNMe2

N	**-0.026571**	**0.5**79843	0.000000
C	-0.026571	-0.221541	1.212275
H	-0.962576	-0.780319	1.277284
H	0.032814	0.428350	2.085229
H	0.768462	1.204664	0.000000
H	0.797956	-0.950570	1.265689
C	-0.026571	-0.221541	-1.212275
H	-0.962576	-0.780319	-1.277284
H	0.032814	0.428350	-2.085229
H	0.797956	-0.950570	-1.265689

FADH- (Figure 5a)

N	-2.563503	-1.311238	0.042966
C	-3.746472	-0.664795	0.219490
O	-4.832460	-1.225944	0.383507
N	-3.710634	0.738596	0.221289
C	-2.590643	1.540300	0.027781
O	-2.666164	2.783593	0.046180
C	-1.413621	0.793394	-0.186013
N	-0.200363	1.473154	-0.461230
C	0.983754	0.814251	-0.224964
C	2.198396	1.477147	-0.082347
C	3.409571	0.797920	0.083475
C	4.693789	1.572678	0.211912
C	3.400002	-0.593087	0.130750
C	4.671401	-1.378606	0.310609
C	2.174004	-1.266859	0.012907
C	0.967793	-0.602430	-0.172874
N	-0.250134	-1.283604	-0.331200
C	-1.464154	-0.585364	-0.147107
C	-0.256221	-2.726592	-0.303647
H	-4.589125	1.208734	0.367008
H	2.196888	2.560776	-0.118095
H	4.509238	2.645327	0.155966
H	5.404863	1.315770	-0.578944
H	5.197639	1.370969	1.161834
H	5.386527	-1.196047	-0.497946
H	4.466175	-2.449002	0.331588
H	5.184666	-1.123042	1.242999
H	2.178672	-2.345404	0.063478
H	0.385737	-3.120631	-1.095870
H	-1.279638	-3.054356	-0.447135
H	0.103049	-3.120877	0.655765
H	-0.248858	2.460493	-0.260745

FADH$^-$•••HNMe2 (Figure 5b)

N	0.981444	-1.777267	2.352207
C	2.423200	-1.600000	2.260656
H	2.837155	-2.337207	1.573435
H	2.879165	-1.754499	3.243784
H	0.597928	-1.805029	1.413630
N	2.272945	1.632462	-0.252369
C	3.457577	1.156090	-0.723102
O	4.511899	1.793178	-0.731057
N	3.459594	-0.151376	-1.234911
C	2.377125	-1.021544	-1.286215
O	2.489189	-2.180836	-1.726850
C	1.191186	-0.451895	-0.781120
N	0.031120	-1.265823	-0.664624
C	-1.190344	-0.628266	-0.543447
C	-2.394396	-1.265720	-0.813314
C	-3.631771	-0.650443	-0.602486
C	-4.904066	-1.398818	-0.896173
C	-3.657939	0.655355	-0.118870
C	-4.959481	1.369430	0.129702
C	-2.444450	1.310650	0.133851
C	-1.209561	0.701682	-0.060348
C	1.206738	0.838496	-0.291259
C	-0.027167	2.684265	0.779422
H	-2.362602	-2.283961	-1.184006
H	-5.529621	-1.502249	-0.004741
H	-5.512780	-0.887120	-1.647361
H	-4.690041	-2.400211	-1.268829
H	-5.562743	1.450541	-0.779682
H	-5.577604	0.849834	0.868344
H	-4.783797	2.379500	0.499567
H	-2.479099	2.326238	0.498445
H	0.999284	2.990901	0.946005
H	-0.498765	3.400247	0.094990
H	4.342056	-0.498465	-1.573913
N	-0.000138	1.350009	0.229055
H	0.076838	-2.089505	-1.246420
H	-0.583603	2.690859	1.720238
H	2.719792	-0.603255	1.903981
C	0.336022	-0.708495	3.094144
H	-0.747213	-0.820593	3.033409
H	0.622675	-0.762815	4.149076
H	0.593475	0.297289	2.729155

FADH$^-$•••HNMe2 (Figure 5c)

N	-1.605081	3.524242	0.670136
C	-3.049842	3.385335	0.585075
H	-3.320685	3.069834	-0.420387
H	-3.529695	4.344292	0.806079

H	-1.171282	2.704004	0.258771
N	-1.898268	-2.340749	0.373255
C	-3.158813	-2.124776	-0.086704
O	-4.107405	-2.891690	0.088269
N	-3.372971	-0.946342	-0.816508
C	-2.428800	0.033253	-1.091065
O	-2.716010	1.044613	-1.762786
C	-1.156206	-0.242416	-0.550372
N	-0.132752	0.740216	-0.726063
C	1.168183	0.310864	-0.479182
C	2.259690	1.077375	-0.869922
C	3.580107	0.718299	-0.591871
C	4.712724	1.602981	-1.038283
C	3.817224	-0.464102	0.105017
C	5.216343	-0.906505	0.439808
C	2.725704	-1.251586	0.491159
C	1.404077	-0.903228	0.223847
C	-0.955118	-1.432953	0.136299
C	0.591287	-2.960225	1.325280
H	2.062560	2.001816	-1.400996
H	5.312608	1.953022	-0.193141
H	5.397434	1.078581	-1.711316
H	4.337618	2.480420	-1.564355
H	5.830267	-1.036502	-0.456616
H	5.736216	-0.178794	1.070513
H	5.206236	-1.856855	0.973363
H	2.925653	-2.173431	1.016533
H	-0.369853	-3.421974	1.523804
H	1.198702	-3.646815	0.722785
H	-4.303005	-0.799525	-1.173712
N	0.337291	-1.724528	0.629800
H	-0.281833	1.308083	-1.547932
H	1.119688	-2.772243	2.264482
H	-3.456136	2.639433	1.287905
C	-1.129180	3.677326	2.036590
H	-0.038575	3.672380	2.049911
H	-1.466705	4.635949	2.442423
H	-1.483724	2.887218	2.719621