Table S1. Continuous Shape Measures for low spin five-coordinate Fe^{II} porphyrin complexes [Fe(porf)L].

Refcode	L	S(vOC-5)	S(TPY-5)
$[Fe(tmp)CN]^-$ (100 K)	CN^-	0.135	1.007
BEPDEF	CS	0.311	1.605
KINMUP	NO_2^-	0.134	1.184
YEQPIU	CO	0.244	1.505
YEQPOA	CO	0.246	1.512

Table S2. Continuous Shape Measures for high spin five-coordinate Fe^{II} porphyrin complexes.

Refcode	L	S(vOC-5)	S(TPY-5)	Spin State assignment
$[Fe(tmp)CN]^-$ (400 K)	CN^-	1.433	0.047	Magnetism
FEXBAL	CH_3COO^-	1.763	0.023	Mössbauer
FEXBAL10	CH_3COO^-	1.760	0.024	Mössbauer
FEXBEP	PhO^-	1.622	0.113	Mössbauer
FUHVUZ	tBu-Im	0.957	0.439	Bond distances
GEJQES	NO_3^-	1.162	0.144	Magnetism
JELMIW	EtS^-	2.098	0.258	Mössbauer
KAXXAJ	py	1.578	0.598	NMR
MAQLEW	Me-Im	1.189	0.421	Mössbauer
MAQLEW	Me-Im	1.256	0.140	Mössbauer
MAYLOO	Me-Im	1.938	0.374	Mössbauer
MAYLUU	Me-Im	1.930	0.094	Mössbauer
MIYZUP	Me-Im	0.829	0.334	Mössbauer
NOCVIK	Cl^-	1.917	0.103	NMR
SEHPOL	Me_2-Im	1.135	0.170	Mössbauer
SEHPUR	Me-Im	0.995	0.326	Mössbauer
SIBZIM	Me-Im	1.627	0.179	Mössbauer
TALLAU	Me-Im	1.319	0.309	Mössbauer
TALLEY	Me_2-Im	1.029	0.297	Mössbauer
TALLIC	Me_2-Im	1.232	0.430	Mössbauer
TALLOI	Me_2-Im	0.908	0.349	Mössbauer

Im = imidazole

Table S3. Atomic Coordinates for the Optimized Structure of $[Fe(tmp)CN]^-$ in the S = 0 state.

Fe	0.8226412081	0.0930874665	1.9415599722
N	-1.0985634025	0.1864154021	1.514356626
N	0.7762304095	-1.8554507721	1.6457365664
N	0.3891919448	-0.1141364274	4.9447994441
N	2.7887215419	0.0210435297	2.0625715266
N	0.9113669224	2.062199601	1.9351968794
C	3.6256992639	1.0459029445	2.4769832274
C	4.9856066022	0.5819076938	2.5342689406
C	4.9846409239	-0.7126315521	2.1238348189
C	3.6169106384	-1.0743839695	1.8617518402
C	3.2400717653	2.363515246	2.703575022
C	1.975710751	2.8378116652	2.3682162134
C	1.6270370444	4.2317023424	2.3147187529
C	0.3659924107	4.3101005022	1.8167783659
C	-0.0939951812	2.9623851353	1.6103877287
C	-1.3890501915	2.6253312542	1.2267458415
C	-1.8581333687	1.3144896502	1.2369168106
C	-3.2369778448	0.9472736262	1.0532544372
C	-3.328119196	-0.3903760866	1.2703009157
C	-1.9981313917	-0.868188561	1.5355583849
C	-1.6675503663	-2.2123093081	1.6803214612
C	-0.3515060993	-2.6625583219	1.6531113934
C	0.0271805138	-4.0429413011	1.5116498115
C	1.37864319	-4.0763131085	1.3830941814
C	1.8500889681	-2.7219916991	1.498543628
C	3.1942280298	-2.3621108502	1.5437922967
C	4.2384727088	-3.4373633429	1.3365412971
C	0.5565636261	-0.0343264697	3.7881090416
C	-2.7855462632	-3.228583927	1.7536373171
C	-2.3557611495	3.7367088542	0.8801015391
C	4.2673438726	3.3435725912	3.2255151587
H	-1.8363132225	4.5921028417	0.4478388887
H	-3.0923890028	3.4055941566	0.1474331524
H	-2.9016193034	4.0909264137	1.7621636059
H	-3.6506687465	-2.8200642735	2.2767700253
H	-3.1190296755	-3.5490701055	0.7591571369
H	-2.4718407896	-4.1175375298	2.3006243009
H	4.9941552724	2.8448612561	3.8667065571
H	4.8194855082	3.8353298863	2.4153453904
H	3.7947611684	4.1228809967	3.8240569122
H	5.1545083552	-3.0230960029	0.9149340777
H	4.5018402277	-3.9357772154	2.276644145
H	3.8854778006	-4.2026301669	0.6448421744
H	2.2734931137	5.0539010316	2.5833655712
H	-0.2080095689	5.20752233	1.6411052834
H	-4.0457324401	1.6248543736	0.8237939034
H	-4.2173324459	-1.0004871113	1.2143573001
H	-0.6507297128	-4.8825374687	1.473166545
H	1.9975622326	-4.9519429419	1.2563940934
H	5.838396069	-1.3686260219	2.0422378547
H	5.8434722793	1.1759947442	2.8116736415

Table S4. Atomic Coordinates for the Optimized Structure of $[Fe(tmp)CN]^-$ in the S = 2 state.

Fe	0.2230729074	0.1448872618	2.8694015258
N	0.4482202873	2.138922489	2.2854587215
N	2.3239306067	-0.0199316282	2.7811523607
N	0.1420139102	-1.9111087017	2.4953270644
N	-0.2610454685	0.3555555874	6.0961927053
N	-1.7558335571	0.2550309984	2.1493921535
C	-2.4620506212	1.4099113394	1.8709944356
C	-3.8282404145	1.0603983676	1.538641368
C	-3.930555667	-0.2891113313	1.610077465
C	-2.629965468	-0.8030620197	1.9883404046
C	-1.9405770278	2.7057883699	1.8715197471
C	-0.5797869368	3.026789505	2.0498176423
C	-0.0492186328	4.3589223798	1.9886438508
C	1.2980837102	4.2683367736	2.1982453645
C	1.6062322233	2.8796030374	2.3898530527
C	2.9029842942	2.3797886515	2.6251560172
C	3.2258628321	1.0270221472	2.7551963213
C	4.570484888	0.4950923149	2.8439520558
C	4.4692999658	-0.8546046161	2.9110086864
C	3.0597354334	-1.1866633353	2.8663479436
C	2.5367964797	-2.4817489601	2.871639025
C	1.1772374962	-2.802121062	2.682799966
C	0.6632227895	-4.1412251517	2.6369024797
C	-0.6847922542	-4.0507895828	2.4325210445
C	-1.0097295357	-2.6551054423	2.3498674926
C	-2.3089405849	-2.1550504585	2.1300543448
C	-3.4097321247	-3.1875272551	2.0006595817
C	-0.0878499383	0.2806748489	4.9419074325
C	3.4783184571	-3.6540803288	3.0545502691
C	4.0119235164	3.4092628131	2.6949223346
C	-2.8739177978	3.8723936179	1.6217889879
H	4.4867572805	-3.3320626671	3.3018995808
H	3.1401118776	-4.301355457	3.868245266
H	3.5373452097	-4.2710614442	2.1511896451
H	-4.3961887868	-2.7303740607	1.9910497157
H	-3.3065318025	-3.7793560692	1.0841813187
H	-3.3887927817	-3.8849300443	2.8418379527
H	-3.9178042608	3.5690039204	1.638984888
H	-2.7510413079	4.6397909063	2.390407264
H	-2.6800168682	4.3473942378	0.6535230581
H	3.7664002126	4.1969698747	3.4118755468
H	4.9544389591	2.9711343408	3.0139450796
H	4.1791378179	3.8918093891	1.7254931639
H	-4.6139065934	1.7439184943	1.2540890467
H	-4.8120153477	-0.8731203238	1.3921903724
H	-1.3821547323	-4.8706941209	2.3419628378
H	1.2426711293	-5.0467402438	2.7419488757
H	5.2917136599	-1.5523439723	2.9573546504
H	5.4878606777	1.0638126728	2.8263901797
H	2.0067891255	5.0833565518	2.2145737254
H	-0.6164582367	5.2598893861	1.8063359881

Table S5. Atomic Coordinates for the Optimized Structure of $[Fe(tmp)(CN)_2]^{2-}$ in the S = 0 state.

Fe	0.0000007488	0.0000001708	-0.0000007823
N	1.9544142116	-0.1417715214	0.4334012123
N	0.6998388177	0.229068615	-3.0894587752
N	-0.106760788	-1.9968143779	-0.1714498226
N	-1.9544127164	0.1417718696	-0.4334028413
N	0.106762259	1.9968147144	0.1714482954
N	-0.6998373806	-0.2290682371	3.089457178
C	4.0604171082	-0.997012305	0.8526318134
C	2.6931157749	-1.302907616	0.5184782679
C	2.8338556052	0.8871463258	0.7083241042
C	4.1494654209	0.3524149604	0.9697041946
C	0.4419299058	0.1442230108	-1.9487242818
C	2.2334478013	-2.6039235865	0.3190164926
C	0.9134947472	-2.9130720946	-0.0063207906
C	-1.2300070572	-2.7341451893	-0.4809237578
C	-0.9084946266	-4.1379382983	-0.5115190631
C	0.4120693872	-4.2504816845	-0.2187466054
C	-2.509889899	-2.2429895446	-0.7340903961
C	-2.8338542224	-0.8871460162	-0.7083252371
C	-2.6931141278	1.3029080071	-0.5184805686
C	-4.0604154313	0.9970127025	-0.852634239
C	-4.1494639278	-0.352414619	-0.9697058178
C	-2.2334460951	2.6039239971	-0.3190190626
C	-0.9134931691	2.9130724604	0.0063187848
C	1.2300083702	2.7341454793	0.4809229336
C	0.908495934	4.1379385866	0.5115182327
C	-0.4120678926	4.2504820286	0.2187449561
C	2.5098911177	2.2429898037	0.7340899766
C	-0.4419284286	-0.1442226524	1.9487226925
C	3.2492879323	-3.7181458217	0.4681764662
C	-3.5838322258	-3.263634134	-1.0506303592
C	-3.2492860653	3.7181462801	-0.46817974
C	3.5838332525	3.2636343283	1.050630788
H	5.0363902509	0.9190305472	1.2131161825
H	4.855206878	-1.7181098179	0.9819998677
H	0.9806866888	-5.1668725584	-0.1579974212
H	-1.6004975501	-4.9396114489	-0.728103404
H	-5.0363887518	-0.9190302016	-1.2131178415
H	-4.8552050738	1.7181102513	-0.9820028527
H	-0.9806851561	5.1668729121	0.1579955445
H	1.6004987459	4.9396117201	0.7281029951
H	2.8053231718	-4.6983055291	0.3080066818
H	4.0702708451	-3.6108245814	-0.2499174424
H	3.6945399219	-3.7222547127	1.4693972648
H	-4.549107207	-2.7959159172	-1.2321500471
H	-3.3315689259	-3.8474742226	-1.9431166818
H	-3.7164161174	-3.9742478995	-0.226969853
H	-2.805321155	4.6983060312	-0.3080106228
H	-3.6945380304	3.7222545799	-1.4694005494
H	-4.0702690122	3.6108256394	0.2499142238
H	4.54910768	2.7959159294	1.2321529509
H	3.7164190329	3.9742471846	0.2269697756
H	3.3315684236	3.8474754518	1.9431159806

Table S6. Atomic Coordinates for the Optimized Structure of $[Ru(tmp)CN]^-$ in the S = 0 state.

Ru	0.825109364	0.0986507942	1.9523363854
N	-1.1748840075	0.1925926454	1.5506910645
N	0.7695963713	-1.9223866801	1.6804223111
N	0.4016999049	-0.102312731	5.0194615068
N	2.864400543	0.0137922895	2.0942887966
N	0.9117317376	2.1430234482	1.9635291368
C	3.7207030369	1.0901429889	2.2762390719
C	5.0747062413	0.6049726888	2.3532575297
C	5.0342524053	-0.7475493971	2.233655843
C	3.6529191005	-1.131781767	2.0843142046
C	3.3469006735	2.4350840614	2.3468610574
C	2.0468966009	2.9143015869	2.1668989866
C	1.6805010356	4.3069357652	2.1310579399
C	0.3404881685	4.3741192083	1.920136802
C	-0.1555982769	3.0235478434	1.8270454832
C	-1.4877364091	2.6577301987	1.6224340041
C	-1.9434122066	1.3435589301	1.4775067433
C	-3.3101234569	0.9820805269	1.2096500314
C	-3.3691472391	-0.3744369598	1.1384940407
C	-2.0377057785	-0.879590729	1.3572145617
C	-1.6712999191	-2.2278421714	1.3478852341
C	-0.3609628565	-2.6987576117	1.4676763919
C	0.030508521	-4.0802040548	1.3622022264
C	1.3802127331	-4.1365015987	1.5218639507
C	1.8476320715	-2.7920447339	1.7329814526
C	3.1847467129	-2.4397816076	1.9414364221
C	4.1834781889	-3.5791703846	1.9770947244
C	0.5616865824	-0.0264223619	3.8595908702
C	-2.7584961811	-3.262685052	1.1399487157
C	-2.5376127179	3.7456595232	1.5174219427
C	4.4420947151	3.4565354157	2.5812273611
H	-2.1367371756	4.7246897633	1.7673227655
H	-2.9538302195	3.805823247	0.5058680424
H	-3.3688753546	3.5537038463	2.2006881243
H	-3.7364152691	-2.8782795478	1.4236283248
H	-2.8178667311	-3.5852936392	0.0936779462
H	-2.5766394886	-4.1500400491	1.7476089602
H	5.25288519	3.0378683201	3.1763468263
H	4.873336019	3.8178175449	1.6396967721
H	4.0648960916	4.3223720799	3.1247137025
H	5.1539010918	-3.2572417983	2.3470334299
H	3.8380828917	-4.3793974451	2.6354809288
H	4.333988417	-4.0154613884	0.9830293519
H	2.357366718	5.1423168959	2.2281434557
H	-0.2435485206	5.2766411073	1.8253552701
H	-4.1300730092	1.6729102231	1.0801022867
H	-4.2473414889	-0.9673423716	0.9326391014
H	-0.632150499	-4.910604692	1.1691295445
H	2.0000422273	-5.0200678124	1.4858690597
H	5.8841225107	-1.412857993	2.2325406796
H	5.9600659401	1.2131646347	2.460840635

Table S7. Atomic Coordinates for the Optimized Structure of $[Ru(tmp)CN]^-$ in the S = 2 state.

Ru	0.1530563683	0.1840857802	3.3516328072
N	0.4389089956	2.1903256266	2.3701598469
N	2.322975869	-0.0190378584	2.7913284531
N	0.1295457541	-1.929171747	2.5704985181
N	-0.3572804485	0.358035127	6.6349228302
N	-1.7536389569	0.2568887888	2.158640966
C	-2.4473901034	1.4087653004	1.8869166541
C	-3.8133611267	1.0720235908	1.5494659362
C	-3.9215102092	-0.2824222691	1.6146213733
C	-2.6221589092	-0.7967566755	1.9930495828
C	-1.9314397001	2.7190037308	1.885649199
C	-0.5791360917	3.0602799869	2.0578747085
C	-0.0272615392	4.3893518786	1.8922640556
C	1.3127766508	4.2985190738	2.1005567357
C	1.608465503	2.9119083774	2.3978437074
C	2.8931918855	2.3933235117	2.6357171796
C	3.2096209866	1.02765052	2.7649469645
C	4.5580692354	0.5095639209	2.8466235799
C	4.4652647459	-0.8456564767	2.9113570484
C	3.0565250867	-1.1803420251	2.871318166
C	2.5314888339	-2.4828421968	2.8708701777
C	1.1757616308	-2.811612515	2.6809937571
C	0.6783330374	-4.1609419642	2.5310365836
C	-0.6641596175	-4.0730256281	2.3251996527
C	-1.0070527044	-2.6677037553	2.3451734566
C	-2.3000667264	-2.1578412378	2.1258173131
C	-3.4150447975	-3.1682062094	1.9399004077
C	-0.1765569582	0.2991867081	5.4792149704
C	3.4958846958	-3.6443424304	3.0106409692
C	4.0570393793	3.3643376439	2.6852197668
C	-2.9199353992	3.8324550081	1.59816232
H	4.4510816512	-3.3268686007	3.4231558946
H	3.0954837691	-4.4066996609	3.6814463843
H	3.6934497426	-4.1268853452	2.0462769353
H	-4.3859132763	-2.7388556767	2.1813163781
H	-3.4621955279	-3.5381327698	0.9085913546
H	-3.2769728551	-4.0308554933	2.5921285496
H	-3.8439516072	3.6899405575	2.1615476364
H	-2.5235121099	4.8053797945	1.8802783933
H	-3.1870884036	3.8772077589	0.5357427635
H	3.7232550405	4.3817268452	2.8779515294
H	4.7519086455	3.1011428537	3.4845539633
H	4.6240540202	3.3722430187	1.7466839095
H	-4.5933434398	1.7670238718	1.2737342324
H	-4.8049593091	-0.8645038278	1.3963791674
H	-1.3432828978	-4.8950519888	2.1508037042
H	1.2692290075	-5.0653313161	2.5540855634
H	5.291878749	-1.5394344606	2.9552169979
H	5.4683367658	1.0915150096	2.831654901
H	2.0243335469	5.1077014883	2.0266049663
H	-0.5692078813	5.2842283568	1.624039088

Table S8. Energies of the d-MO for the systems [Fe(TRP)$(CN)_2$], [Fe(TRP)CN, S=0] and [Fe(TRP)CN, S=2] (R=Me, Ph) with TPSSh functional

	[Fe(TMP)$(CN)_2$][α]	[Fe(TMP)(CN),S=0][α]	[Fe(TMP)(CN),S=2][α]
d_{xz}	2353	1139	14826
d_{yz}	2355	1657	16680
d_{xy}	0	0	0
$d_{x^2-y^2}$	36997	38081	27026
d_{z^2}	39312	27886	19970

	[Fe(TPP)$(CN)_2$][α]	[Fe(TPP)(CN),S=0][α]	[Fe(TPP)(CN),S=2][α]
d_{xz}	2502	1328	14481
d_{yz}	2504	1837	16504
d_{xy}	0	0	0
$d_{x^2-y^2}$	37831	38527	22270
d_{z^2}	37921	27963	19197

Table S9. Shape measures and geometrical parameters for the Fe coordination sphere in crystal structures of deoxyhaemoglobins and myoglobins.

PDB-ID	δ (Å)	S(vOC-5)	S(SPY-5)
3qjd_Fe4853	0.291	0.768	0.356
3qjd_Fe4795	0.349	1.057	0.263
3qjd_Fe4752	0.294	0.845	0.304
3qjd_Fe4709	0.373	1.294	0.165
2hhb_Fe4431	0.448	1.467	0.124
2hhb_Fe4752	0.294	1.024	0.211
2hhb_Fe4795	0.349	1.222	0.388
2hhb_Fe4853	0.291	1.09	0.456
1fdh_Fe4451	0.599	2.246	0.298
1fdh_Fe4494	0.497	2.246	0.2
1fdh_Fe4537	0.599	2.246	0.298
1fdh_Fe4580	0.497	2.246	0.2
2dhb_Fe2246	0.369	1.305	0.737
2dhb_Fe2289	0.326	0.775	0.432
1hbh_Fe4531	0.37	1.688	0.349
1hbh_Fe4574	0.313	1.341	0.32
1hbh_Fe4617	0.359	1.444	0.366
1hbh_Fe4660	0.389	1.507	0.451
1hda_Fe4391	0.421	2.245	0.344
1hda_Fe4434	0.332	1.376	0.212
1hda_Fe4477	0.402	1.616	0.179
1hda_Fe4520	0.307	1.661	0.749
1hga_Fe4389	0.343	2.013	0.918
1hga_Fe4432	0.31	1.087	0.284
1hga_Fe4475	0.389	1.683	0.321
1hga_Fe4518	0.546	2.331	0.132
1hgc_Fe4434	0.227	0.917	0.497
1hgc_Fe4522	0.252	0.933	0.525
1bz0_Fe4389	0.44	2.007	0.245
1bz0_Fe4432	0.369	1.419	0.177
1bz0_Fe4475	0.417	1.693	0.228
1bz0_Fe4518	0.369	1.399	0.21
1ibe_Fe2214	0.402	1.577	0.164
1ibe_Fe2257	0.342	1.764	0.556
1kd2_Fe4389	0.43	1.736	0.16
1kd2_Fe24432	0.333	1.225	0.29
1kd2_Fe4475	0.35	1.434	0.292
1kd2_Fe4518	0.298	1.006	0.287
1lfl_Fe8777	0.154	0.551	1.052
1lfl_Fe8820	0.157	2.225	1.455
1lfl_Fe8863	0.089	0.311	0.879
1lfl_Fe8906	0.081	0.796	1.127
1lfl_Fe8949	0.166	0.968	1.066
1lfl_Fe8992	0.129	0.95	0.754
1lfl_Fe9035	0.08	0.853	1.305
1lfl_Fe9078	0.065	0.59	0.939

1hba_Fe4511	0.489	2.194	0.244
1hba_Fe4556	0.331	1.089	0.166
1hba_Fe4425	0.404	1.538	0.189
1hba_Fe4468	0.368	1.306	0.14
1hbb_Fe4431	0.409	1.513	0.165
1hbb_Fe4474	0.357	1.248	0.18
1hbb_Fe4517	0.533	2.304	0.145
1hbb_Fe4560	0.381	1.355	0.136
1y0a_Fe4371	0.372	1.271	0.177
1y0a_Fe4414	0.351	1.191	0.145
1y0a_Fe4457	0.466	1.761	0.05
1y0a_Fe4500	0.334	1.084	0.138
1y7z_Fe4385	0.386	1.554	0.247
1y7z_Fe4428	0.339	1.217	0.185
1y7z_Fe4471	0.475	1.994	0.129
1y7z_Fe4514	0.362	1.354	0.121
1y0t_Fe4391	0.396	1.799	0.276
1y0t_Fe4434	0.309	1.346	0.27
1y0t_Fe4477	0.492	2.378	0.218
1y0t_Fe4520	0.32	1.377	0.276
1xye_Fe4371	0.547	2.591	0.204
1xye_Fe4414	0.367	1.53	0.183
1xye_Fe4457	0.533	2.463	0.296
1xye_Fe4500	0.201	1.157	0.526
1xz2_Fe4389	0.478	1.967	0.177
1xz2_Fe4432	0.404	1.442	0.098
1xze_Fe4475	0.436	1.816	0.199
1xze_Fe4518	0.361	1.114	0.231
1xz4_Fe4371	0.457	1.964	0.176
1xz4_Fe4414	0.464	1.67	0.15
1xz4_Fe4457	0.473	2.039	0.182
1xz4_Fe4500	0.364	0.965	0.241
1y5k_Fe4385	0.422	1.705	0.212
1y5k_Fe4428	0.401	1.077	0.148
1y5k_Fe4471	0.512	2.198	0.265
1y5k_Fe4514	0.322	1.741	0.464
1dxt_Fe4447	0.44	1.933	0.27
1dxt_Fe4490	0.356	1.241	0.219
1dxt_Fe4533	0.424	1.913	0.379
1dxt_Fe4576	0.442	1.485	0.21
1xxt_Fe4389	0.395	1.446	0.185
1xxt_Fe4432	0.367	1.277	0.13
1xxt_Fe4475	0.467	2.108	0.106
1xxt_Fe4572	0.379	1.272	0.097
1dxu_Fe4433	0.547	2.34	0.219
1dxu_Fe4481	0.313	1.171	0.349
1dxu_Fe4524	0.456	1.768	0.161
1dxu_Fe4572	0.351	1.209	0.277
1y45_Fe4387	0.432	1.649	0.225
1y45-Fe4430	0.317	0.893	0.302

1y45_Fe4473	0.471	1.952	0.29
1y45_Fe4516	0.264	1.079	0.45
1y83_Fe4375	0.426	1.698	0.202
1y83_Fe4418	0.295	0.971	0.289
1y83_Fe4461	0.478	1.927	0.058
1y83_Fe4504	0.308	1.071	0.173
1y0c_Fe4383	0.406	1.537	0.165
1y0c_Fe4426	0.301	1.045	0.237
1y0c_Fe4469	0.519	2.35	0.212
1y0c_Fe4512	0.378	1.274	0.081
1y7c_Fe4387	0.402	1.64	0.295
1y7c_Fe4430	0.284	1.047	0.299
1y7c_Fe4473	0.504	2.257	0.179
1y7c_Fe4516	0.325	1.186	0.186
1y22_Fe4387	0.418	1.757	0.304
1y22_Fe4430	0.308	1.126	0.229
1y22_Fe4473	0.516	2.278	0.155
1y22_Fe4516	0.336	1.249	0.17
1y4p_Fe4381	0.477	1.665	0.168
1y4p_Fe4424	0.353	1.15	0.26
1y4p_Fe4467	0.516	1.82	0.111
1y4p_Fe4510	0.342	1.337	0.194
1y4q_Fe4379	0.389	1.478	0.215
1y4q_Fe4422	0.319	1.212	0.313
1y4q_Fe4465	0.501	2.176	0.139
1y4q_Fe4508	0.315	1.136	0.17
1y4r_Fe4379	0.38	1.358	0.142
1y4r_Fe4422	0.354	1.285	0.162
1y4r_Fe4465	0.503	2.253	0.19
1y4r_Fe4508	0.364	1.388	0.114
1y4v_Fe4389	0.313	1.104	0.276
1y4v_Fe4432	0.327	1.197	0.22
1y4v_Fe4475	0.42	1.621	0.101
1y4v_Fe4518	0.342	1.298	0.138
1y09_Fe4379	0.483	2.129	0.259
1y09_Fe4422	0.357	1.408	0.314
1y09_Fe4465	0.604	2.79	0.279
1y09_Fe4508	0.339	1.627	0.385
1y31_Fe4377	0.392	1.512	0.199
1y31_Fe4420	0.293	1.069	0.24
1y31_Fe4463	0.456	1.958	0.116
1y31_Fe4506	0.329	1.278	0.185
1y35_Fe4389	0.404	1.608	0.241
1y35_Fe4432	0.312	1.134	0.249
1y35_Fe4475	0.49	2.138	0.155
1y35_Fe4518	0.341	1.215	0.132
1y46_Fe4387	0.511	2.215	0.208
1y46_Fe4430	0.387	1.475	0.239
1y46_Fe4473	0.518	2.303	0.187
1y46_Fe4516	0.256	1.285	0.592

1y4b_Fe4383	0.401	1.848	0.415
1y4b_Fe4426	0.404	1.685	0.151
1y4b_Fe4469	0.508	2.271	0.204
1y4b_Fe4512	0.246	1.31	0.486
1y4f_Fe4373	0.456	1.911	0.278
1y4f_Fe4416	0.335	1.03	0.281
1y4f_Fe4459	0.467	1.711	0.139
1y4f_Fe4502	0.283	0.971	0.335
1y4g_Fe4371	0.47	1.892	0.241
1y4g_Fe4414	0.33	0.985	0.3
1y4g_Fe4457	0.452	1.488	0.216
1y4g_Fe4500	0.29	0.93	0.359
1xz7_Fe4373	0.509	1.963	0.141
1xz7_Fe4416	0.341	1.076	0.202
1xz7_Fe4459	0.461	1.672	0.067
1xz7_Fe4502	0.248	1.057	0.353
1xy0_Fe4375	0.352	1.36	0.326
1xy0_Fe4418	0.357	1.364	0.167
1xy0_Fe4461	0.492	2.167	0.157
1xy0_Fe4504	0.326	1.144	0.213
1xz5_Fe4379	0.379	1.404	0.192
1xz5_Fe4422	0.379	1.466	0.144
1xz5_Fe4465	0.498	2.143	0.143
1xz5_Fe4508	0.333	1.173	0.203
1xzu_Fe4420	0.325	1.214	0.203
1xzu_Fe4463	0.317	1.243	0.356
1xzu_Fe4506	0.263	0.833	0.289
1xzv_Fe4381	0.336	1.256	0.29
1xzv_Fe4424	0.354	1.311	0.139
1xzv_Fe4467	0.494	2.094	0.123
1xzv_Fe4510	0.354	1.263	0.158
1y2z_Fe4385	0.415	1.656	0.228
1y2z_Fe4428	0.326	1.181	0.222
1y2z_Fe4471	0.503	2.184	0.135
1y2z_Fe4514	0.326	1.204	0.196
1y0w_Fe4391	0.47	1.76	1.5
1y0w_Fe4434	0.374	1.258	1.49
1y0w_Fe4477	0.537	2.038	0.093
1y0w_Fe4520	0.234	1.096	0.498
1y7d_Fe4385	0.421	1.7	0.239
1y7d_Fe4428	0.325	1.164	0.215
1y7d_Fe4471	0.445	1.891	0.143
1y7d_Fe4514	0.382	1.414	0.105
1y7g_Fe4385	0.381	1.559	0.311
1y7g_Fe4428	0.362	1.434	0.252
1y7g_Fe4471	0.539	2.365	0.132
1y7g_Fe4514	0.282	0.907	0.219
1y85_Fe4369	0.379	1.577	0.349
1y85_Fe4412	0.378	1.445	0.119
1y85_Fe4455	0.509	2.226	0.11

1y85_Fe4498	0.349	1.207	0.131
1y5f_Fe4385	0.424	1.698	0.205
1y5f_Fe4428	0.3	1.258	0.348
1y5f_Fe4471	0.505	2.236	0.152
1y5f_Fe4514	0.308	1.112	0.182
1dxv_Fe4427	0.535	2.366	0.223
1dxv_Fe4475	0.326	1.238	0.355
1dxv_Fe4518	0.445	1.798	0.251
1dxv_Fe4566	0.345	1.357	0.288

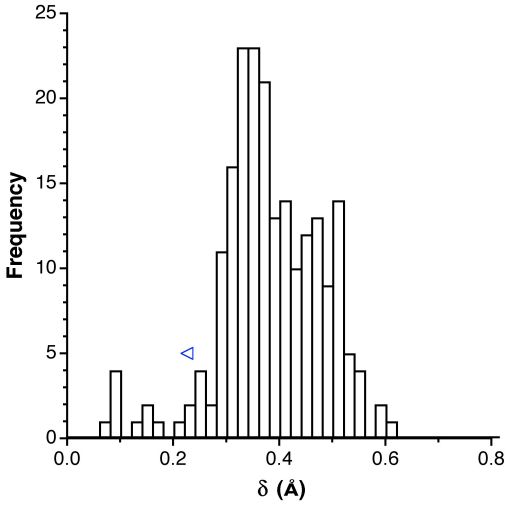

Figure S1. Distribution of out of plane displacements of the Fe atom in deoxyhaemoglobin and myoglobin crystal structures obtained from the PDB.

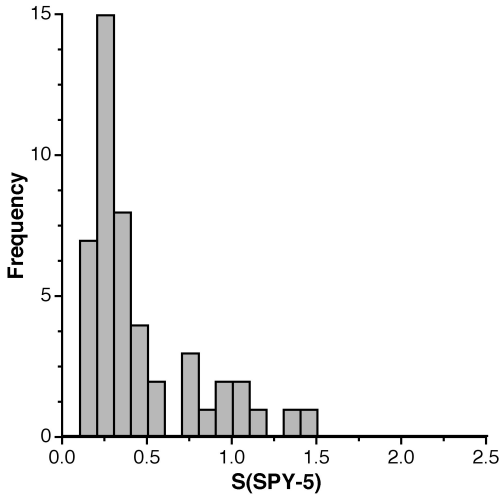

Figure S1. Distribution of square pyramidal (SPY-5) shape measures for the coordination spheres of the Fe atom in deoxyhaemoglobin and myoglobin crystal structures obtained from the PDB.

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