10.1071/CH04103_AC

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PDB Code	Organism	Resolution	Mutations	Fe-AspOD1	Fe-TyrOH$_{ax}$	Fe-TyrOH$_{eq}$	Fe-HisNE2	Fe-CO_3^{2-} O1	Fe-CO_3^{2-} O2
N-lobe of Lactoferrins									
1lfg	Human	2.2	Wild	1.932	1.897	2.202	2.064	2.063	2.129
1b0l	Human	2.2	Wild	2.146	1.817	2.035	2.087	2.138	2.007
1n76	Human	3.4	Wild	1.896	1.944	1.960	2.170	1.956	2.440
1vfe	Human	2.3	R121S	2.112	1.769	2.028	2.267	2.443	2.092
1vfd	Human	2.3	R121E	1.916	2.026	1.806	1.964	1.976	2.228
1h45	Human	1.95	R210G	2.249	2.065	2.198	2.292	2.320	2.303
1h44	Human	2.0	R210L	2.128	2.040	2.258	2.244	2.225	2.308
1eh3	Human	2.0	R210K	2.081	2.002	2.132	2.305	2.167	2.161
1h43	Human	2.2	R210E	2.094	2.012	2.084	2.226	2.139	2.531
1h76	Porcine	2.15	Wild	2.054	1.813	2.030	2.202	2.082	2.185
1ce2	Bovine	2.5	Wild	2.206	1.960	1.892	2.102	2.073	2.257
1blf	Bovine	2.8	Wild	1.945	1.987	1.920	2.077	1.874	2.210
1biy	Buffalo	3.37	Wild	2.062	2.206	1.703	2.000	2.272	1.923
1hse	Human	2.2	H253M	2.010	1.871	2.106	-*	2.177	2.119
N-lobe of Ovotransferrins									
1iej	Chicken	1.65	Wild	2.133	1.966	1.871	2.123	2.056	2.085
1ovt	Chicken	2.4	Wild	2.178	2.040	1.838	2.078	1.845	2.088
1nnt	Hen	2.3	Wild	1.914	1.774	2.013	2.261	2.270	2.095
1dot	Duck	2.3	Wild	1.982	2.059	1.978	2.040	1.506	2.779
N-lobe of serum transferrins									
1a8e	Human	1.6	Wild	2.030	1.796	1.972	2.036	2.055	2.240
1a8f	Human	1.8	Wild	2.022	1.898	1.986	2.105	1.964	2.233
1d3k	Human	1.8	Wild	2.039	1.856	1.900	2.107	1.997	2.264
1d4n	Human	2.0	Wild	2.388	2.002	2.093	2.171	2.127	2.598
1n84	Human	2.05	Wild	2.360	2.032	2.057	2.270	2.408	2.635
1n7x	Human	2.1	Wild	2.339	1.956	2.142	2.339	2.426	2.594
1tfd	Human	2.3	Wild	1.891	2.041	2.097	2.204	2.078	2.056
1b3e	Human	2.5	Wild	2.013	1.906	1.892	2.118	2.015	2.020
1fqe	Human	1.8	K206A	2.117	2.038	1.983	2.154	2.167	2.220
1fqf	Human	2.1	K296A	1.935	2.048	2.023	2.088	2.005	2.369
1n7w	Human	2.2	L66W	2.165	2.040	2.069	2.170	2.360	2.407
1oqh	Human	2.4	R124A	2.141	2.077	1.972	2.378	2.213	2.011
1jnf	Rabbit	2.6	Wild	2.145	1.826	1.772	2.143	1.925	1.962
1oqg	Human	1.9	D63E	2.016*	1.999	1.876	2.196	2.047	2.128
1jqf	Human	1.85	H249Q	2.101	1.886	1.983	2.349*	2.175	2.151
1dtg	Human	2.4	H249E	2.109	1.637	1.599	2.089*	1.986	1.973
C-lobe of Lactoferrins									
1lfg	Human	2.2	Wild	2.089	2.034	1.854	2.121	2.082	2.019
1b0l	Human	2.2	Wild	2.008	1.848	2.004	2.194	2.010	2.286
1n76	Human	3.4	Wild	2.063	2.044	1.963	2.429	2.193	2.001
1h76	Porcine	2.15	Wild	2.015	1.870	1.883	2.189	2.081	2.066
1ce2	Bovine	2.5	Wild	2.005	1.985	2.034	2.052	2.109	2.320
1blf	Bovine	2.8	Wild	1.940	1.910	1.885	2.067	1.893	2.139
1biy	Buffalo	3.37	Wild	1.822	2.060	1.965	2.388	1.792	2.111
C-lobe of Ovotransferrins									
1ovt	Chicken	2.4	Wild	2.336	1.897	1.828	2.161	1.897	2.145
1dot	Duck	2.3	Wild	3.136	2.818	1.958	2.736	2.058	2.109
C-lobe of serum transferrins									
1jnf	Rabbit	2.6	Wild	2.398	1.856	1.697	2.092	1.875	2.245
Ferric-binding proteins of Bacteria									
1mrp	*Haemophilus Influenzae*	1.6	Wild	2.082	1.917	1.776	2.189	2.094*	2.019*
1d9y	*Neisseria Gonorrhoeae*	2.2	Wild	2.031	1.880	1.836	2.192	2.099*	2.231*

Table 1: Iron-ligand distances for proteins of the transferrin family present in the Protein Data Bank (PDB). Results for some bacterial ferric-binding proteins are also shown. Distances are in Å.

Models	Model 2H	Model 2	Model 3
Fe-AspOD1	1.96	1.96	1.87
Fe-TyrO$^{-}_{ax}$	2.28	1.97	5.47
Fe-TyrO$^{-}_{eq}$	1.90	1.90	1.89
Fe-HisNE2	2.11	2.06	2.06
Fe-CO$^{2-}_{3}$O1	2.09	2.06	1.98
Fe-CO$^{2-}_{3}$O2	2.20	3.17	2.21

Table 2: Geometry-optimized distances (in Å) for models including second sphere ligands. Model 2H is model 2 but for which an optimization of hydrogen positions was performed before the full optimization.

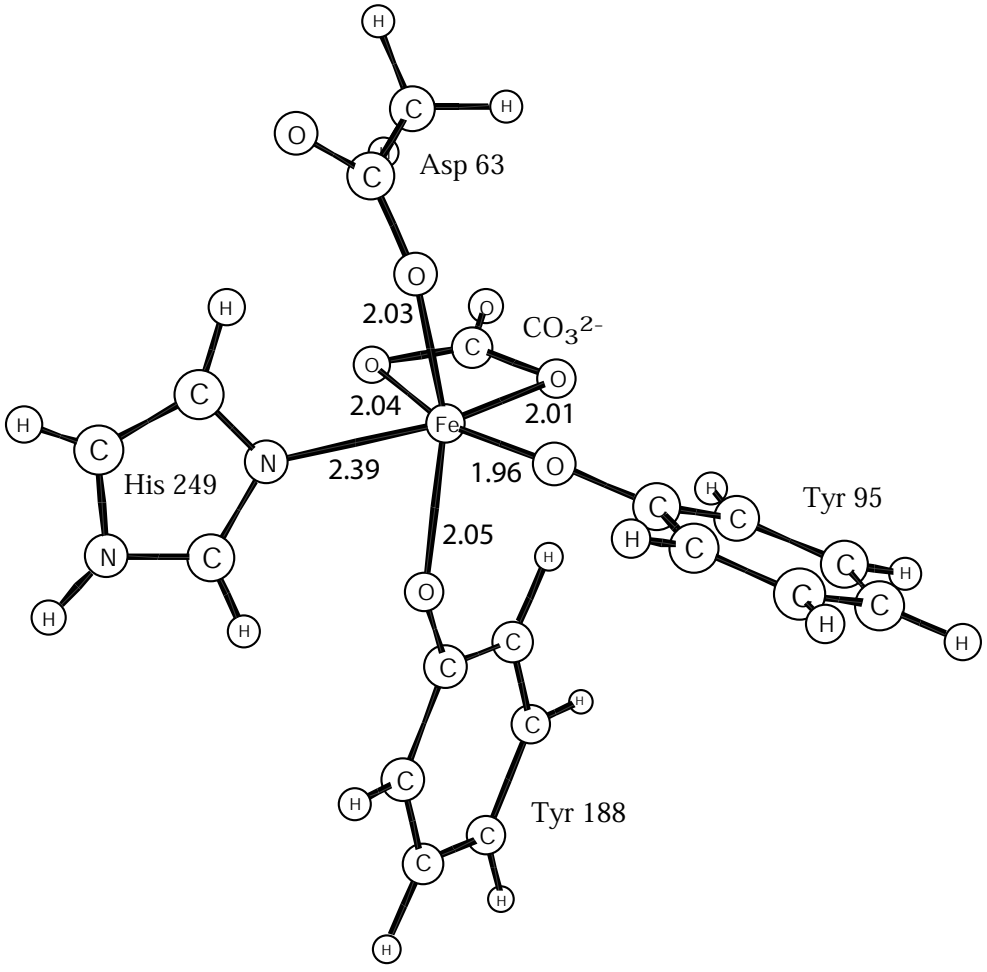

Figure 1: Geometry-optimized structure of the first-shell cluster model of the iron-binding site in the high-spin state and with a protonated histidine. Distances are in Å.

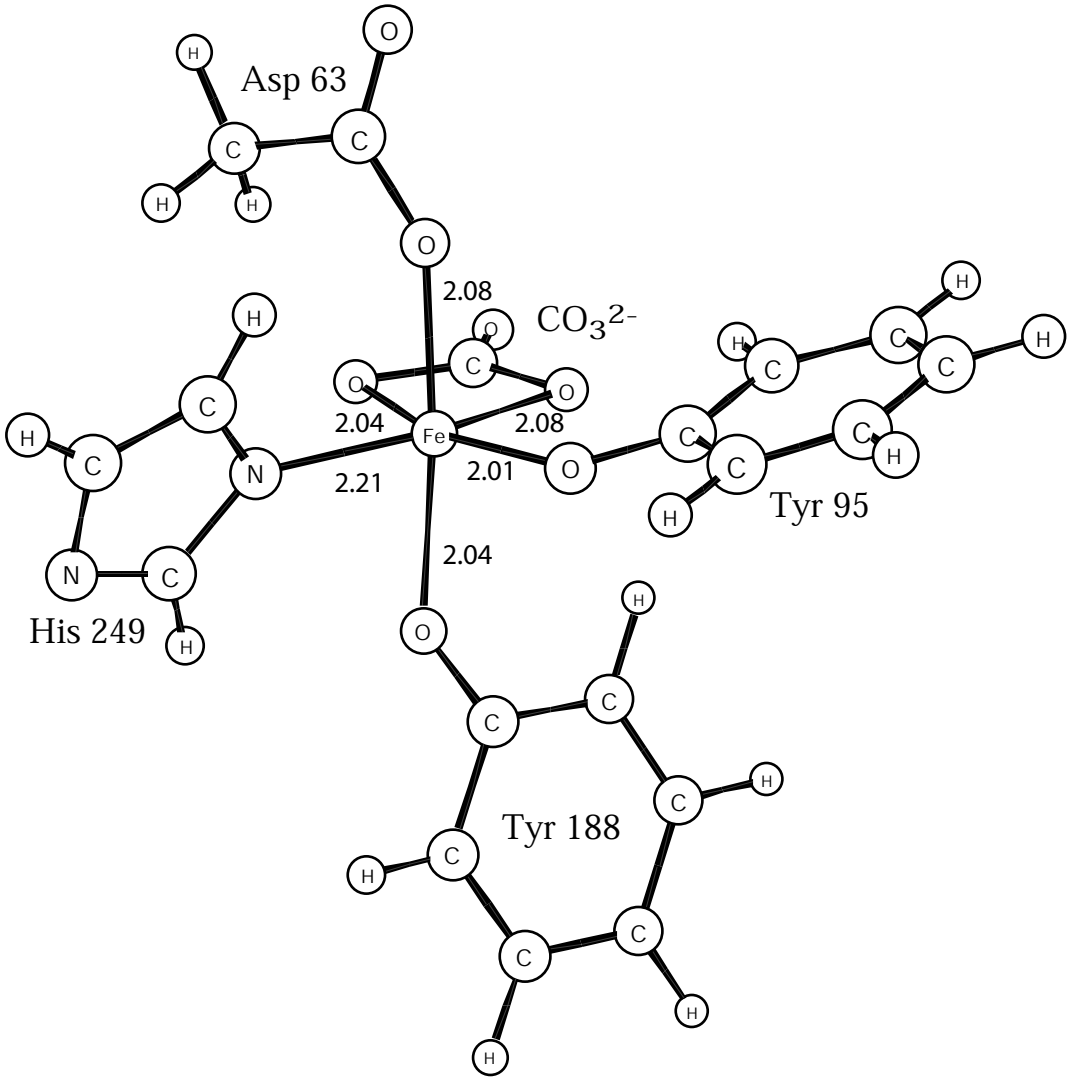

Figure 2: Geometry-optimized structure of the first-shell cluster model of the iron-binding site in the high-spin state and with a deprotonated histidine. Distances are in Å.

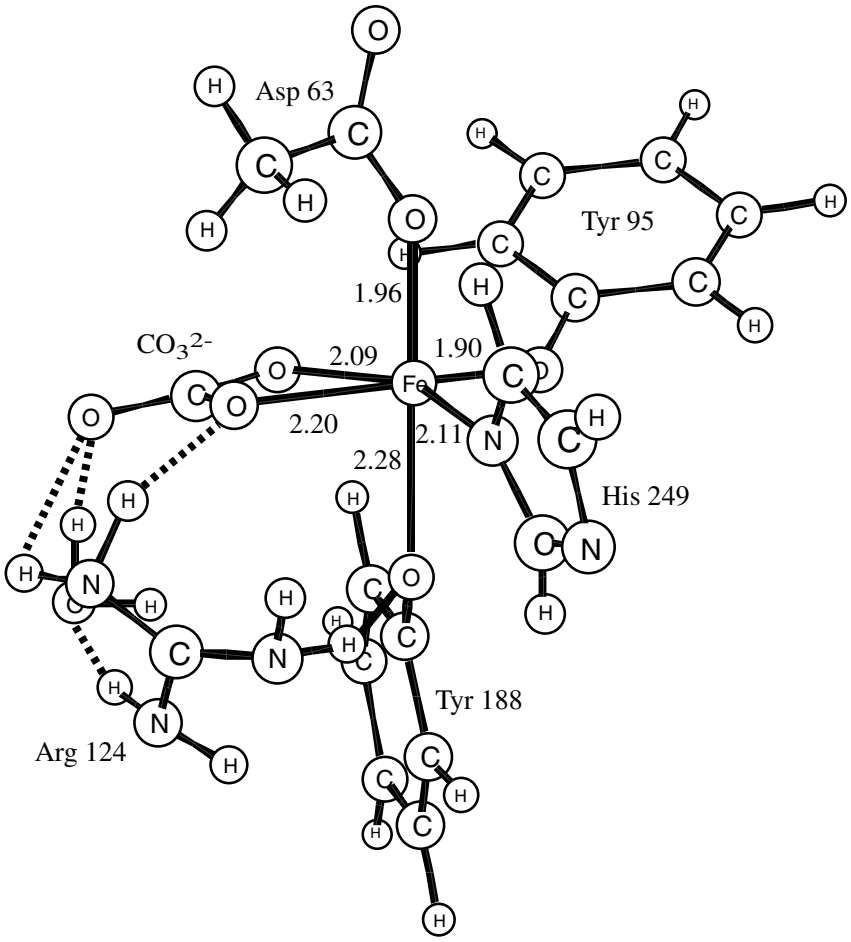

Figure 3: Geometry-optimized structure of the cluster model of the iron-binding site containing a guanidium ion and a water molecule. This structure was obtained with a preliminary optimization of the hydrogen positions. Distances are in Å.

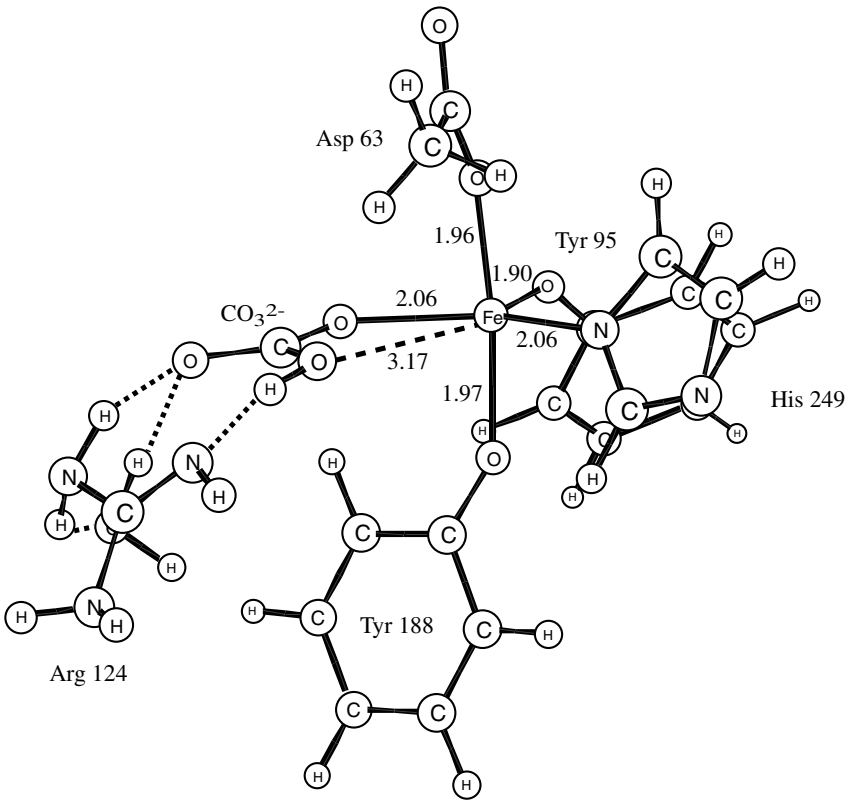

Figure 4: Geometry-optimized structure of the cluster model of the iron-binding site containing a guanidium ion and a water molecule. This structure was obtained without a preliminary optimization of the hydrogen positions. Distances are in Å.

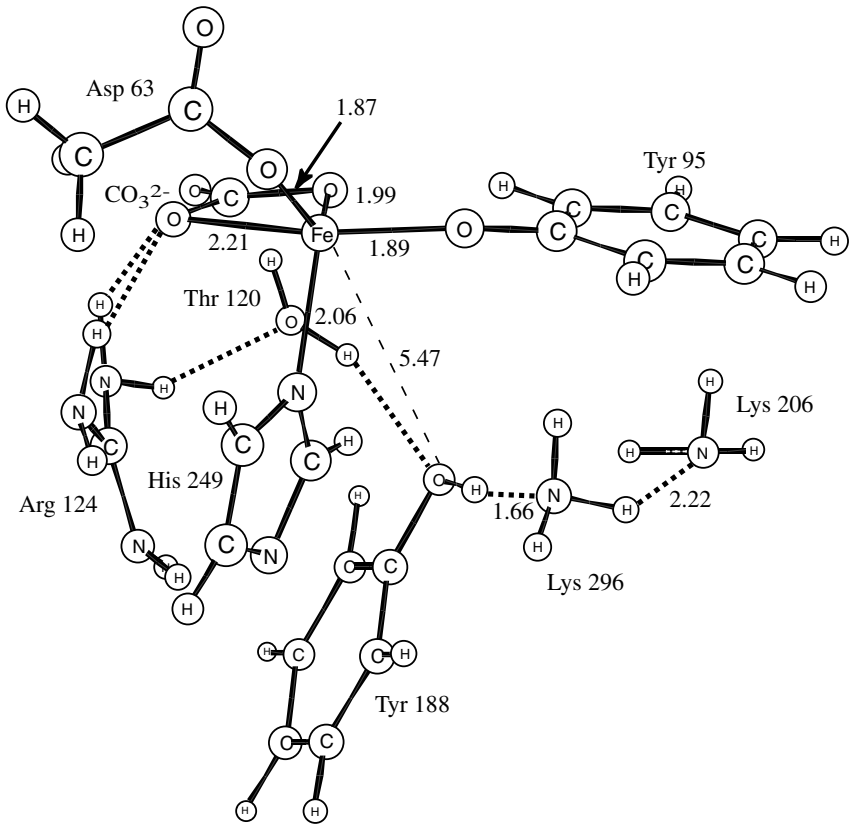

Figure 5: Geometry-optimized structure of the cluster model of the iron-binding site containing a guanidium ion, a water molecule, an ammonium ion and an ammonia molecule. A proton transfer from ammonium to the oxygen atom of Tyr 188 occurs. Distances are in Å.