Supporting Information

for

Redox-Specific Allosteric Modulation of the Conformational Dynamics of κB DNA by Pirin in the NF-κB Supramolecular Complex

Charles Adeniran and Donald Hamelberg*

Department of Chemistry and the Center for Diagnostics & Therapeutics, Georgia State University, Atlanta, Georgia 30302-3965

*To whom correspondence should be addressed, Dr. Donald Hamelberg, P. O. Box 3965, Atlanta, GA 30302-3965. Email: dhamelberg@gsu.edu; Tel: 404-413-5564, Fax: 404-513-5505

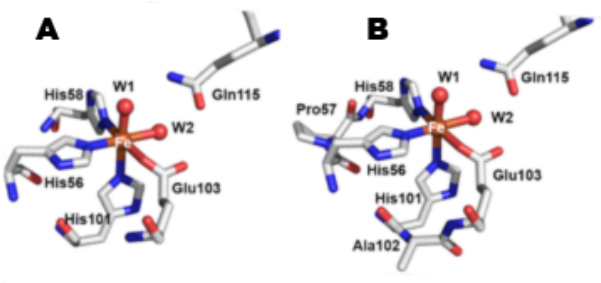

Figure S1. Residues included in the QM region and the RESP charge fitting procedure. The hydrogen atoms are not shown but are included in the calculations. (A) Residues treated in the QM region during QM/MM minimization. (B) Residues included in the QM region during a single point energy calculation to obtain the electrostatic potential and to calculate the partial charges of the atoms using the RESP charge fitting procedure.

Table S1. Partial charges of the atoms in the residues at the iron center of the Fe(II) and Fe(III) forms of Pirin.

	Fe(II)			**Fe(III)**		
	His56	**His58**	**His101**	**His56**	**His58**	**His101**
N	-0.2824	-0.7333	-0.0965	0.0814	-0.6056	0.0412
H	0.0970	0.3954	-0.0846	-0.0252	0.3355	-0.1036
CA	0.5477	0.0810	0.1301	-0.3582	-0.2237	-0.0235
HA	-0.0379	0.0784	0.0978	0.2476	0.1578	0.1191
CB	-0.5482	-0.3323	-0.4762	-0.5614	-0.1528	-0.4717
HB2	0.1571	0.1165	0.1781	0.2238	0.0697	0.2141
HB3	0.1571	0.1165	0.1781	0.2238	0.0697	0.2141
CG	0.3847	0.3728	0.2258	0.2374	0.3986	0.0443
ND1	-0.3467	-0.5428	-0.3489	-0.0604	-0.4977	-0.1582
HD1	0.3410	0.4290	0.3686	0.2875	0.4278	0.3494
CE1	0.0177	0.0705	0.0261	-0.1367	0.0787	-0.1053
HE1	0.1823	0.1433	0.1837	0.2225	0.1563	0.1963
NE2	-0.1666	0.0997	-0.2988	-0.1578	-0.0656	-0.1772
CD2	-0.3555	-0.4448	-0.0859	-0.2467	-0.3720	0.0084
HD2	0.2045	0.2655	0.1181	0.1842	0.2692	0.0898
C	-0.3648	0.6331	0.2613	0.3444	0.7851	0.3804
O	-0.1110	-0.4809	-0.3354	-0.3758	-0.4930	-0.4288
	Pro57			**Pro57**		
N	0.4385			0.0659		
CD	-0.0119			0.0804		
HD2	0.0539			0.0353		
HD3	0.0539			0.0353		
CG	-0.3127			-0.2138		
HG2	0.1237			0.1059		
HG3	0.1237			0.1059		
CB	0.0759			0.0388		
HB2	0.0584			0.0421		
HB3	0.0584			0.0421		
CA	-0.5379			-0.2968		
HA	0.1279			0.1156		
C	0.7397			0.6765		

O	-0.4995	-0.5394
	Ala102	**Ala102**
N	-0.5091	-0.4409
H	0.3007	0.3005
CA	0.3273	0.1850
HA	-0.0366	0.0260
CB	-0.4494	-0.4148
HB1	0.1271	0.1306
HB2	0.1271	0.1306
HB3	0.1271	0.1306
C	0.7539	0.8220
O	-0.5609	-0.5731
	Glu103	**Glu103**
N	-0.8500	-0.8863
H	0.4221	0.4376
CA	-0.1017	-0.4297
HA	0.1673	0.2893
CB	-0.0466	-0.0040
HB2	0.0354	0.0452
HB3	0.0354	0.0452
CG	-0.1095	-0.0235
HG2	0.0502	0.0449
HG3	0.0502	0.0449
CD	0.5381	0.5159
OE1	-0.5466	-0.4714
OE2	-0.5271	-0.4566
C	0.6640	0.8759
O	-0.5146	-0.5644
	Wat1	**Wat1**
O	-0.8791	-0.8533
H1	0.4823	0.4872
H2	0.4823	0.4872
	Wat2	**Wat2**
O	-0.9599	-0.9097
H1	0.4882	0.5009
H2	0.4882	0.5009
	Gln115	**Gln115**
N	-0.2853	-0.2038
H	0.2082	0.2201

CA	-0.2083	-0.4373
HA	0.2117	0.2710
CB	0.0836	-0.2229
HB2	0.0025	0.1166
HB3	0.0025	0.1166
CG	-0.2601	-0.1657
HG2	0.0607	0.0687
HG3	0.0607	0.0687
CD	0.8261	0.6725
OE1	-0.6308	-0.4808
NE2	-1.0033	-0.9378
HE21	0.4494	0.3896
HE22	0.4494	0.3896
C	0.5755	0.7134
O	-0.4681	-0.5092
	Fe(II)	**Fe(III)**
Fe	0.6724	1.007

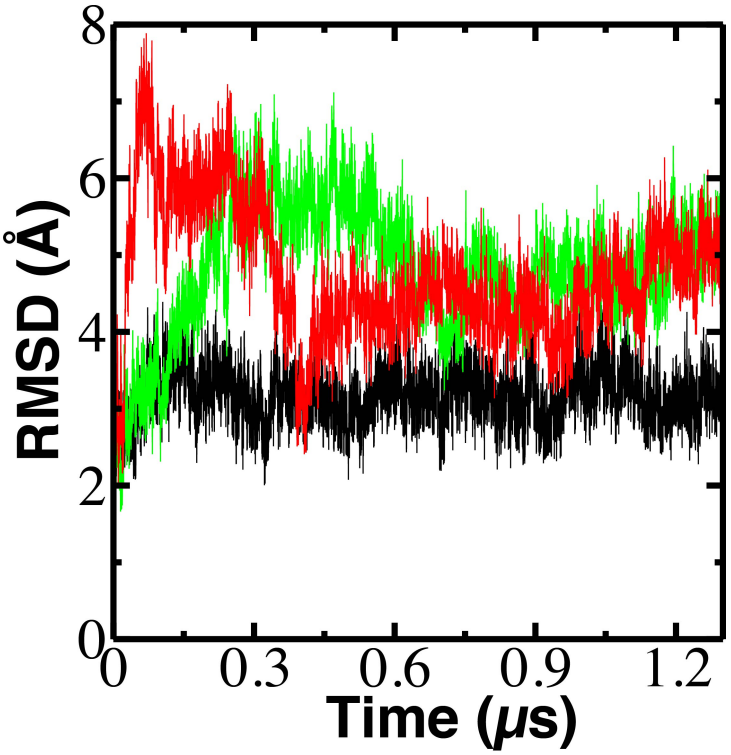

Figure S2. Root mean square deviation of the Cα atoms of the p65 in the p65-DNA complex (black), the Fe(III) form of the Pirin-p65-DNA supramolecular complex (green), and the Fe(II) form of the Pirin-p65-DNA supramolecular (red) during the entire 1.3 μs MD simulation.

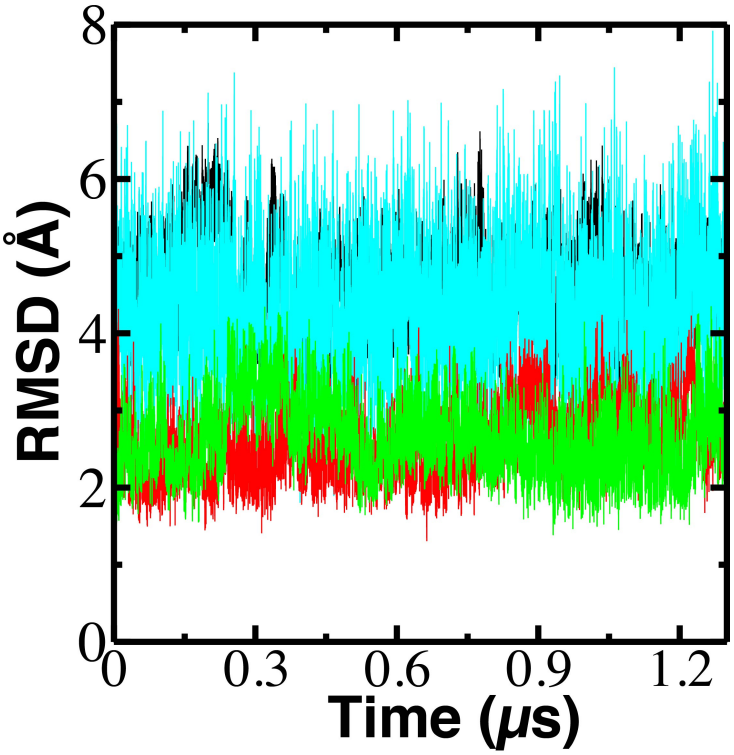

Figure S3. Root-mean-square deviation (RMSD) of the heavy atoms of the free DNA (cyan), the DNA in the p65-DNA complex (black), the DNA in the Fe(III) form of the Pirin-p65-DNA supramolecular complex (green), and the DNA in the Fe(II) form of the Pirin-p65-DNA supramolecular complex (red) during the entire 1.3 μs MD simulation.

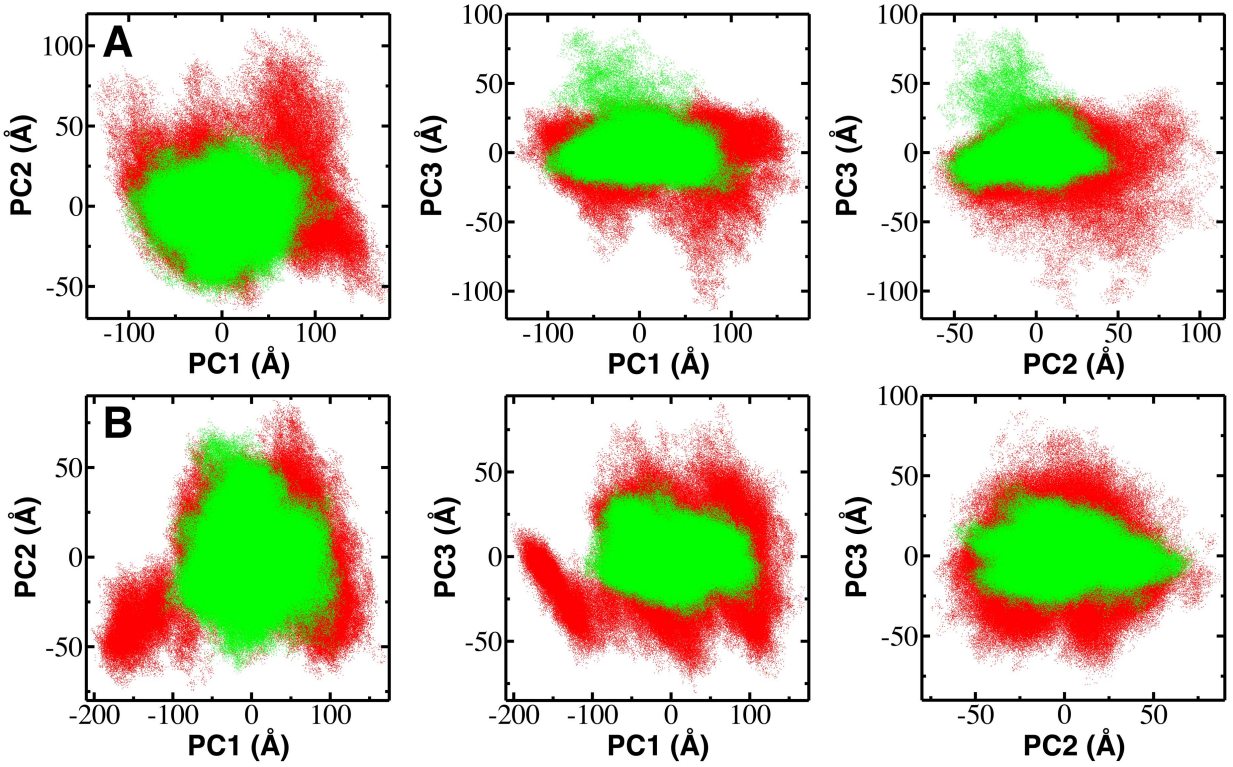

Figure S4. Principal Component Analysis of the motions of Pirin in the supramolecular complexes. Projection of the top three principal components of the Fe(III) form of Pirin (green) and the Fe(II) form of Pirin (red) in the Pirin-p65-DNA supramolecular complexes on either side of the homodimeric p65 in the supramolecular complexes, (A) and (B). Each dot represents a conformation.