S3_Text: Supplementary tables

Table A Partial charges on non hydrogen atoms of the metal binding residues before and after *ab-initio* calculations

Residue name	***Atom***	***AMBER charge***	***MS1 charge***		***MS2 charge***
			HIS79	***HIS98***	***HIS106***
HIS	N	-0.42	-0.42	-0.42	-0.42
	CA	0.02	0.02	0.02	0.02
	CB	-0.05	0.10	0.32	-0.22
	CG	-0.03	-0.14	0.08	0.03
	ND1	-0.38	-0.09	-0.23	-0.13
	CE1	0.21	-0.15	-0.15	-0.06
	NE2	-0.57	-0.12	-0.17	-0.08
	CD2	0.13	-0.02	-0.16	-0.13
	C	0.60	0.60	0.60	0.60
	O	-0.57	-0.57	-0.57	-0.57
			GLU83	***GLU172***	***GLU105***
GLU	N	-0.52	-0.52	-0.52	-0.52
	CA	0.04	0.04	0.04	0.04
	CB	0.06	0.25	0.25	-0.10
	CG	0.01	-0.05	-0.05	0.16
	CD	0.81	0.57	0.57	0.56
	OE1	-0.82	-0.62	-0.62	-0.56
	OE2	-0.82	-0.62	-0.62	-0.56
	C	0.54	0.54	0.54	0.54
	O	-0.58	-0.58	-0.58	-0.58
			GLN175		
GLN	N	-0.42	-0.42		
	CA	0.00	0.00		
	CB	0.00	0.00		
	CG	-0.06	0.00		
	CD	0.70	0.22		
	OE1	-0.61	-0.24		
	NE2	-0.94	-0.59		
	C	0.60	0.60		
	O	-0.57	-0.57		

					MET10
MET	N	-0.42			-0.42
	CA	-0.02			-0.02
	CB	0.03			0.04
	CG	0.00			0.04
	SD	-0.27			0.08
	CE	-0.05			-0.05
	C	0.60			0.60
	O	-0.57			-0.57
					CYS102
CYS	N	-0.42			-0.42
	CA	0.04			0.04
	CB	-0.08			-0.18
	SG	-0.11			-0.46
	C	0.60			0.60
	O	-0.57			-0.30
HOH	O	-1			-0.81
FE	FE	2	0.92		0.46

Table B Molecular Dynamics Protocol

Parameters	***MD protocol***
Time step for integration	2fs
Temperature	300K
Temperature coupling	Langevin dynamics
Pressure	1 bar
Electrostatic Interactions	Particle mesh Ewald
Water model	TIP3P
Force Field	ff99SB
Metal ion force field	Modified using MCPB
Size of cubic box	12 Å away from the farthest atom in all directions
Minimization	500 steps [SD] + 2500 steps [CG]
Equilibration	20ps + 50ps + 50ps = 120 ps
Length of production run	100 ns

Table C: List of dynamically stable hydrogen bonds between protein subunits and DNA.

System	*Chain A*			*Chain B*			*Chain C*			*Chain D*		
	DNA	*Protein*	*%O*	*DNA*	*Protein*	*%O*	*DNA*	*Protein*	*%O*	*DNA*	*Protein*	*%O*
FU-nm	10/O2P	28/N	99.3				13'/O2P	60/NH1	71.9	5/O1P	27/NH2	94.7
	10/O1P	27/NH2	98.4				13'/O2P	60/NE	59.1	24'/O2P	37/OG	84.0
	9/O1P	29/NH1	93.9							5/O1P	27/NE	79.7
	9/O2P	29/NH2	90.5							24'/O2P	40/OG1	66.3
	10/O1P	27/NE	75.0							4/O2P	29/NH1	53.5
	17'/O2P	43/NE2	69.4							6/O2P	42/OG	53.3
	18'/O2P	47/NH2	65.6							22'/O2P	47/NH2	53.1
	17'/O2P	47/NH1	62.0									
	11/O2P	27/NH2	53.6									
	17'/O2P	50/NH2	51.8									
FU-m	18'/O2P	7/OG1	62.5	20/O2P	7/OG1	73.5	13'/O1P	27/NH2	99.6	23'/O2P	11/OH	99.7
	17'/O1P	7/N	58.3	21/O2P	37/N	63.0	16/O2P	37/OG	95.1	24'/O2P	37/OG	99.7
	11/O2P	27/NH1	55.1	21/O2P	37/OG	62.5	12'/O1P	29/NH1	81.2	5/O1P	27/NH2	99.7
	17'/O2P	8/OG1	53.6	**20/N4*	*43/OE1*	*56.7*	13'/O1P	27/NE	76.3	22'/O2P	47/NH1	95.4
				20/O2P	36/NE2	56.5	12'/O2P	29/NE	74.2	4/O2P	29/NH2	78.5
				21/O2P	40/OG1	55.4	16/O2P	40/OG1	72.1	4/O1P	29/NH1	78.0
							14/O1P	7/OG1	52.7	24'/O2P	40/OG1	76.6
										**23'/N7*	*43/NE2*	*71.7*

* Hydrogen bonds involving DNA bases are marked in red and italicized. All other hydrogen bonds are formed between the phosphate group of DNA and protein residue.
%O represents percentage occupancy of the hydrogen bonds.

Table D List of residues forming dynamically stable clusters in the protein-DNA bipartite network

	Chain A	*Chain B*	*Chain C*	*Chain D*
FU-nm	d12 40 d19' 39 d20' 37	60 d8' 27	28 60 d12'	d7 d24' 37 d25' 39 d6
	28 27 d10 60 d9 26		29 d14' 27 28 d13' 60 d12'	36 40 d23'

	d19' 40 44 43 50 d17' 47 d18' ***7***			27 42 d5
	60 d11 27 d10 28 29 d9 26			26 42 d6 27 d5 28 29 d4
				7 37 40 d24' 36 d23'
FU-m	d19' 43 d18' 40	43 d20 40 d21 39 d22 37	d15' 39 d17 37 d16 40 d15	d7 d22' 43 d23' 40 d24' 37 d25' 39 d6
	47 d16' ***8***	36 40 d20 ***2***	26 28 27 d13' 60 d12'	26 28 27 d5 60 d4
	60 d10 27	***7*** 37 40 d21 36 d20 ***2***	36 40 d15	36 40 d23'
	7 d17' ***2***	50 d18 47 d19 ***8***	37 40 d16 36 d15 ***7*** d14 47 d13	***2 4 7*** 11 37 39 d24' 36 d23'
	6 d18' ***7 8*** 47 d17'***2***	60 d8' 27	60 d14' 27 28 d13' 26 29 d12'	60 d6 27 28 d5 26 29 d4
	60 d10 d11 27			43 47 d22'

* Network are generated at MEC = 2%. Cluster colours represent the different clusters obtained from bipartite network from different DNA entities, blue [nucleobases], green [deoxyribose sugar] and phosphate [orange]. Bold and underlined residues represent the N-terminal region. Also, note that DNA residues have a prefix 'd'.

Table E Top 20 protein-DNA pairs that contribute maximally to the free energy contribution in FU-nm and FU-m.

FU-nm			FU-m		
DNA	***P***	***E (kcal/mol)***	***DNA***	***P***	***E (kcal/mol)***
10	**27A**	**-20.903**	**5**	**27D**	**-21.594**
13'	**27C**	**-20.877**	**13'**	**27C**	**-20.080**
5	**27D**	**-16.351**	**4**	**29D**	**-13.838**
17'	**50A**	**-15.320**	**5**	**29C**	**-12.468**
17'	**47A**	**-14.580**	**17'**	**47A**	**-12.240**
4	**29D**	**-12.808**	**13'**	**60C**	**-12.227**
9	**29A**	**-12.154**	**19**	**47B**	**-11.606**
7'	**27B**	**-11.849**	**7'**	**27B**	**-11.179**
22'	**47D**	**-11.377**	**14**	**47C**	**-10.754**
13'	**60C**	**-10.501**	**15'**	**50A**	**-10.552**
24'	**37D**	**-10.339**	**22'**	**47D**	**-10.021**
8'	**60B**	**-9.723**	**10**	**60A**	**-9.389**
11	**27A**	**-9.130**	**18**	**50B**	**-9.276**
18'	**47A**	**-8.848**	**24'**	**37D**	**-8.775**

12’	60C	-8.205	10	27A	-8.525
12’	27A	-8.050	11	27A	-8.393
11’	29C	-7.616	5	60D	-8.373
6	27D	-7.362	16	37C	-7.700
24’	26D	-6.972	14’	60C	-6.595
24’	13D	-6.672	17’	7A	-6.563

*** Pairs are coloured based on protein residue location in the DNA binding domain. Orange represents protein residues from the 2nd helix, blue represents residues from the DBHs and red for N-terminal residues.**

Table F Mean and standard deviation values of the different parameters used to monitor the geometry of the metal center. Values are provided for individual subunit of all the metallated system studied (M1, M2, D-m and FU). Standard deviation is calculated over all the snapshots. The distance values are compared to experimental values obtained from (Feese *et.al.* J Biol Chem. 2001;276(8):5959-66 and Wisedchaisri G *et.al.* Journal of molecular biology. 2004;342(4):1155-69), representing the crystal structures IFX7 and 1U8R. Mean and standard deviation of these values are obtained from individual monomeric subunits of the crystal structure as provided in the literature. The angles are compared to expected values (text book) of the given geometry (distorted trigonal bipyramidal geometry for MS1 and octahedral geometry for MS2).

Parameter	M1	M2	Dm-A	Dm-B	FU-A	FU-B	FU-C	FU-D	Known
Distance between Fe and coordinating ligands									
Fe-79@NE2	2.05±0.06	2.07±0.06	2.08±0.06	2.05±0.06	2.08±0.06	2.05±0.06	2.07±0.06	2.07±0.06	2.05±0.10
Fe-83@OE2	1.99±0.06	1.99±0.06	1.98±0.06	1.99±0.06	1.98±0.06	1.99±0.06	1.99±0.06	1.98±0.06	1.99±0.10
Fe-98@ND1	2.06±0.06	2.07±0.05	2.07±0.06	2.06±0.06	2.07±0.06	2.06±0.06	2.06±0.06	2.06±0.06	2.07±0.09
Fe-172@OE1	2.05±0.06	2.04±0.06	2.01±0.07	2.04±0.06	2.00±0.06	2.02±0.06	2.03±0.06	1.99±0.06	1.92±0.11
Fe-175@OE1	2.02±0.06	2.03±0.06	2.00±0.06	2.01±0.07	2.01±0.06	2.01±0.06	2.00±0.06	2.01±0.07	1.94±0.14
Fe-10@SD	NA	2.37±0.06	2.39±0.07	2.39±0.06	2.39±0.07	2.37±0.06	2.39±0.06	2.39±0.06	2.32±0.11
Fe-102@O	NA	1.83±0.06	1.83±0.06	1.83±0.06	1.83±0.06	1.83±0.06	1.84±0.06	1.84±0.06	2.06±0.13
Fe-102@SG	NA	2.19±0.07	2.18±0.07	2.19±0.07	2.18±0.07	2.19±0.06	2.19±0.07	2.18±0.07	2.88±0.30
Fe-105@OE1	NA	1.98±0.06	1.96±0.06	1.97±0.06	1.96±0.06	1.96±0.06	1.97±0.06	1.97±0.06	1.97±0.08
Fe-106@NE2	NA	2.13±0.06	2.14±0.06	2.14±0.06	2.15±0.06	2.14±0.06	2.14±0.06	2.13±0.06	2.13±0.07
Angle between Fe and two coordinating ligands									
98@ND1-Fe-172@OE1	89.3±2.49	89.4±2.53	87.0±3.07	88.5±2.69	85.8±2.61	88.5±2.66	89.2±2.84	89.2±2.84	~90
172@OE1-Fe-79@NE2	87.0±2.96	88.9±3.13	92.2±3.47	88.6±3.39	92.7±3.30	87.8±3.23	89.1±3.33	92.2±3.02	~90

79@NE2-Fe-83@OE2	89.5±2.58	90.1±2.76	91.6±2.73	90.3±2.80	92.1±2.53	90.3±2.74	90.9±2.78	91.8±2.61	~90
83@OE2-Fe-175@OE1	90.4±2.93	89.2±2.94	90.3±2.90	90.2±2.99	90.4±2.89	90.4±2.98	90.0±2.89	90.2±2.94	~90
175@OE1-Fe-98@ND1	130.5±2.3	130.9±2.2	131.2±2.4	130.6±2.3	131.6±2.3	130.1±2.2	130.3±2.3	131.4±2.3	~120
105@OE2-Fe-106@NE2	NA	76.8±2.52	78.0±3.88	76.5±2.57	76.6±2.79	76.4±2.59	76.3±2.55	76.6±2.62	~90
106@NE2-Fe-102@O	NA	80.6±2.49	80.9±2.54	80.6±2.43	80.2±2.44	80.1±2.40	79.8±2.47	80.7±2.49	~90
102@O-Fe-102@SG	NA	107.3±2.6	107.6±2.8	107.0±2.6	106.8±2.6	107.4±2.5	107.2±2.6	107.1±2.8	~90

Table G

Coordinates of the metal centers used to generate the electrostatic parameters using MCPB.

Metal Site1 sidechain model for force constants:

```
REMARK
ATOM     627  CB  HIF     1       6.261  41.034   3.476
ATOM     628  CG  HIF     1       5.188  41.773   2.727
ATOM     629  ND1 HIF     1       4.801  43.044   3.085
ATOM     630  CD2 HIF     1       4.441  41.427   1.654
ATOM     631  CE1 HIF     1       3.847  43.454   2.266
ATOM     632  NE2 HIF     1       3.621  42.494   1.389
ATOM    2415  HB2 HIF     1       7.021  41.755   3.778
ATOM    2416  HB3 HIF     1       6.703  40.302   2.800
ATOM    2417  HD1 HIF     1       5.178  43.586   3.849
ATOM    2418  HE1 HIF     1       3.402  44.440   2.398
ATOM    2419  HD2 HIF     1       4.390  40.533   1.032
ATOM     661  CB  GLF     2       0.120  38.748   2.987
ATOM     662  CG  GLF     2       0.586  40.176   2.719
ATOM     663  CD  GLF     2       1.075  40.440   1.316
ATOM     664  OE1 GLF     2       1.603  39.502   0.685
ATOM     665  OE2 GLF     2       0.964  41.577   0.806
ATOM    2451  HB2 GLF     2       0.947  38.072   2.771
ATOM    2452  HB3 GLF     2      -0.712  38.528   2.319
ATOM    2453  HG2 GLF     2      -0.239  40.867   2.895
ATOM    2454  HG3 GLF     2       1.413  40.420   3.386
ATOM     785  CB  HIM     3      -0.523  44.821   0.179
ATOM     786  CG  HIM     3       0.820  45.444  -0.116
ATOM     787  ND1 HIM     3       1.967  44.704  -0.160
ATOM     788  CD2 HIM     3       1.155  46.741  -0.348
ATOM     789  CE1 HIM     3       2.985  45.518  -0.417
ATOM     790  NE2 HIM     3       2.512  46.756  -0.539
ATOM    2577  HB2 HIM     3      -0.624  43.888  -0.375
ATOM    2578  HB3 HIM     3      -1.318  45.506  -0.115
```

```
ATOM   2579  HE1 HIM     3       3.997  45.119  -0.492
ATOM   2580  HE2 HIM     3       3.071  47.573  -0.741
ATOM   2581  HD2 HIM     3       0.587  47.670  -0.402
ATOM   1340  CB  GLM     4       5.396  44.105  -3.202
ATOM   1341  CG  GLM     4       5.831  42.753  -2.638
ATOM   1342  CD  GLM     4       4.678  41.969  -2.022
ATOM   1343  OE1 GLM     4       3.643  42.572  -1.668
ATOM   1344  OE2 GLM     4       4.767  40.735  -1.923
ATOM   3134  HB2 GLM     4       6.273  44.585  -3.637
ATOM   3135  HB3 GLM     4       5.024  44.709  -2.375
ATOM   3136  HG2 GLM     4       6.256  42.145  -3.437
ATOM   3137  HG3 GLM     4       6.580  42.907  -1.861
ATOM   1366  CB  GLC     5       0.188  44.691  -3.464
ATOM   1367  CG  GLC     5       0.083  43.242  -3.885
ATOM   1368  CD  GLC     5       0.852  42.315  -2.959
ATOM   1369  OE1 GLC     5       0.810  42.457  -1.747
ATOM   1370  NE2 GLC     5       1.565  41.359  -3.532
ATOM   3156  HB2 GLC     5       1.250  44.888  -3.315
ATOM   3157  HB3 GLC     5      -0.333  44.769  -2.510
ATOM   3158  HG2 GLC     5      -0.963  42.935  -3.876
ATOM   3159  HG3 GLC     5       0.487  43.125  -4.891
ATOM   3160 HE21 GLC     5       2.096  40.717  -2.960
ATOM   3161 HE22 GLC     5       1.575  41.275  -4.538
ATOM   1779 FE   FE1     6       2.243  42.623  -0.240
ATOM     54  C   CH3     7       5.687  40.325   4.716
ATOM     55  H1  CH3     7       6.484  39.801   5.236
ATOM     56  H2  CH3     7       4.928  39.613   4.408
ATOM     57  H3  CH3     7       5.244  41.060   5.382
ATOM     58  C   CH3     8      -0.327  38.573   4.450
ATOM     59  H1  CH3     8      -0.652  37.550   4.610
ATOM     60  H2  CH3     8      -1.148  39.250   4.661
ATOM     61  H3  CH3     8       0.504  38.796   5.112
ATOM     62  C   CH3     9      -0.677  44.514   1.680
ATOM     63  H1  CH3     9      -1.651  44.068   1.861
ATOM     64  H2  CH3     9      -0.590  45.434   2.249
ATOM     65  H3  CH3     9       0.101  43.823   1.991
ATOM     66  C   CH3    10       4.300  43.936  -4.270
ATOM     67  H1  CH3    10       4.012  44.912  -4.651
ATOM     68  H2  CH3    10       3.435  43.452  -3.828
ATOM     69  H3  CH3    10       4.678  43.327  -5.085
ATOM     70  C   CH3    11      -0.422  45.625  -4.525
ATOM     71  H1  CH3    11      -0.332  46.656  -4.196
ATOM     72  H2  CH3    11      -1.470  45.380  -4.664
ATOM     73  H3  CH3    11       0.106  45.499  -5.466
```

Metal Site1 large model for RESP charges:

```
REMARK
ATOM    615  CH3 ACE     1       7.776  38.196   7.083
ATOM    616  C   ACE     1       6.562  38.865   6.446
```

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ATOM    617  O   ACE     1       5.436  38.697   6.905
ATOM   3582 HH31 ACE     1       7.483  37.580   7.933
ATOM   3583 HH32 ACE     1       8.264  37.574   6.333
ATOM   3584 HH33 ACE     1       8.466  38.971   7.416
ATOM    623  N   HIF     2       6.831  39.649   5.384
ATOM    624  CA  HIF     2       5.710  40.317   4.720
ATOM    625  C   HIF     2       4.658  39.317   4.259
ATOM    626  O   HIF     2       3.458  39.467   4.490
ATOM    627  CB  HIF     2       6.261  41.034   3.476
ATOM    628  CG  HIF     2       5.188  41.773   2.727
ATOM    629  ND1 HIF     2       4.801  43.044   3.085
ATOM    630  CD2 HIF     2       4.441  41.427   1.654
ATOM    631  CE1 HIF     2       3.847  43.454   2.266
ATOM    632  NE2 HIF     2       3.621  42.494   1.389
ATOM   2413  H   HIF     2       7.785  39.760   5.071
ATOM   2414  HA  HIF     2       5.241  41.016   5.413
ATOM   2415  HB2 HIF     2       7.021  41.755   3.778
ATOM   2416  HB3 HIF     2       6.703  40.302   2.800
ATOM   2417  HD1 HIF     2       5.178  43.586   3.849
ATOM   2418  HE1 HIF     2       3.402  44.440   2.398
ATOM   2419  HD2 HIF     2       4.390  40.533   1.032
ATOM    633  N   NME     3       5.133  38.287   3.539
ATOM    634  CH3 NME     3       4.207  37.337   2.913
ATOM   3585  H   NME     3       6.130  38.168   3.430
ATOM   3586 HH31 NME     3       4.354  37.344   1.833
ATOM   3587 HH32 NME     3       4.397  36.335   3.299
ATOM   3588 HH33 NME     3       3.181  37.625   3.141
ATOM    653  CH3 ACE     4       1.836  38.348   7.562
ATOM    654  C   ACE     4       0.588  38.471   6.689
ATOM    655  O   ACE     4      -0.549  38.374   7.178
ATOM   3589 HH31 ACE     4       1.572  38.285   8.618
ATOM   3590 HH32 ACE     4       2.379  37.450   7.268
ATOM   3591 HH33 ACE     4       2.465  39.223   7.396
ATOM    657  N   GLF     5       0.799  38.556   5.367
ATOM    658  CA  GLF     5      -0.328  38.561   4.441
ATOM    659  C   GLF     5      -1.171  37.293   4.557
ATOM    660  O   GLF     5      -2.398  37.412   4.566
ATOM    661  CB  GLF     5       0.120  38.748   2.987
ATOM    662  CG  GLF     5       0.586  40.176   2.719
ATOM    663  CD  GLF     5       1.075  40.440   1.316
ATOM    664  OE1 GLF     5       1.603  39.502   0.685
ATOM    665  OE2 GLF     5       0.964  41.577   0.806
ATOM   2449  H   GLF     5       1.743  38.617   5.012
ATOM   2450  HA  GLF     5      -0.970  39.416   4.654
ATOM   2451  HB2 GLF     5       0.947  38.072   2.771
ATOM   2452  HB3 GLF     5      -0.712  38.528   2.319
ATOM   2453  HG2 GLF     5      -0.239  40.867   2.895
ATOM   2454  HG3 GLF     5       1.413  40.420   3.386
ATOM    666  N   NME     6      -0.539  36.124   4.637
ATOM    667  CH3 NME     6      -1.273  34.862   4.794
ATOM   3592  H   NME     6       0.469  36.094   4.590
ATOM   3593 HH31 NME     6      -1.056  34.208   3.950
```

```
ATOM   3594 HH32 NME     6      -0.965  34.375   5.719
ATOM   3595 HH33 NME     6      -2.343  35.066   4.830
ATOM    775  CH3 ACE     7      -3.620  43.182   3.653
ATOM    776  C   ACE     7      -2.223  43.694   3.299
ATOM    777  O   ACE     7      -1.350  43.680   4.160
ATOM   3596 HH31 ACE     7      -3.681  42.902   4.705
ATOM   3597 HH32 ACE     7      -4.343  43.970   3.444
ATOM   3598 HH33 ACE     7      -3.840  42.314   3.032
ATOM    781  N   HIM     8      -1.966  44.082   2.052
ATOM    782  CA  HIM     8      -0.623  44.536   1.689
ATOM    783  C   HIM     8      -0.178  45.731   2.516
ATOM    784  O   HIM     8       0.967  45.699   3.027
ATOM    785  CB  HIM     8      -0.523  44.821   0.179
ATOM    786  CG  HIM     8       0.820  45.444  -0.116
ATOM    787  ND1 HIM     8       1.967  44.704  -0.160
ATOM    788  CD2 HIM     8       1.155  46.741  -0.348
ATOM    789  CE1 HIM     8       2.985  45.518  -0.417
ATOM    790  NE2 HIM     8       2.512  46.756  -0.539
ATOM   2575  H   HIM     8      -2.700  44.062   1.359
ATOM   2576  HA  HIM     8       0.090  43.728   1.851
ATOM   2577  HB2 HIM     8      -0.624  43.888  -0.375
ATOM   2578  HB3 HIM     8      -1.318  45.506  -0.115
ATOM   2579  HE1 HIM     8       3.997  45.119  -0.492
ATOM   2580  HE2 HIM     8       3.071  47.573  -0.741
ATOM   2581  HD2 HIM     8       0.587  47.670  -0.402
ATOM    791  N   NME     9      -0.986  46.782   2.660
ATOM    792  CH3 NME     9      -0.511  47.937   3.432
ATOM   3599  H   NME     9      -1.905  46.770   2.241
ATOM   3600 HH31 NME     9      -0.503  48.822   2.796
ATOM   3601 HH32 NME     9      -1.175  48.106   4.280
ATOM   3602 HH33 NME     9       0.498  47.742   3.794
ATOM   1330  CH3 ACE    10       4.063  41.378  -7.077
ATOM   1331  C   ACE    10       3.759  42.597  -6.227
ATOM   1332  O   ACE    10       2.684  43.163  -6.353
ATOM   3603 HH31 ACE    10       3.288  41.219  -7.826
ATOM   3604 HH32 ACE    10       5.022  41.529  -7.572
ATOM   3605 HH33 ACE    10       4.124  40.506  -6.426
ATOM   1336  N   GLM    11       4.614  42.945  -5.247
ATOM   1337  CA  GLM    11       4.294  43.971  -4.279
ATOM   1338  C   GLM    11       3.974  45.337  -4.876
ATOM   1339  O   GLM    11       3.144  46.053  -4.317
ATOM   1340  CB  GLM    11       5.396  44.105  -3.202
ATOM   1341  CG  GLM    11       5.831  42.753  -2.638
ATOM   1342  CD  GLM    11       4.678  41.969  -2.022
ATOM   1343  OE1 GLM    11       3.643  42.572  -1.668
ATOM   1344  OE2 GLM    11       4.767  40.735  -1.923
ATOM   3132  H   GLM    11       5.509  42.483  -5.175
ATOM   3133  HA  GLM    11       3.420  43.668  -3.703
ATOM   3134  HB2 GLM    11       6.273  44.585  -3.637
ATOM   3135  HB3 GLM    11       5.024  44.709  -2.375
ATOM   3136  HG2 GLM    11       6.256  42.145  -3.437
ATOM   3137  HG3 GLM    11       6.580  42.907  -1.861
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ATOM   1345  N   NME    12       4.609  45.735  -5.969
ATOM   1346  CH3 NME    12       4.352  47.043  -6.564
ATOM   3606  H   NME    12       5.287  45.126  -6.406
ATOM   3607 HH31 NME    12       5.274  47.624  -6.577
ATOM   3608 HH32 NME    12       3.990  46.914  -7.584
ATOM   3609 HH33 NME    12       3.600  47.569  -5.976
ATOM   1356  CH3 ACE    13       0.817  46.499  -7.958
ATOM   1357  C   ACE    13      -0.077  46.485  -6.742
ATOM   1358  O   ACE    13      -1.041  47.245  -6.620
ATOM   3610 HH31 ACE    13       0.390  47.112  -8.752
ATOM   3611 HH32 ACE    13       1.789  46.900  -7.671
ATOM   3612 HH33 ACE    13       0.937  45.476  -8.314
ATOM   1362  N   GLC    14       0.350  45.759  -5.699
ATOM   1363  CA  GLC    14      -0.392  45.719  -4.452
ATOM   1364  C   GLC    14      -0.340  47.079  -3.763
ATOM   1365  O   GLC    14      -1.279  47.388  -3.038
ATOM   1366  CB  GLC    14       0.188  44.691  -3.464
ATOM   1367  CG  GLC    14       0.083  43.242  -3.885
ATOM   1368  CD  GLC    14       0.852  42.315  -2.959
ATOM   1369  OE1 GLC    14       0.810  42.457  -1.747
ATOM   1370  NE2 GLC    14       1.565  41.359  -3.532
ATOM   3154  H   GLC    14       1.205  45.226  -5.775
ATOM   3155  HA  GLC    14      -1.432  45.462  -4.655
ATOM   3156  HB2 GLC    14       1.250  44.888  -3.315
ATOM   3157  HB3 GLC    14      -0.333  44.769  -2.510
ATOM   3158  HG2 GLC    14      -0.963  42.935  -3.876
ATOM   3159  HG3 GLC    14       0.487  43.125  -4.891
ATOM   3160 HE21 GLC    14       2.096  40.717  -2.960
ATOM   3161 HE22 GLC    14       1.575  41.275  -4.538
ATOM   1371  N   NME    15       0.717  47.853  -3.960
ATOM   1372  CH3 NME    15       0.916  49.144  -3.312
ATOM   3613  H   NME    15       1.446  47.556  -4.593
ATOM   3614 HH31 NME    15       1.832  49.118  -2.722
ATOM   3615 HH32 NME    15       0.995  49.923  -4.070
ATOM   3616 HH33 NME    15       0.070  49.357  -2.659
ATOM   1779 FE  FE1    16       2.243  42.623  -0.240
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Metal Site 2 sidechain model for force constants:

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REMARK
ATOM     76  CB  MEF     1      11.177  50.490   3.310
ATOM     77  CG  MEF     1       9.946  50.055   4.111
ATOM     78  SD  MEF     1       9.147  48.576   3.427
ATOM     79  CE  MEF     1       8.367  49.275   1.970
ATOM   1847  HB2 MEF     1      11.717  51.243   3.884
ATOM   1848  HB3 MEF     1      10.843  50.924   2.368
ATOM   1849  HG2 MEF     1      10.240  49.830   5.136
ATOM   1850  HG3 MEF     1       9.210  50.859   4.113
ATOM   1851  HE1 MEF     1       8.752  48.781   1.078
ATOM   1852  HE2 MEF     1       7.289  49.128   2.029
ATOM   1853  HE3 MEF     1       8.586  50.342   1.917
ATOM    811  CA  CYF     2       4.124  46.459   4.853
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ATOM   2599  HA  CYF     2       4.923  45.846   4.435
ATOM    812  C   CYF     2       4.623  47.092   6.162
ATOM    813  O   CYF     2       5.797  47.442   6.269
ATOM    814  CB  CYF     2       3.929  47.575   3.825
ATOM   2600  HB2 CYF     2       3.407  47.180   2.954
ATOM   2601  HB3 CYF     2       3.340  48.378   4.267
ATOM    815  SG  CYF     2       5.511  48.287   3.256
ATOM    845  CB  GLT     3       7.257  43.149   6.644
ATOM    846  CG  GLT     3       7.641  44.601   6.305
ATOM    847  CD  GLT     3       7.529  44.885   4.806
ATOM    848  OE1 GLT     3       7.312  43.942   4.036
ATOM    849  OE2 GLT     3       7.629  46.052   4.355
ATOM   2627  HB2 GLT     3       8.060  42.497   6.301
ATOM   2628  HB3 GLT     3       6.339  42.907   6.108
ATOM   2629  HG2 GLT     3       6.977  45.286   6.833
ATOM   2630  HG3 GLT     3       8.671  44.786   6.611
ATOM    854  CB  HIT     4       9.345  46.755   9.979
ATOM    855  CG  HIT     4       9.257  47.092   8.514
ATOM    856  ND1 HIT     4      10.238  46.778   7.618
ATOM    857  CD2 HIT     4       8.273  47.704   7.817
ATOM    858  CE1 HIT     4       9.881  47.183   6.402
ATOM    859  NE2 HIT     4       8.692  47.759   6.498
ATOM   2633  HB2 HIT     4       8.495  47.200  10.496
ATOM   2634  HB3 HIT     4      10.270  47.167  10.382
ATOM   2635  HD1 HIT     4      11.108  46.310   7.830
ATOM   2636  HE1 HIT     4      10.543  47.010   5.554
ATOM   2637  HD2 HIT     4       7.305  48.117   8.099
ATOM   6963 FE   FE2     5       7.280  47.921   4.876
ATOM   7031  O   OH1     6       6.986  50.124   5.514
ATOM   3570  H1  OH1     6       6.135  50.147   5.951
ATOM     44  C   CH3     7      12.107  49.296   3.025
ATOM     45  H1  CH3     7      12.968  49.635   2.457
ATOM     46  H2  CH3     7      11.569  48.547   2.453
ATOM     47  H3  CH3     7      12.440  48.864   3.964
ATOM     48  C   CH3     8       7.044  42.968   8.158
ATOM     49  H1  CH3     8       6.775  41.937   8.366
ATOM     50  H2  CH3     8       6.247  43.624   8.493
ATOM     51  H3  CH3     8       7.961  43.216   8.685
ATOM     52  C   CH3     9       9.331  45.231  10.202
ATOM     53  H1  CH3     9       9.396  45.020  11.265
ATOM     54  H2  CH3     9      10.178  44.783   9.693
ATOM     55  H3  CH3     9       8.410  44.815   9.806
ATOM     56  C   CH3    10       2.834  45.638   5.036
ATOM     57  H1  CH3    10       3.003  44.856   5.770
ATOM     58  H2  CH3    10       2.552  45.191   4.089
ATOM     59  H3  CH3    10       2.036  46.290   5.379
ATOM     60  C   CH3    11       3.479  47.237   7.182
ATOM     61  H1  CH3    11       3.861  47.686   8.094
ATOM     62  H2  CH3    11       3.067  46.258   7.406
ATOM     63  H3  CH3    11       2.700  47.870   6.767
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Metal Site2 large model for RESP charges:

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REMARK
ATOM     64  CH3 ACE     1      14.361  47.494   5.544
ATOM     65  C   ACE     1      13.495  47.805   4.335
ATOM     66  O   ACE     1      13.500  46.974   3.419
ATOM   3581 HH31 ACE     1      14.771  46.486   5.484
ATOM   3582 HH32 ACE     1      15.176  48.216   5.583
ATOM   3583 HH33 ACE     1      13.751  47.586   6.443
ATOM     72  N   MEF     2      12.901  48.990   4.218
ATOM     73  CA  MEF     2      12.104  49.299   3.026
ATOM     74  C   MEF     2      12.910  49.485   1.762
ATOM     75  O   MEF     2      12.625  49.106   0.627
ATOM     76  CB  MEF     2      11.177  50.490   3.310
ATOM     77  CG  MEF     2       9.946  50.055   4.111
ATOM     78  SD  MEF     2       9.147  48.576   3.427
ATOM     79  CE  MEF     2       8.367  49.275   1.970
ATOM   1845  H   MEF     2      13.001  49.676   4.952
ATOM   1846  HA  MEF     2      11.403  48.486   2.837
ATOM   1847  HB2 MEF     2      11.717  51.243   3.884
ATOM   1848  HB3 MEF     2      10.843  50.924   2.368
ATOM   1849  HG2 MEF     2      10.240  49.830   5.136
ATOM   1850  HG3 MEF     2       9.210  50.859   4.113
ATOM   1851  HE1 MEF     2       8.752  48.781   1.078
ATOM   1852  HE2 MEF     2       7.289  49.128   2.029
ATOM   1853  HE3 MEF     2       8.586  50.342   1.917
ATOM     80  N   NME     3      14.159  49.967   1.956
ATOM     81  CH3 NME     3      15.179  50.159   0.934
ATOM   3584  H   NME     3      14.456  50.232   2.884
ATOM   3585 HH31 NME     3      15.460  51.211   0.893
ATOM   3586 HH32 NME     3      16.056  49.559   1.178
ATOM   3587 HH33 NME     3      14.786  49.850  -0.035
ATOM    806  CH3 ACE     4       1.772  43.705   6.099
ATOM    807  C   ACE     4       3.026  44.516   5.828
ATOM    808  O   ACE     4       4.097  44.172   6.343
ATOM   3588 HH31 ACE     4       1.994  42.831   6.712
ATOM   3589 HH32 ACE     4       1.052  44.339   6.617
ATOM   3590 HH33 ACE     4       1.352  43.383   5.146
ATOM    810  N   CYF     5       2.946  45.630   5.088
ATOM    811  CA  CYF     5       4.124  46.459   4.853
ATOM    812  C   CYF     5       4.623  47.092   6.162
ATOM    813  O   CYF     5       5.797  47.442   6.269
ATOM    814  CB  CYF     5       3.929  47.575   3.825
ATOM    815  SG  CYF     5       5.511  48.287   3.256
ATOM   2598  H   CYF     5       2.061  45.903   4.686
ATOM   2599  HA  CYF     5       4.923  45.846   4.435
ATOM   2600  HB2 CYF     5       3.407  47.180   2.954
ATOM   2601  HB3 CYF     5       3.340  48.378   4.267
ATOM    816  N   NME     6       3.750  47.279   7.133
ATOM    817  CH3 NME     6       4.114  47.706   8.467
ATOM   3591  H   NME     6       2.767  47.122   6.961
ATOM   3592 HH31 NME     6       3.620  48.651   8.694
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ATOM   3593 HH32 NME     6       3.802  46.951   9.189
ATOM   3594 HH33 NME     6       5.194  47.838   8.525
ATOM    828  CH3 ACE     7       4.048  44.238  10.128
ATOM    829  C   ACE     7       5.363  43.553   9.821
ATOM    830  O   ACE     7       6.046  43.050  10.732
ATOM   3595 HH31 ACE     7       3.788  44.134  11.181
ATOM   3596 HH32 ACE     7       4.139  45.295   9.878
ATOM   3597 HH33 ACE     7       3.268  43.786   9.514
ATOM    841  N   GLT     8       5.795  43.609   8.555
ATOM    842  CA  GLT     8       7.037  42.942   8.166
ATOM    843  C   GLT     8       8.240  43.444   8.935
ATOM    844  O   GLT     8       9.264  42.762   8.952
ATOM    845  CB  GLT     8       7.257  43.149   6.644
ATOM    846  CG  GLT     8       7.641  44.601   6.305
ATOM    847  CD  GLT     8       7.529  44.885   4.806
ATOM    848  OE1 GLT     8       7.312  43.942   4.036
ATOM    849  OE2 GLT     8       7.629  46.052   4.355
ATOM   2625  H   GLT     8       5.260  44.115   7.864
ATOM   2626  HA  GLT     8       6.948  41.871   8.350
ATOM   2627  HB2 GLT     8       8.060  42.497   6.301
ATOM   2628  HB3 GLT     8       6.339  42.907   6.108
ATOM   2629  HG2 GLT     8       6.977  45.286   6.833
ATOM   2630  HG3 GLT     8       8.671  44.786   6.611
ATOM    850  N   HIT     9       8.185  44.666   9.490
ATOM    851  CA  HIT     9       9.330  45.220  10.185
ATOM    852  C   HIT     9       9.373  44.928  11.676
ATOM    853  O   HIT     9      10.336  45.355  12.342
ATOM    854  CB  HIT     9       9.345  46.755   9.979
ATOM    855  CG  HIT     9       9.257  47.092   8.514
ATOM    856  ND1 HIT     9      10.238  46.778   7.618
ATOM    857  CD2 HIT     9       8.273  47.704   7.817
ATOM    858  CE1 HIT     9       9.881  47.183   6.402
ATOM    859  NE2 HIT     9       8.692  47.759   6.498
ATOM   2631  H   HIT     9       7.336  45.209   9.424
ATOM   2632  HA  HIT     9      10.247  44.812   9.759
ATOM   2633  HB2 HIT     9       8.495  47.200  10.496
ATOM   2634  HB3 HIT     9      10.270  47.167  10.382
ATOM   2635  HD1 HIT     9      11.108  46.310   7.830
ATOM   2636  HE1 HIT     9      10.543  47.010   5.554
ATOM   2637  HD2 HIT     9       7.305  48.117   8.099
ATOM    860  N   NME    10       8.315  44.344  12.229
ATOM    861  CH3 NME    10       8.275  44.116  13.671
ATOM   3598  H   NME    10       7.539  44.058  11.649
ATOM   3599 HH31 NME    10       7.422  44.643  14.099
ATOM   3600 HH32 NME    10       8.178  43.048  13.868
ATOM   3601 HH33 NME    10       9.195  44.486  14.124
ATOM   6963 FE   FE2    11       7.280  47.921   4.876
ATOM   7031  O   OH1    12       6.986  50.124   5.514
ATOM   3570  H1  OH1    12       6.549  50.789   4.981
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