

Supporting Information

Role of Structural Dynamics in Selectivity and Mechanism of Non-Heme Fe(II) and 2-Oxoglutarate-Dependent Oxygenases Involved in DNA Repair

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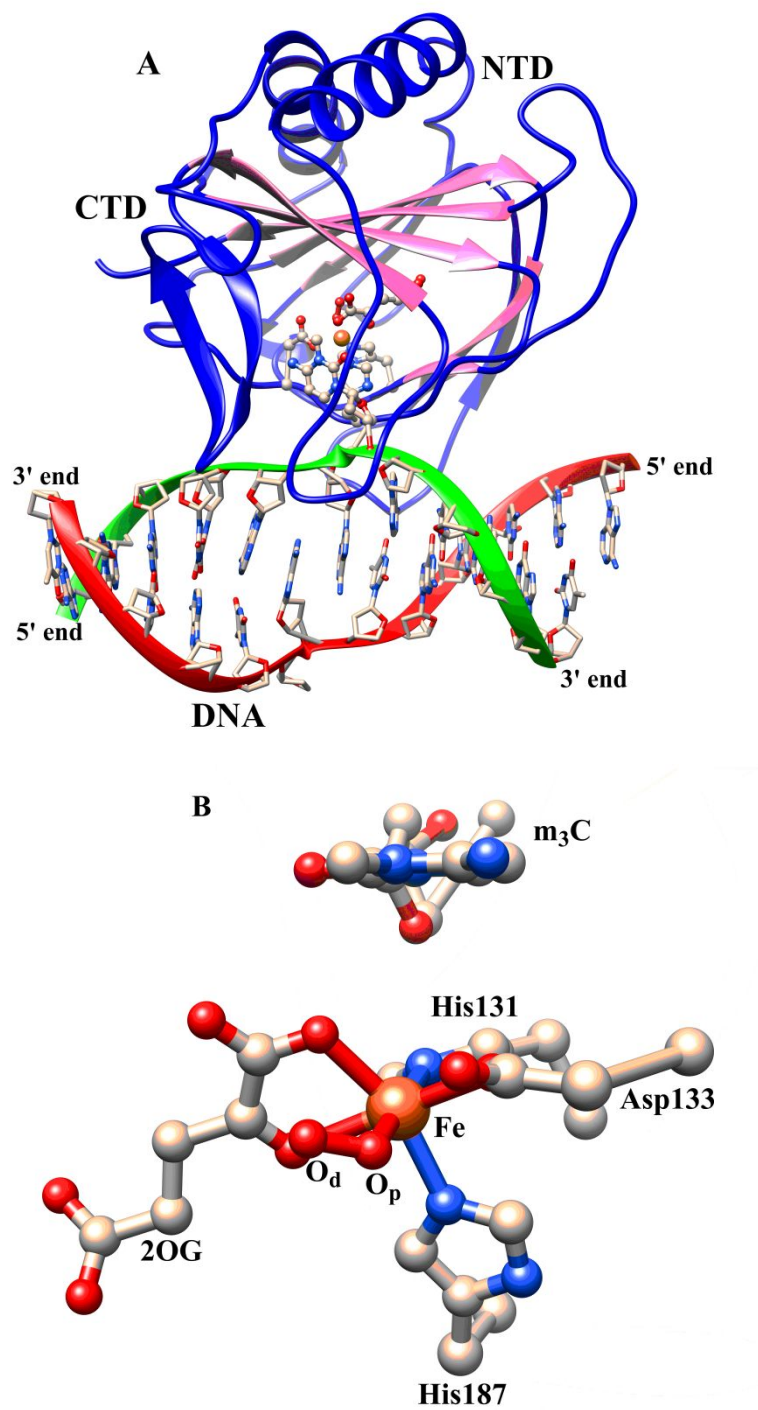


Figure S1 Average structure of AlkB-dsDNA (A) and a view of the AlkB-dsDNA active site (B) derived from the Fe(III)-superoxo MD simulations. Coloring in (A): double stranded beta helix (DSBH) core fold (pink). m₃C: 3-methylcytosine.

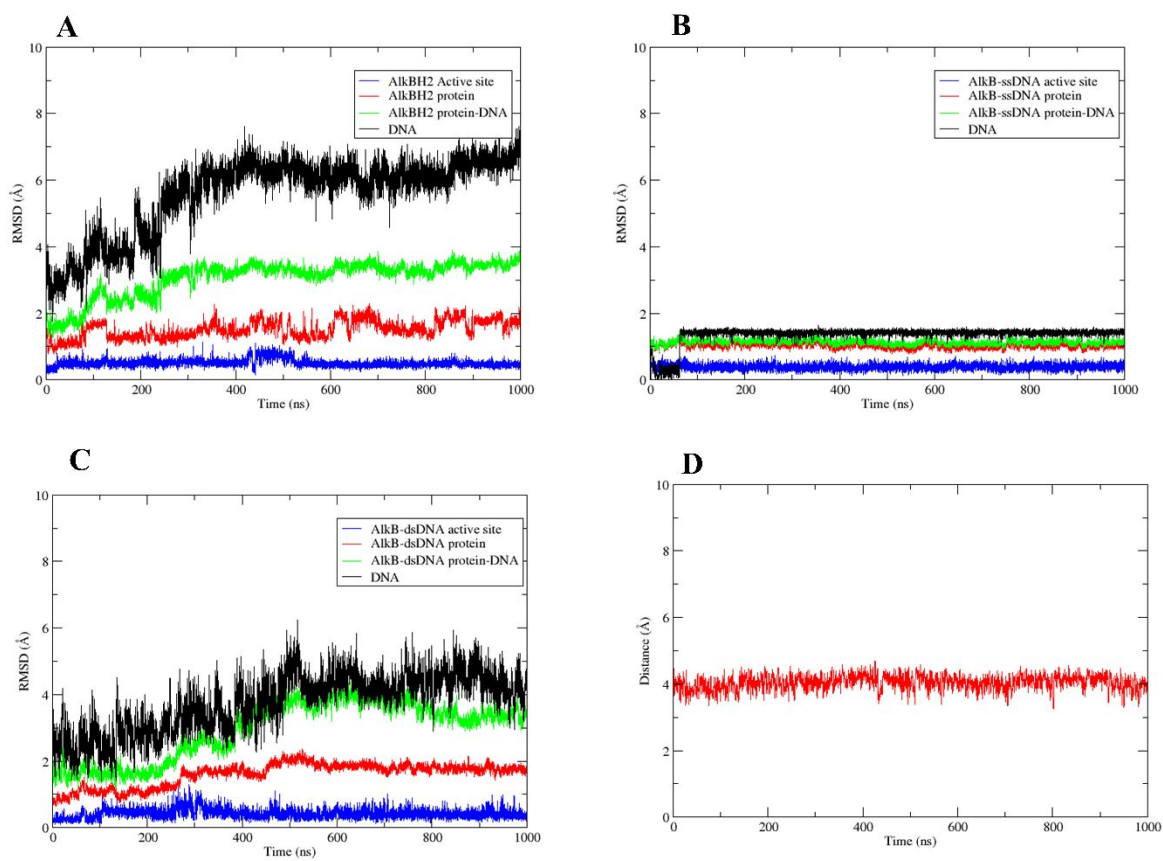


Figure S2 RMSD Plots for AlkBH2-dsDNA (A), AlkB-ssDNA (B), AlkB-dsDNA (C) and plot of the distance between the distal oxygen (O_d) of the superoxide and C2 of 2OG (D) in the AlkBH2-dsDNA Fe(III)-superoxo complex.

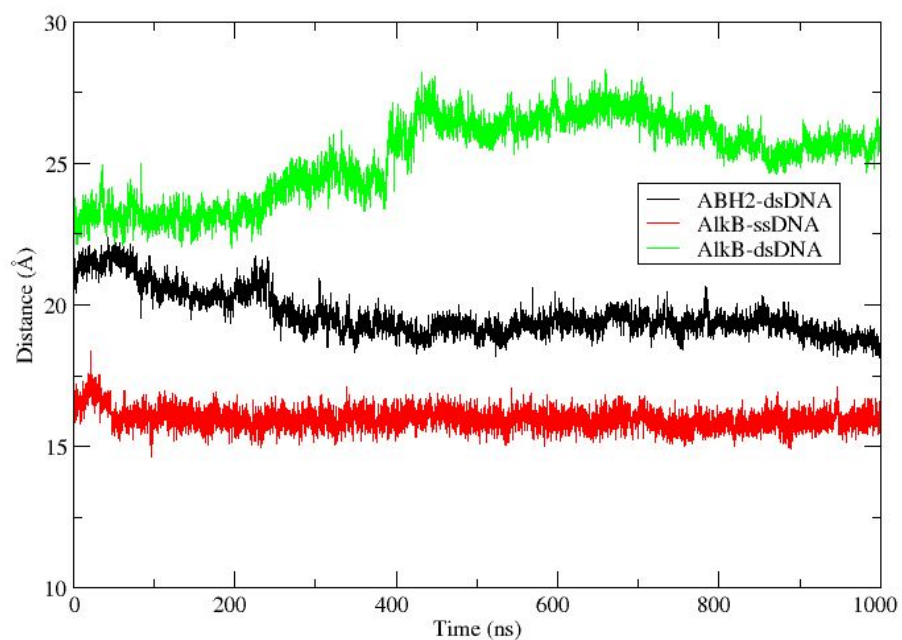


Figure S3 Measured distances between the center of mass of the protein and the DNA molecule in the AlkBH2-dsDNA, AlkB-ssDNA and AlkB-dsDNA complexes, during MD simulations of the Fe(III)-superoxo intermediates.

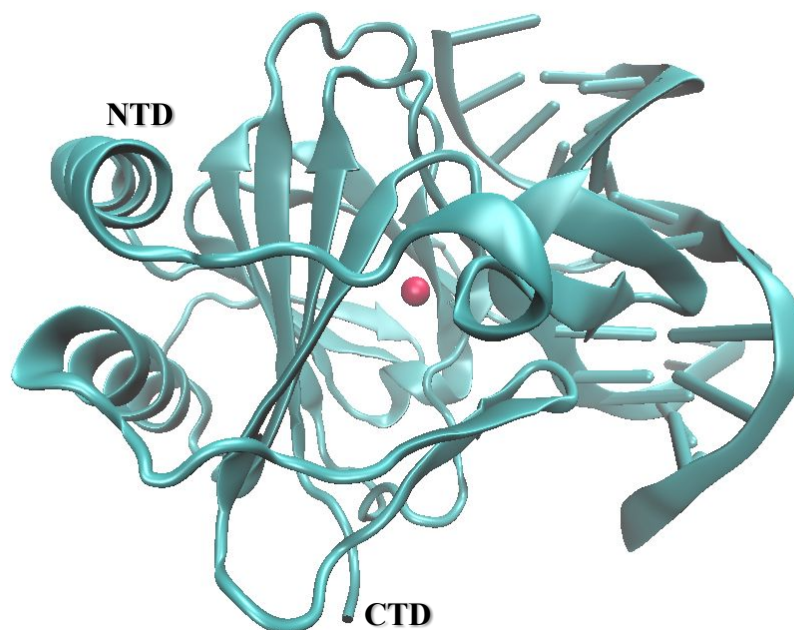


Figure S4 View of the structure of AlkBH2-dsDNA showing the location of the center of mass (in red sphere) of the protein-DNA complex. NTD and CTD are N-terminal Domain and C-terminal Domain, respectively.

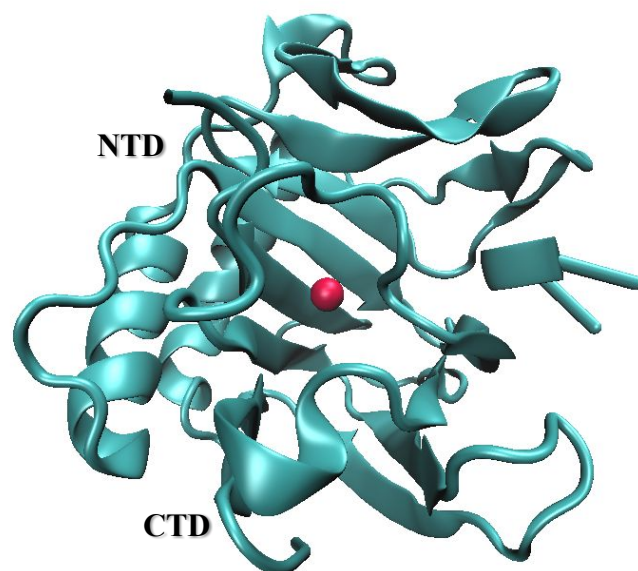


Figure S5 View of the structure of AlkB-ssDNA showing the location of the center of mass (in red sphere) of the protein-DNA complex. NTD and CTD are N-terminal Domain and C-terminal Domain, respectively.

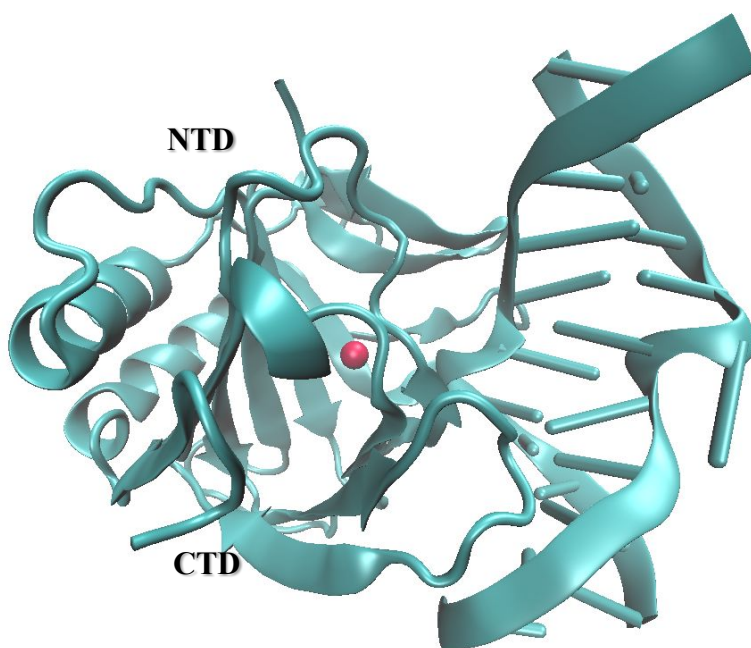


Figure S6 View of the structure of AlkB-dsDNA showing the location of the center of mass (in red sphere) of the protein-DNA complex. NTD and CTD are N-terminal Domain and C-terminal Domain, respectively.

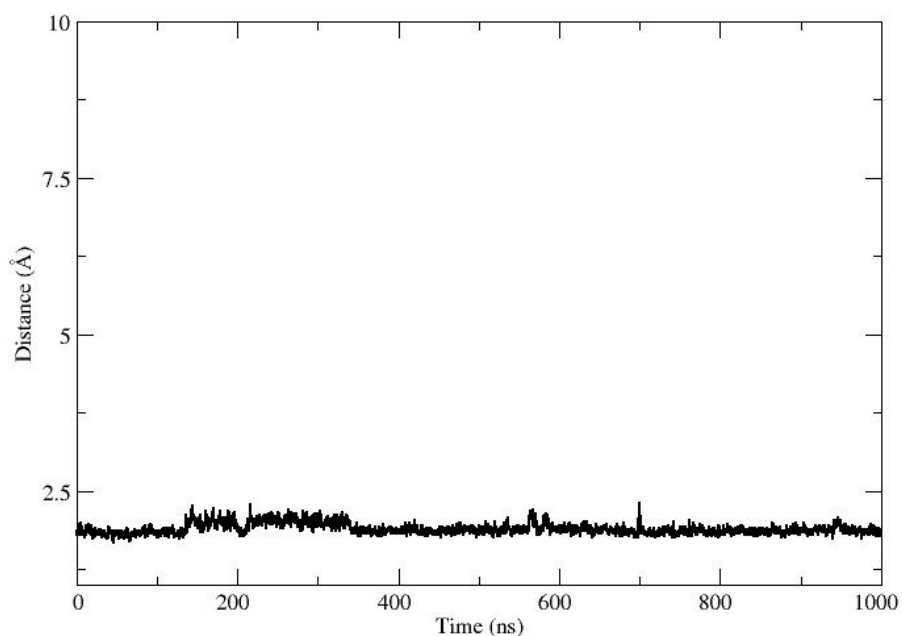


Figure S7 Hydrogen bonding interaction of Arg254 side chain with the non metal ion coordinating carboxylate oxygen of Asp173 in the AlkBH2-dsDNA complex during the Fe(III)-superoxo MD simulations. The distance was measured between the center of mass of the atoms forming the guanidino group of Arg254 and the carboxylate of Asp173.

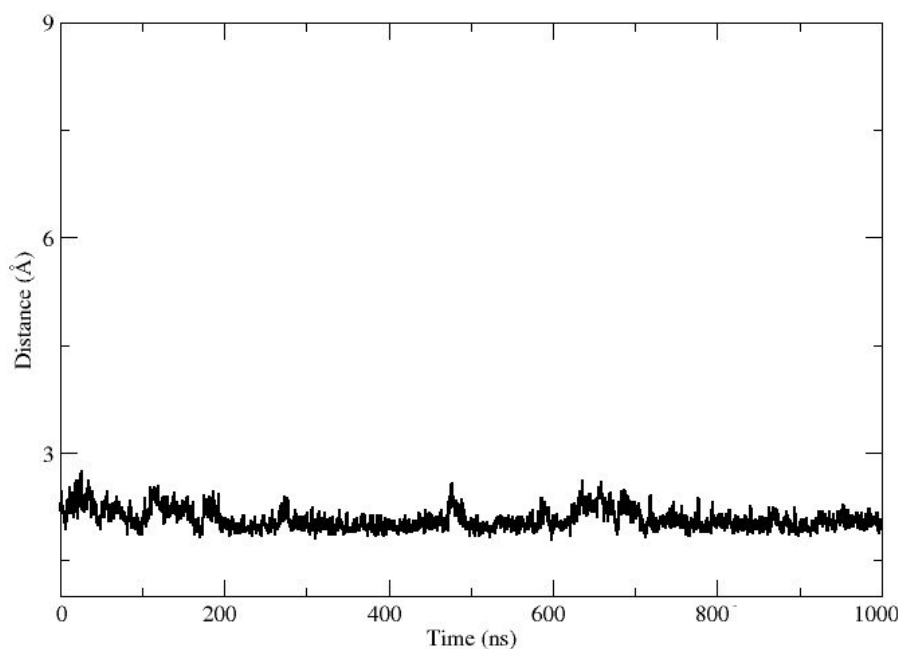


Figure S8 Hydrogen bonding interaction of Arg210 side chain with the non metal ion coordinating carboxylate oxygen of Asp133 in the AlkB-ssDNA complex during the Fe(III)-superoxo MD simulations. The distance was measured between the center of mass of the atoms forming the guanidino group of Arg210 and the carboxylate of Asp133.

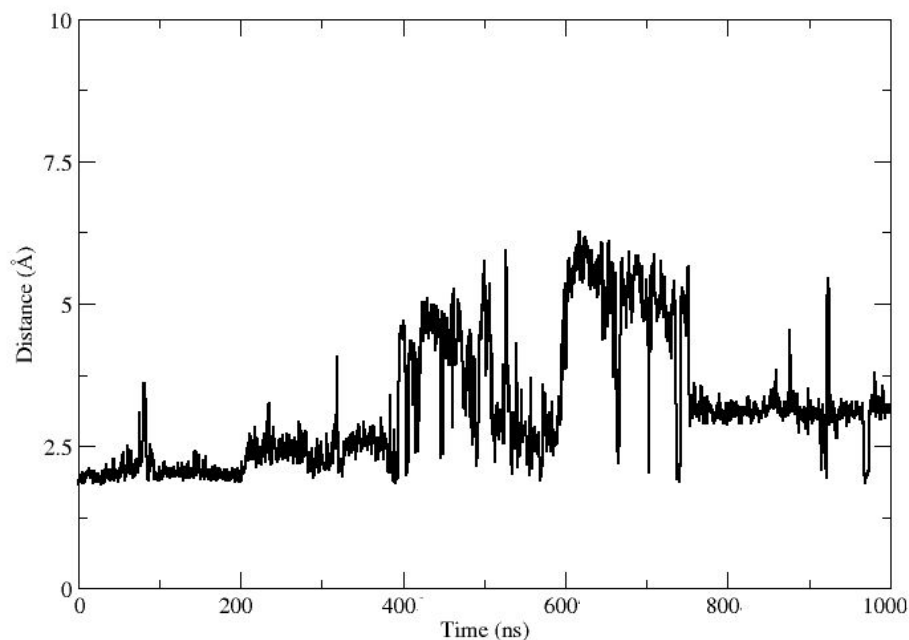


Figure S9 Hydrogen bonding interaction of Arg210 side chain with the non meta ion coordinating carboxylate oxygen of Asp133 in the AlkB-dsDNA complex during the Fe(III)-superoxo MD simulations. The distance was measured between the center of mass of the atoms forming the guanidino group of Arg210 and the carboxylate of Asp133.

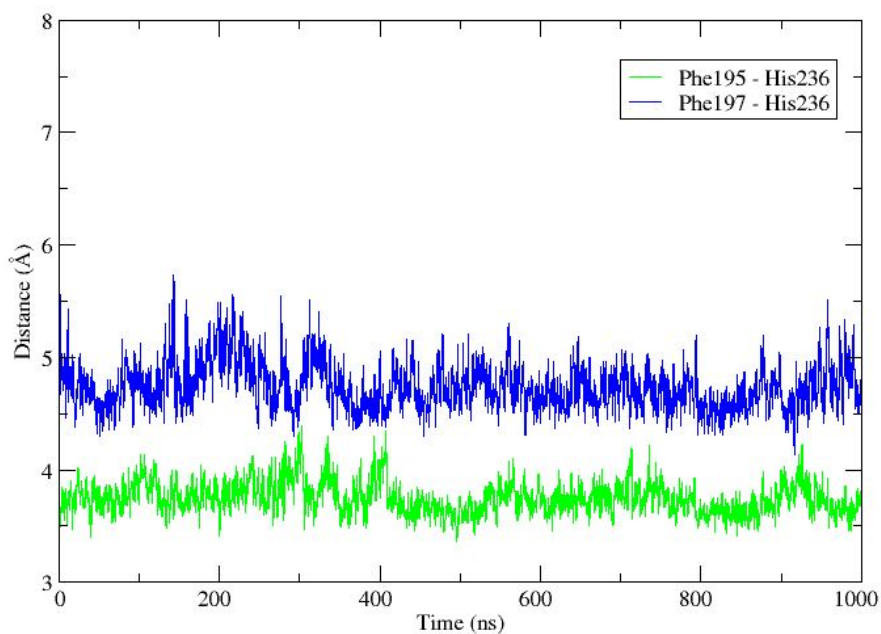


Figure S10 Stacking interaction of the iron coordinating residue His236 (His²) with Phe195 and Phe197 at the Fe(III)-superoxo intermediate stage of the AlkBH2-dsDNA complex. Distances were measured between the center of mass of the atoms forming the imidazole ring of His236 and the phenyl groups of Phe195 and Phe197.

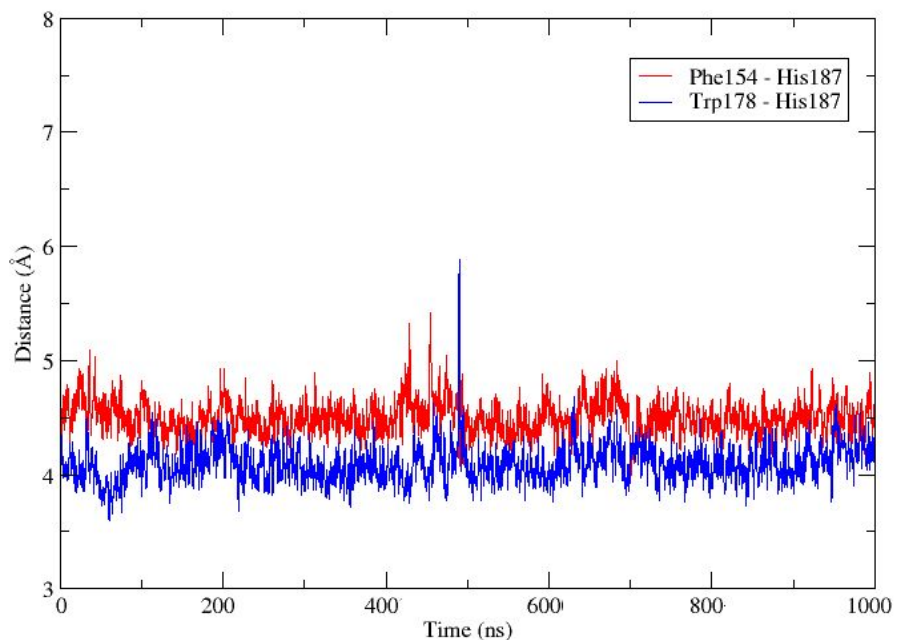


Figure S11 Stacking interactions of the iron coordinating residue His187 (His²) with Phe154 and Trp178 at the Fe(III)-superoxo intermediate stage of the AlkB-ssDNA complex. Distances were measured between the center of mass of the atoms forming the imidazole ring of His187, the phenyl group of Phe154, and the indole group of Trp178.

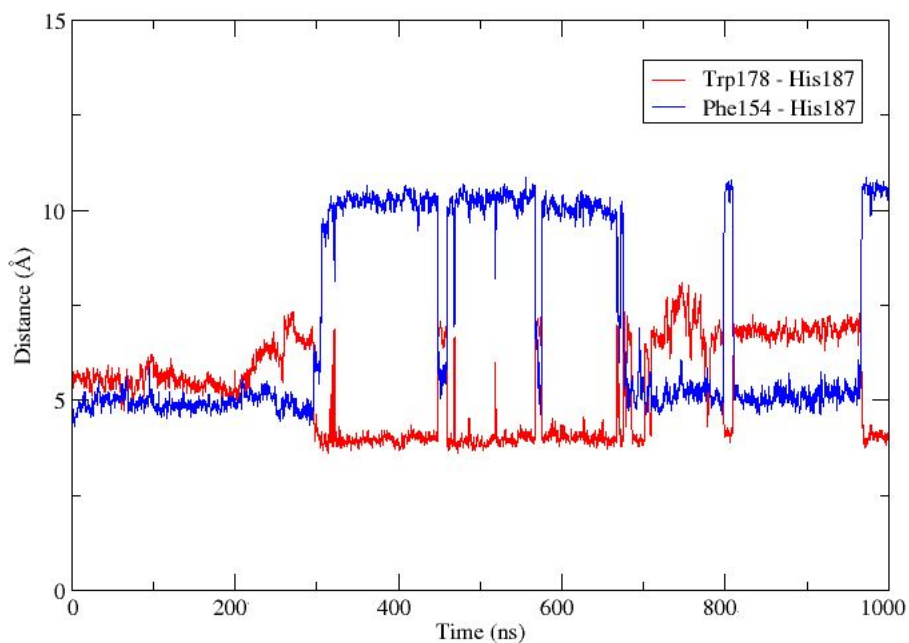


Figure S12 Stacking interactions of the iron coordinating residue His187 (His²) with Phe154 and Trp178 at the Fe(III)-superoxo intermediate stage of the AlkB-dsDNA complex. Distances were measured between the center of mass of the atoms forming the imidazole group of His187, phenyl group of Phe154, and indole group of Trp178.

With AlkBH2-dsDNA, DCCA shows that residues 57-87, belonging to (β 1- β 2) and (α 1), manifest a positive correlation with residues 210-237 (β 11- β 13), and residues 152-197 (β 8- β 10) manifest a positive correlation with residues 210-250 (β 11- β 14) and (α 5) (Figure 2A). Similarly, in AlkB-ssDNA (Fig. S13), residues 17-27 (β 1) show a positive correlation with 174-178 (the loop connecting β 9 to β 10), and residues 114-159 (β 5- β 8) have a positive correlation with residues 164-210 (β 9- β 12) and (α 3). With AlkB-dsDNA (Fig. S14), residues 43-60 (α 1) have a positive correlation with residues 65-93 (β 3- β 4); residues 15-26 (β 1) show a positive correlation with residues 98-113 (α 2); residues 58-63 (β 2) have a positive correlation with 113-128 (β 5); residues 93-133 (α 3) and (β 5- β 6) have positive correlations with residues 128-178 (β 6- β 10); residues 113-184 (β 5- β 8) have a positive correlation with residues 158-191 (β 9- β 11); and residues 123-193 (β 6- β 11) and (α 3) show a negative correlation with the DNA. Figures S15 and S16 contain the annotated secondary structures of AlkBH2-dsDNA and AlkBs, respectively.

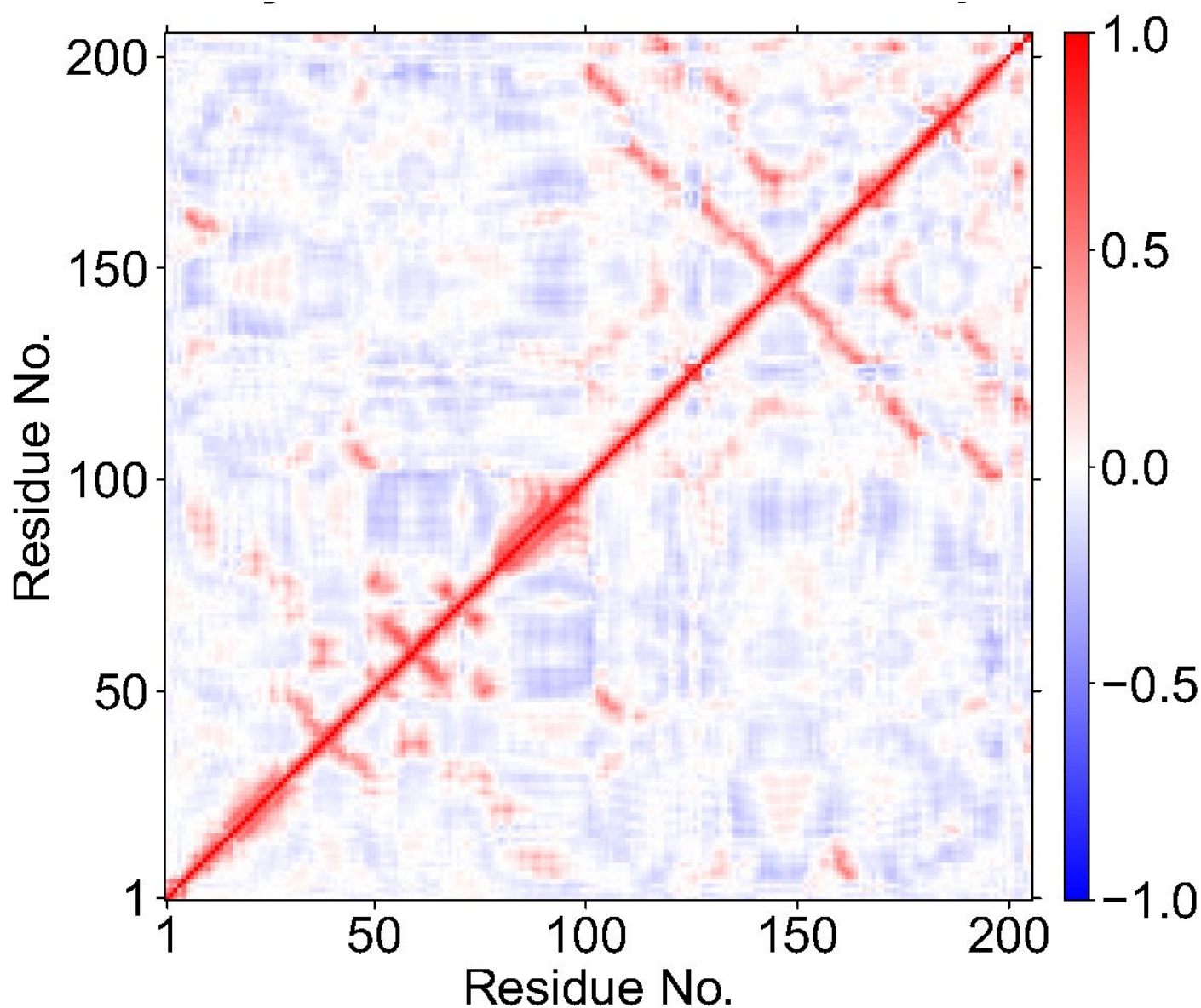


Figure S13 Dynamic cross correlation for the Fe(III)-superoxo intermediate stage of the AlkB-ssDNA complex. Residue numbers 1-200 (protein), 201 (Fe), 202 (O₂), 203 (2OG), 204-206 (DNA) and 205 (m₃C substrate).

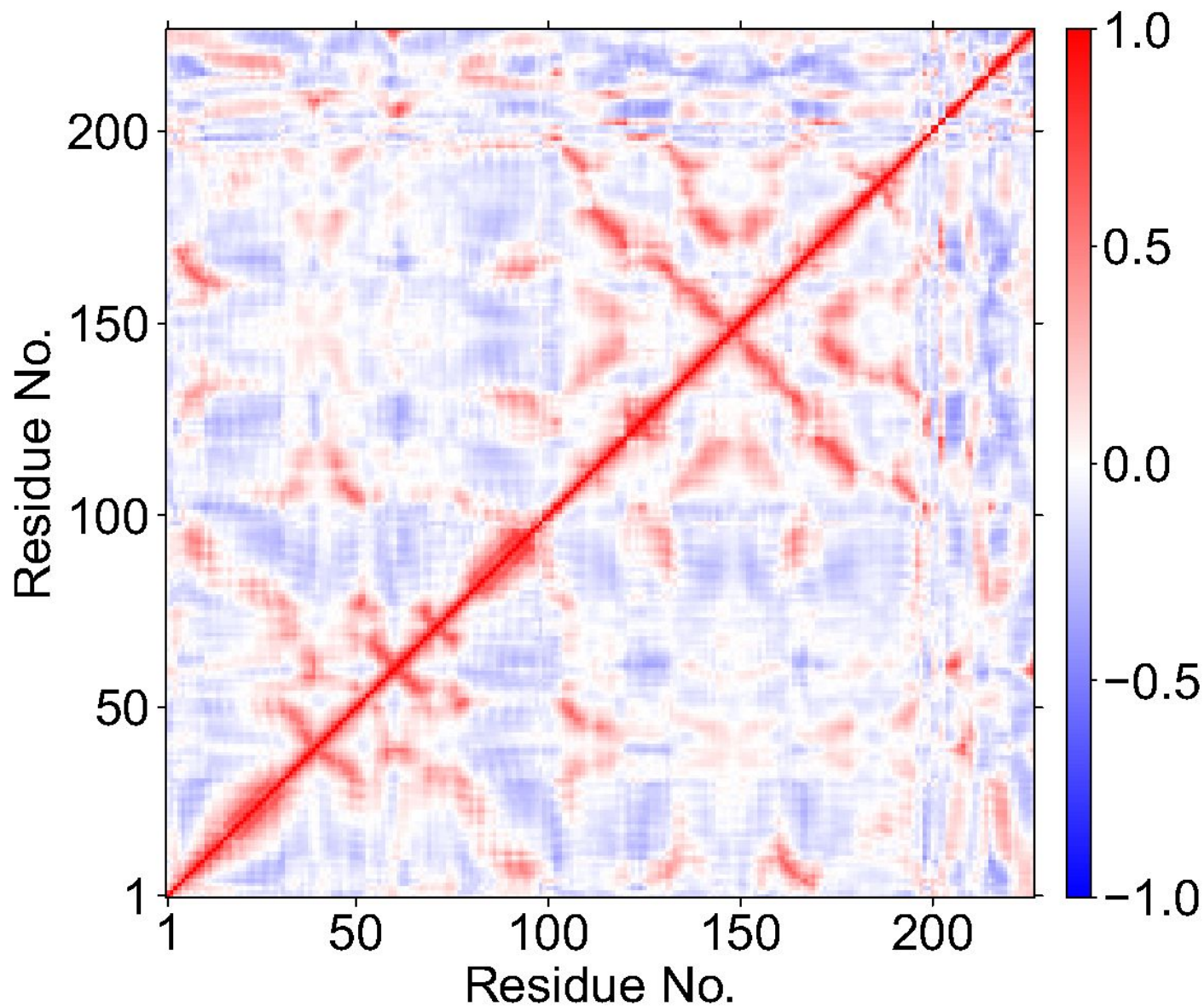


Figure S14 Dynamic cross correlation for the Fe(III)-superoxo intermediate stage of the complex AlkB-dsDNA. Residue numbers 1-201 (protein), 202 (Fe), 203 (O₂), 204 (2OG), 205-229 (DNA) and 211 (m₃C substrate).

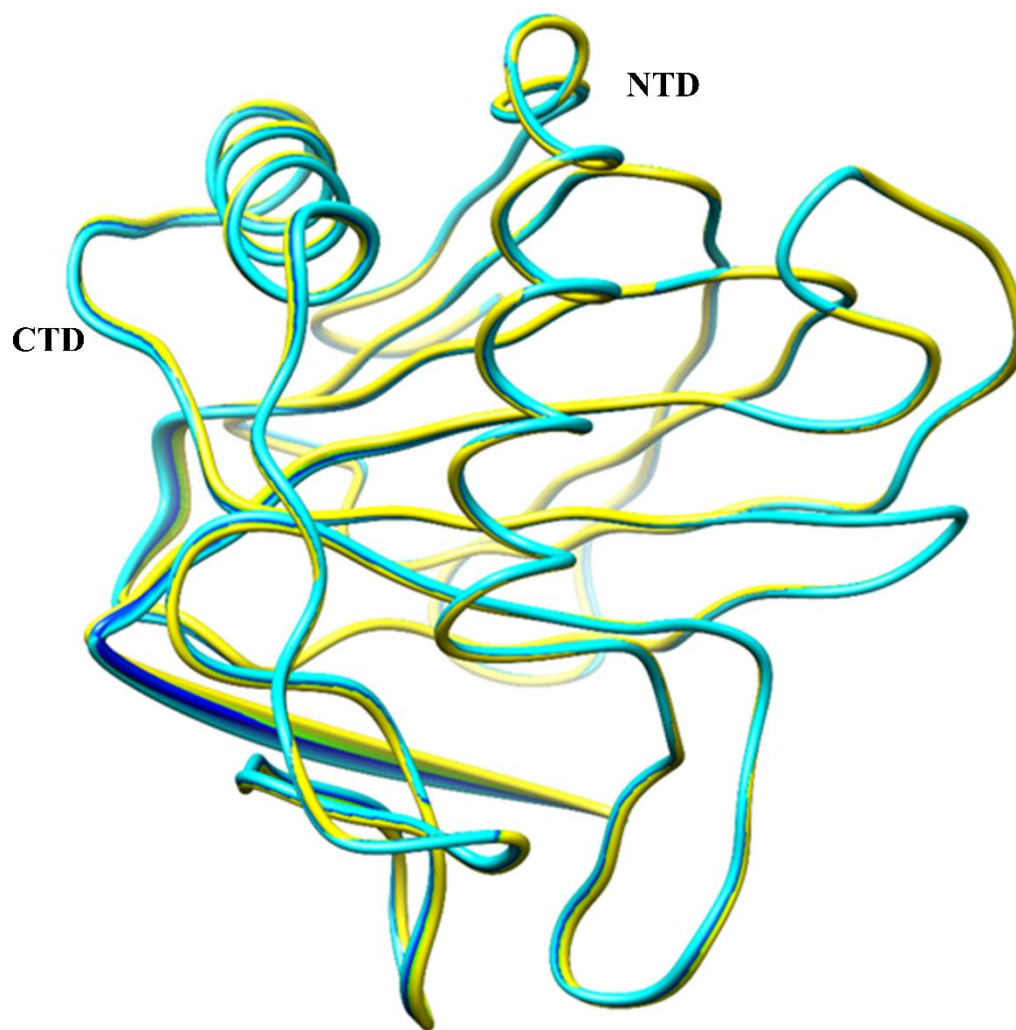


Figure S17 PCA for the AlkB-ssDNA Fe(III)-superoxo MD simulation. Yellow to blue coloring represents the main direction of motion of protein residues. NTD and CTD are N-terminal Domain and C-terminal Domain, respectively.

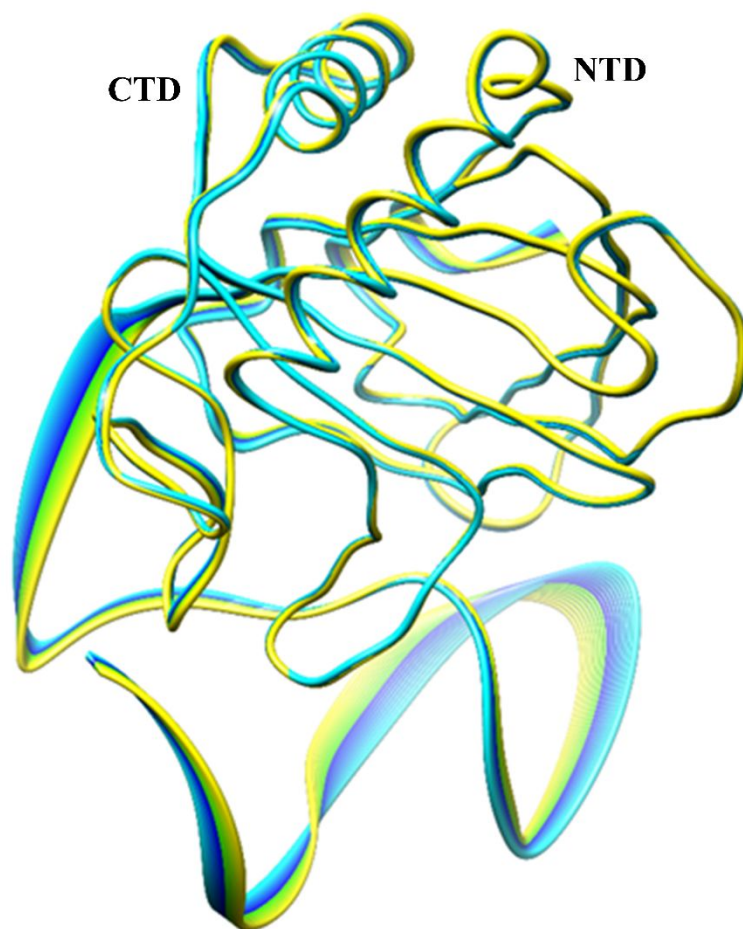


Figure S18 PCA for the AlkB-dsDNA Fe(III)-superoxo MD simulation. Yellow to blue coloring represents the main direction of motion of protein residues. NTD and CTD are N-terminal Domain and C-terminal Domain, respectively.

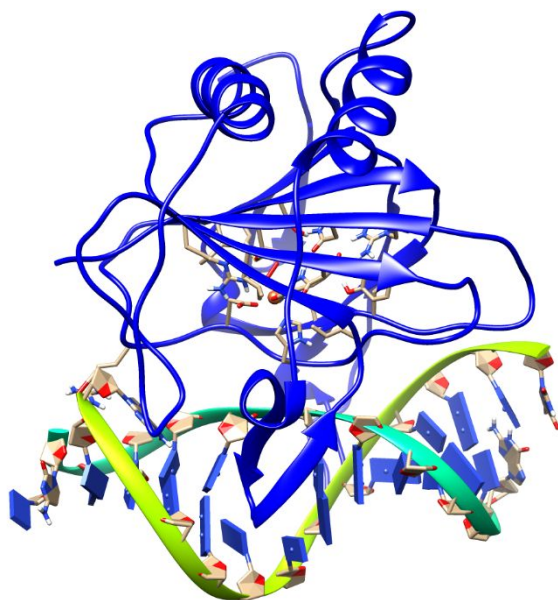


Figure S19 View of an MD structure of AlkBH2-dsDNA with undamaged DNA.

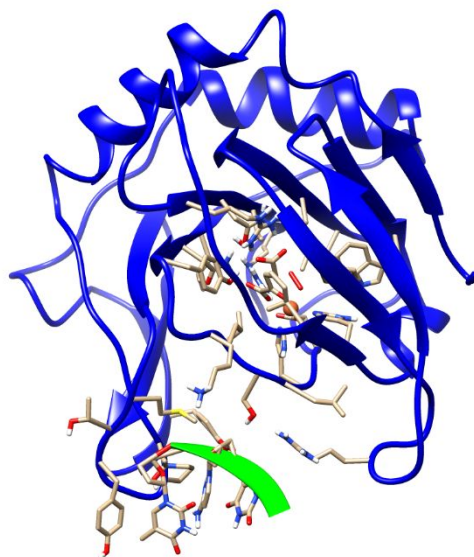


Figure S20 View of an MD structure of AlkB-ssDNA with undamaged DNA.

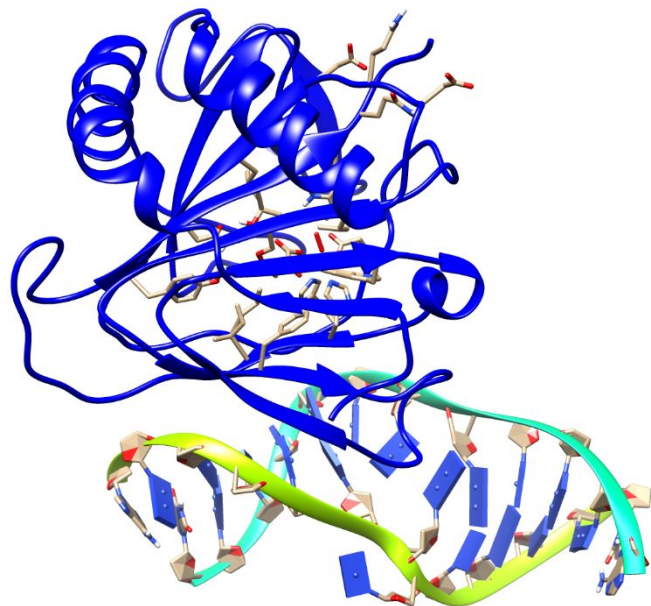


Figure S21 View of an MD structure of AlkB-dsDNA with undamaged DNA.

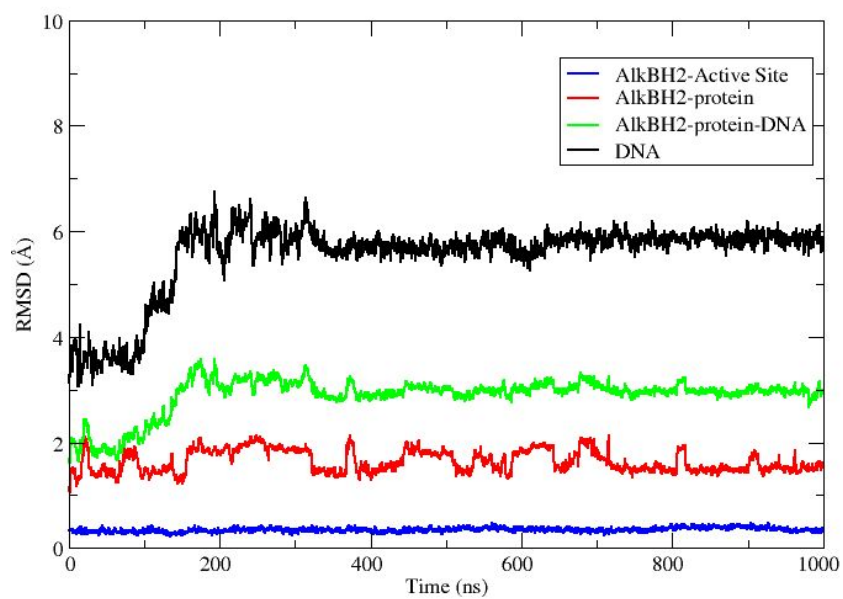


Figure S22 RMSD Plot for AlkBH2-dsDNA with undamaged DNA.

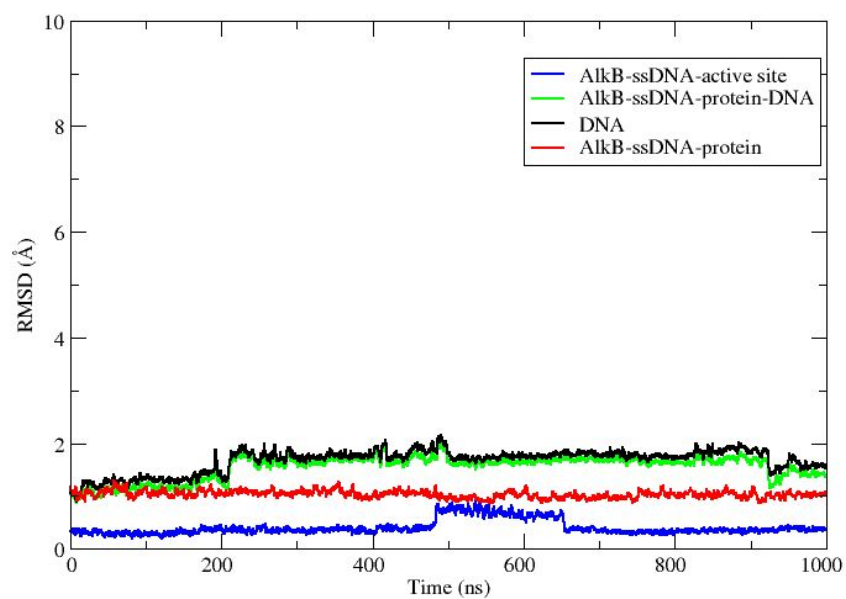


Figure S23 RMSD Plot for AlkB-ssDNA with undamaged DNA.

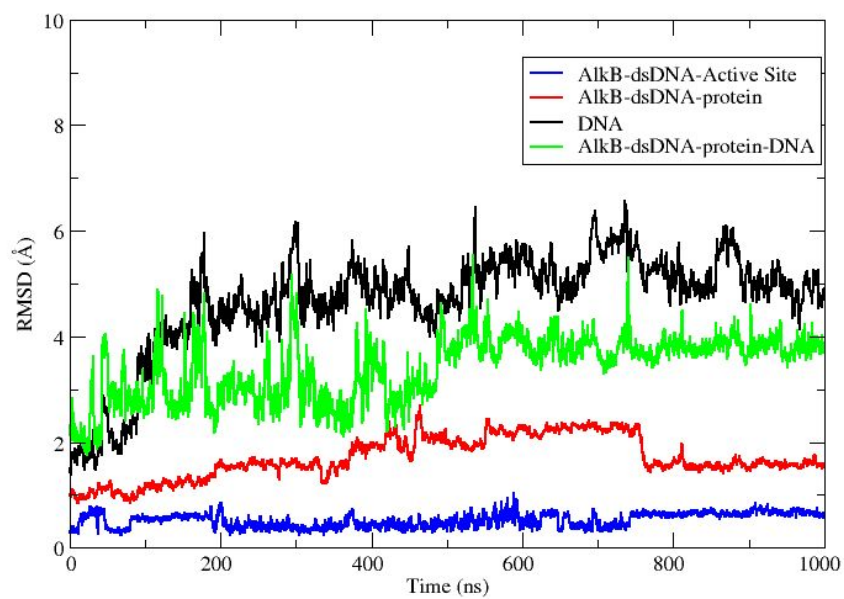


Figure S24 RMSD Plot for AlkB-dsDNA with undamaged DNA.

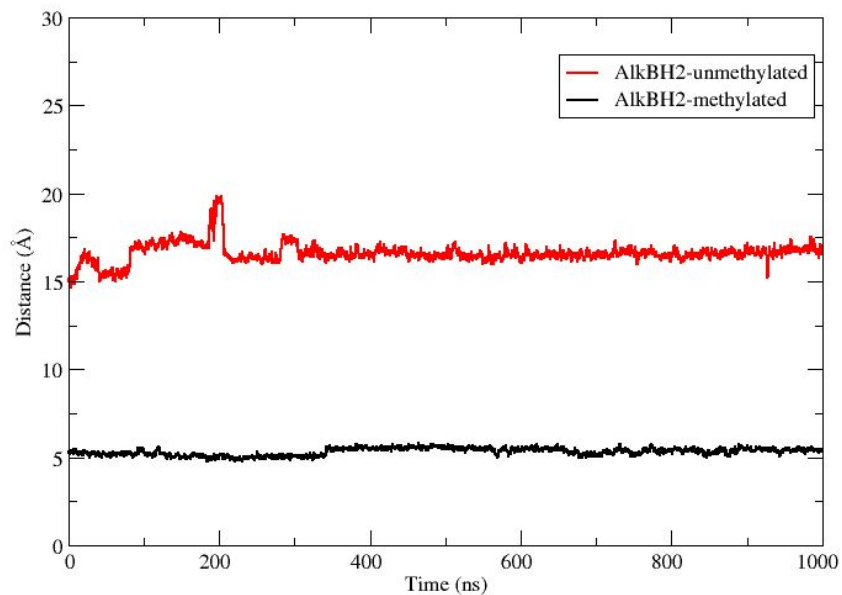


Figure S25 The distance between Fe center (Fe) and N3 of the substrate in the AlkBH2-dsDNA Fe(III)-superoxo complex MD simulations.

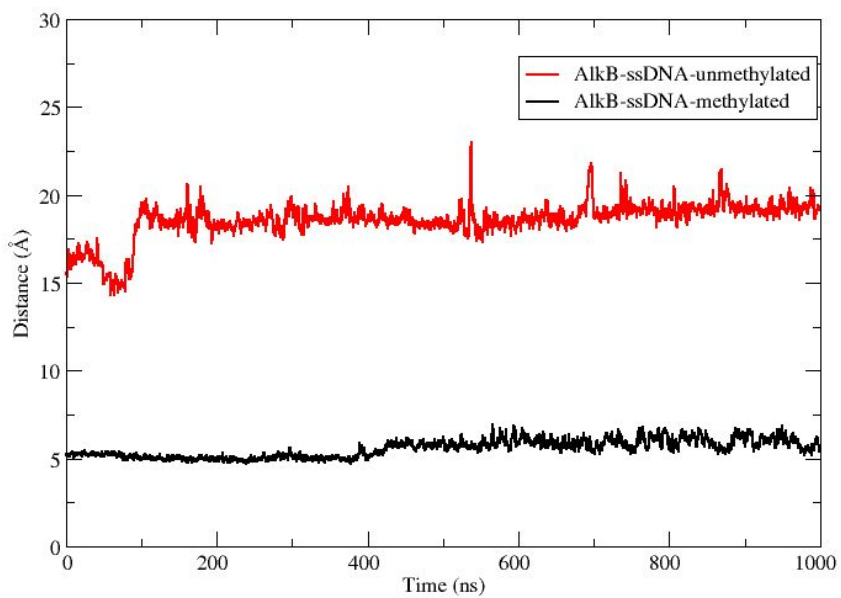


Figure S26 The distance between Fe center (Fe) and N3 of the substrate in the AlkB-ssDNA Fe(III)-superoxo complex MD simulations.

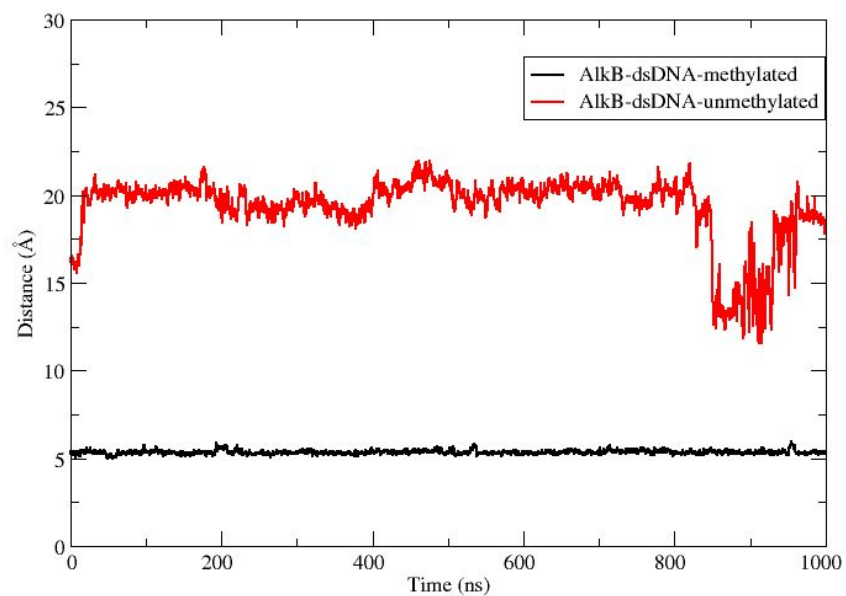


Figure S27 The distance between Fe center (Fe) and N3 of the substrate in the AlkB-dsDNA Fe(III)-superoxo complex MD simulations.

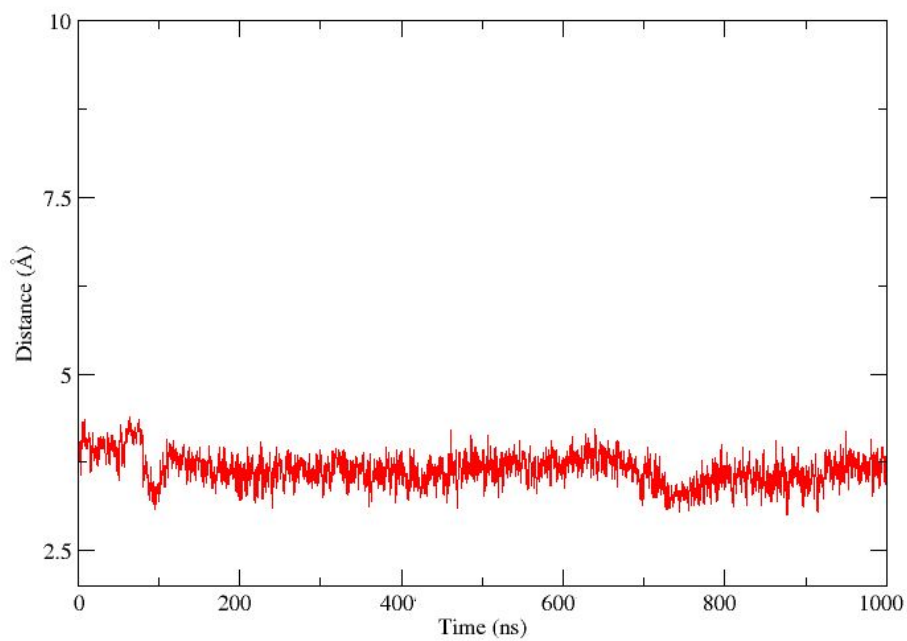


Figure S28 The distance between distal oxygen (O_d) of the superoxide and C2 of 2OG in the AlkB-ssDNA Fe(III)-superoxo complex MD simulations.

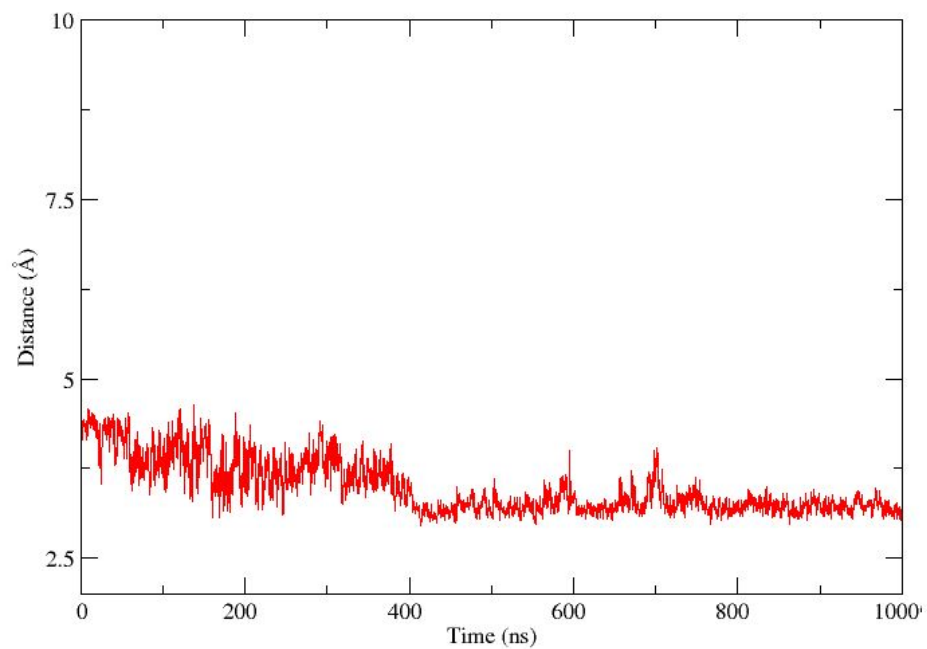


Figure S29 The distance between distal oxygen (O_d) of the superoxide and C2 of 2OG in AlkB-dsDNA Fe(III)-superoxo complex MD simulations.

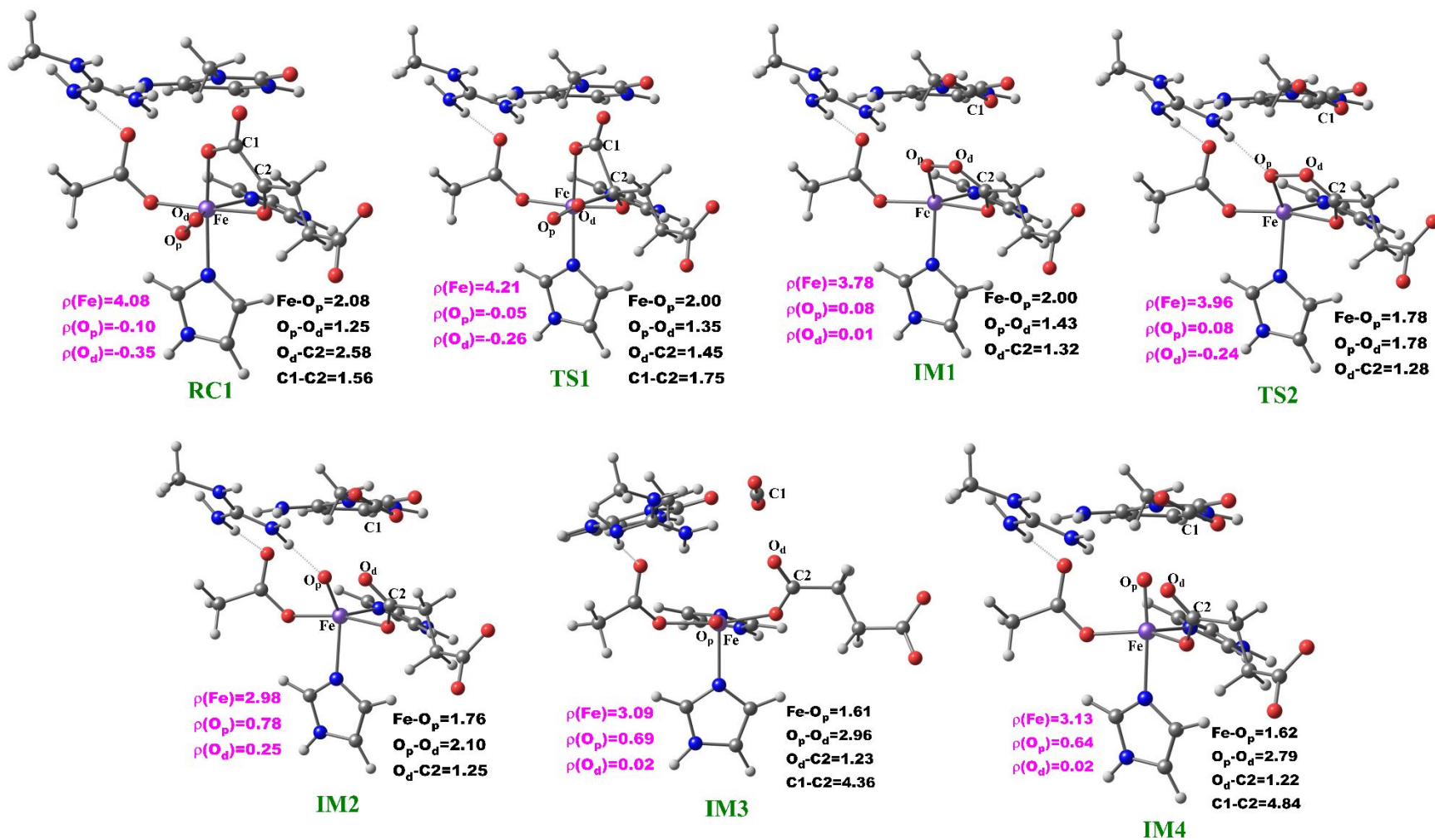


Figure S30 The reaction state geometries of the dioxygen activation step stationary points in AlkB-ssDNA. Distances (Å) and spin densities are in black and pink, respectively.

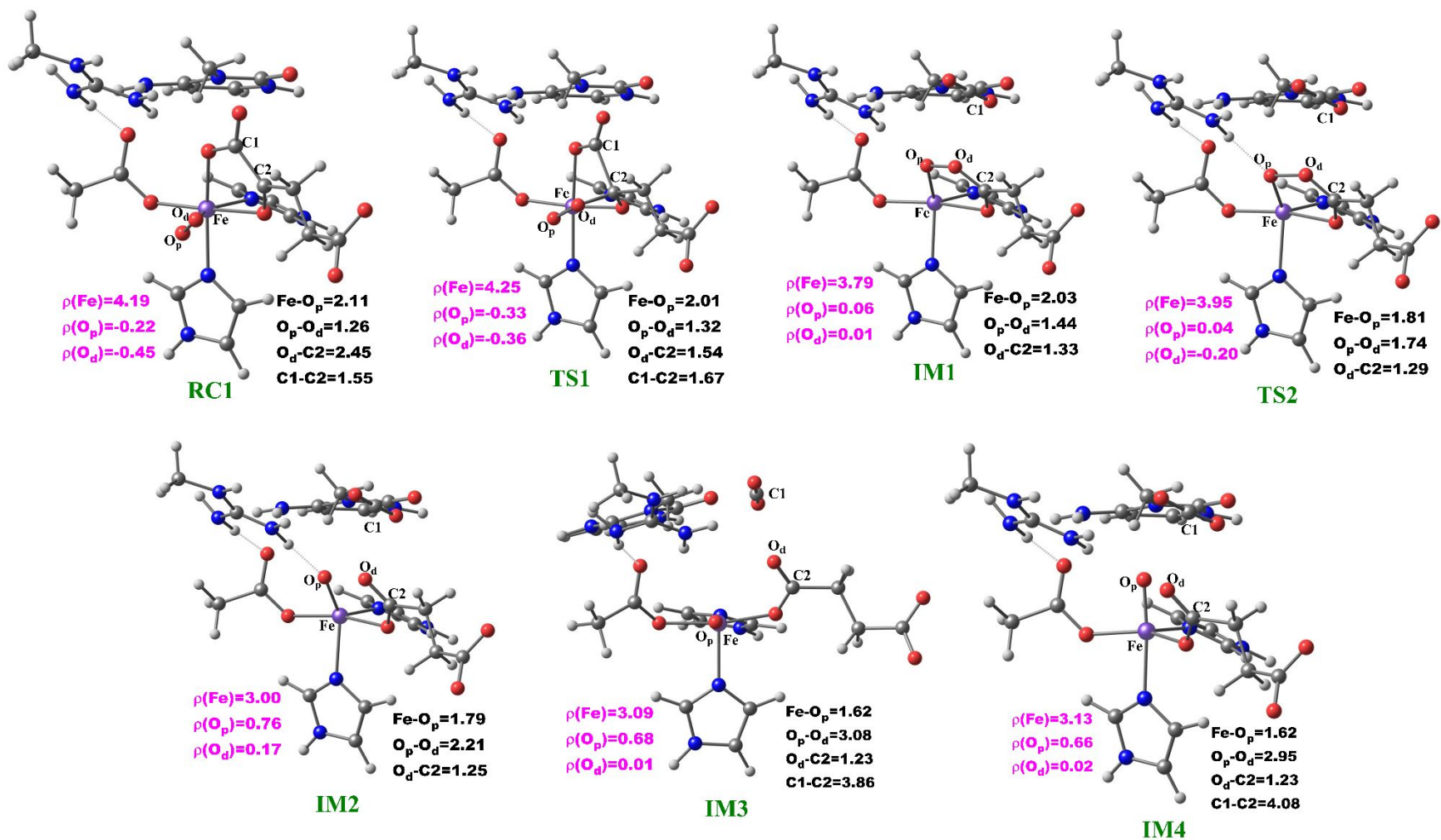


Figure S31 The reaction state geometries of the dioxygen activation step stationary points in AlkB-dsDNA. Distances (Å) and spin densities are in black and pink, respectively.

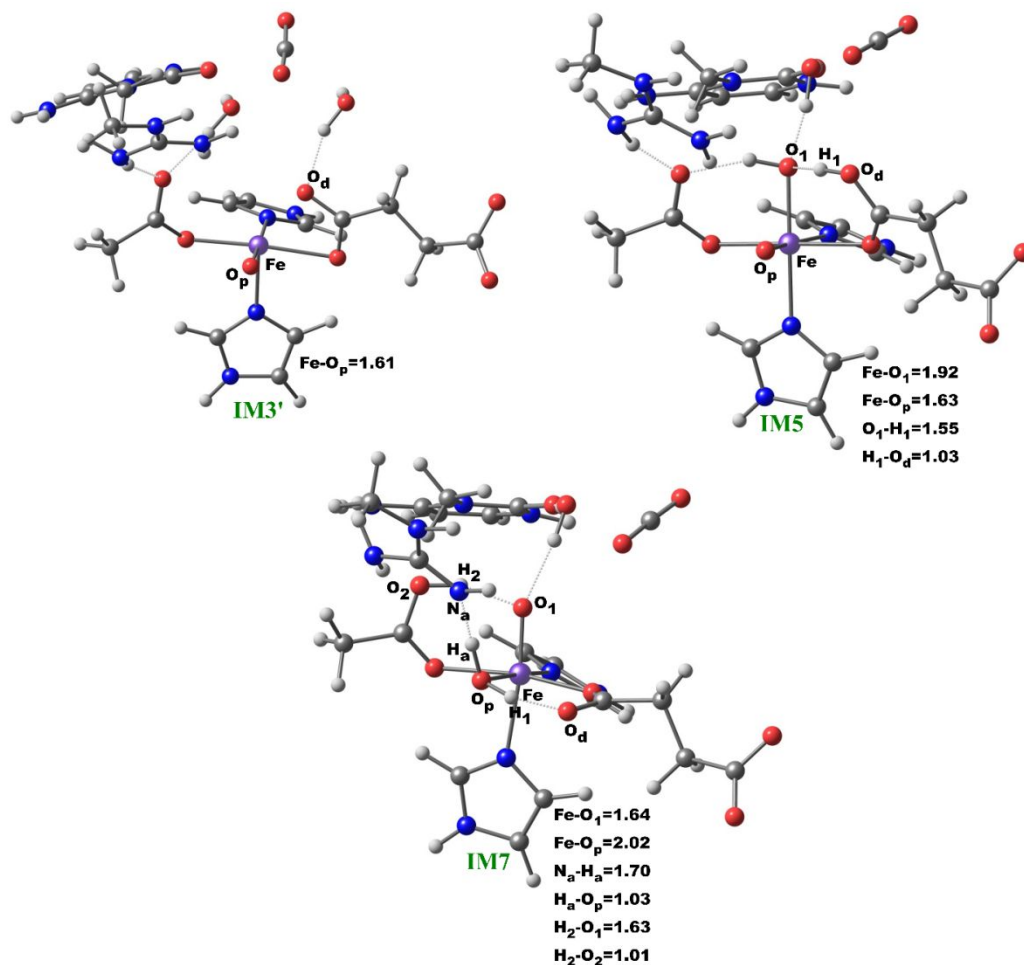


Figure S32 The reaction state geometries (IM3', IM5 and IM7) for the proposed ferryl flip mechanism stationary points in AlkBH2-dsDNA. Distances are in Å.

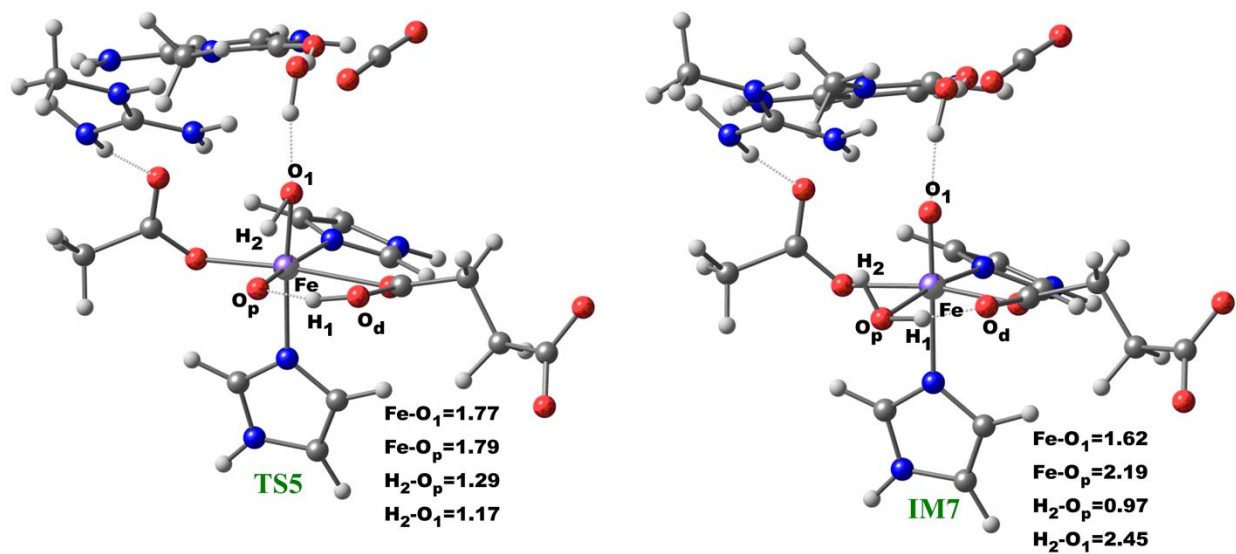


Figure S33 The reaction state geometries for the proposed ferryl flip mechanism stationary points via the direct proton transfer from IM6 in the AlkBH2-dsDNA complex. Distances are in Å.

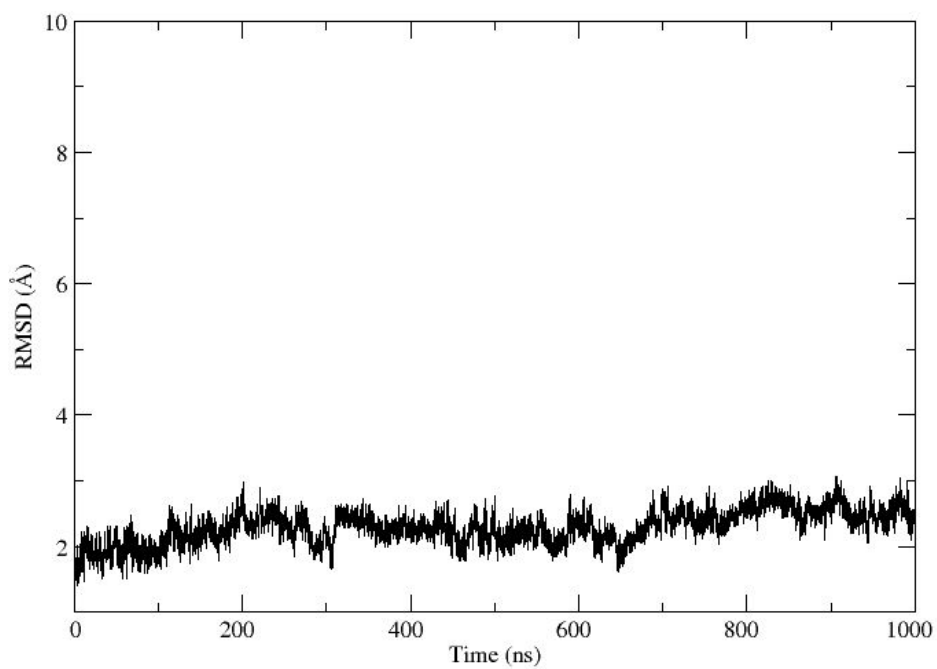


Figure S34 RMSD plot for the Protein-DNA complex of AlkBH2-dsDNA Fe(II) five-coordinate enzyme-substrate complex MD Simulations.

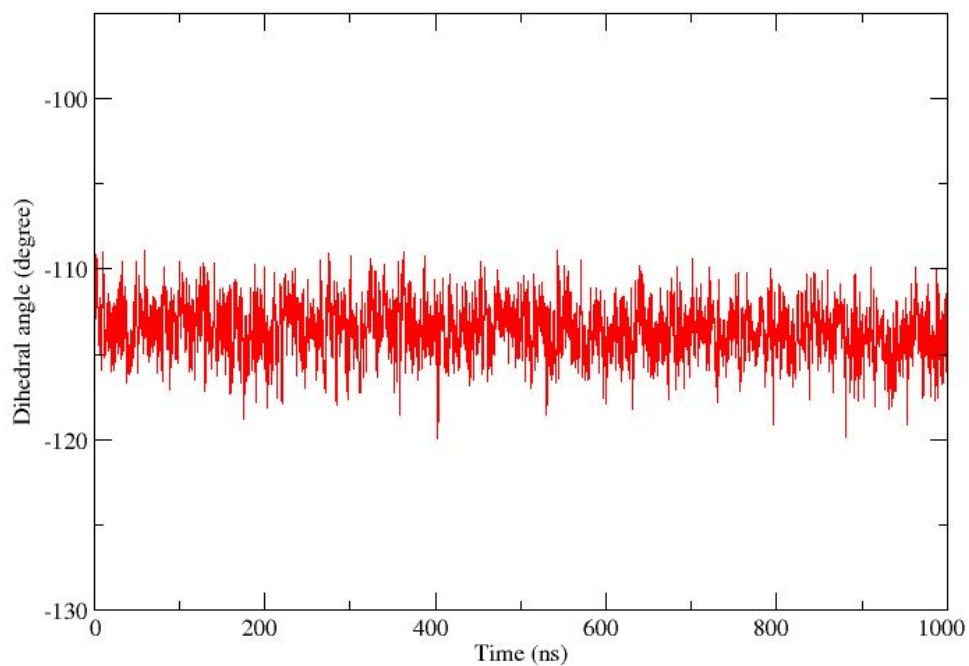


Figure S35 The N^ϵ (His¹)-Fe-O5-O2 dihedral angle in AlkBH2-dsDNA Fe(II) five-coordinate enzyme-substrate complex MD Simulations.

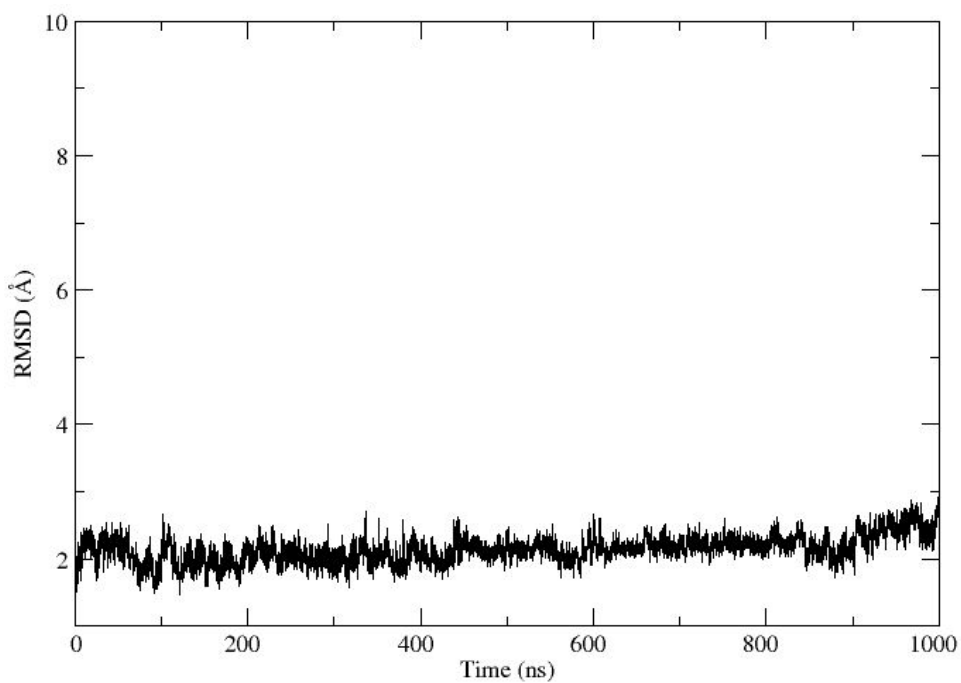


Figure S36 RMSD plot for the Protein-DNA complex of AlkBH2-dsDNA “in-line” Fe(III)-superoxo complex MD simulations.

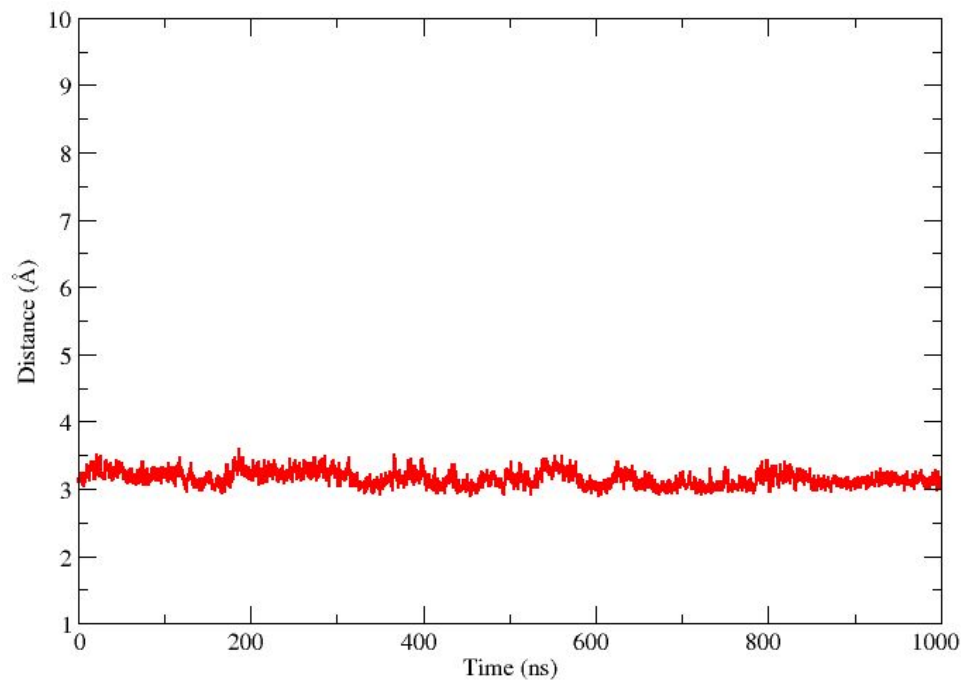


Figure S37 The distance between distal oxygen (O_d) of the superoxide and C2 of 2OG in AlkBH2-dsDNA “in-line” Fe(III)-superoxo complex MD simulations.

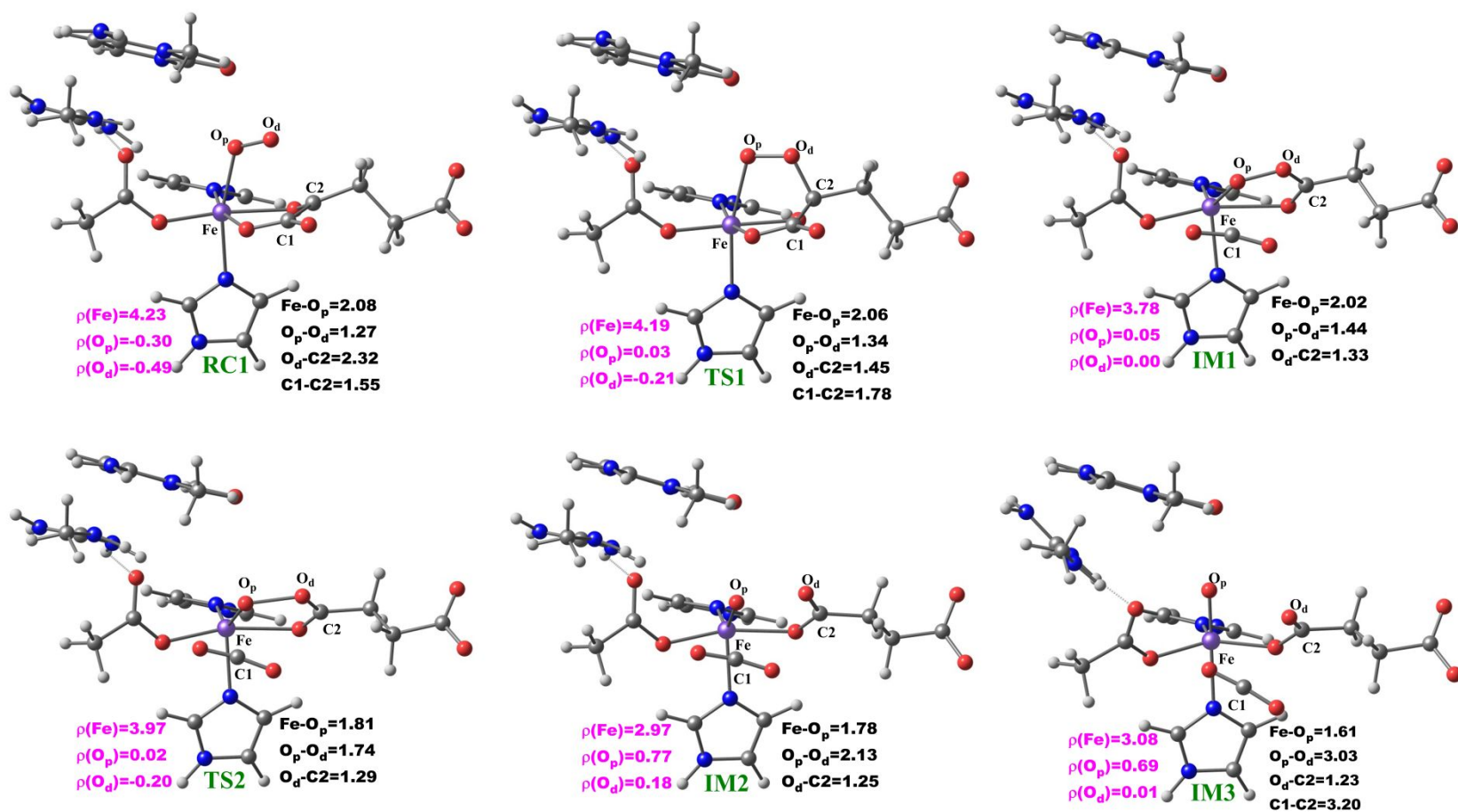


Figure S38 The reaction state geometries of the dioxygen activation step stationary points of AlkBH2-dsDNA via ‘in-line’ Fe(III)-superoxo complex. Distances (Å) and spin densities are in black and pink, respectively.

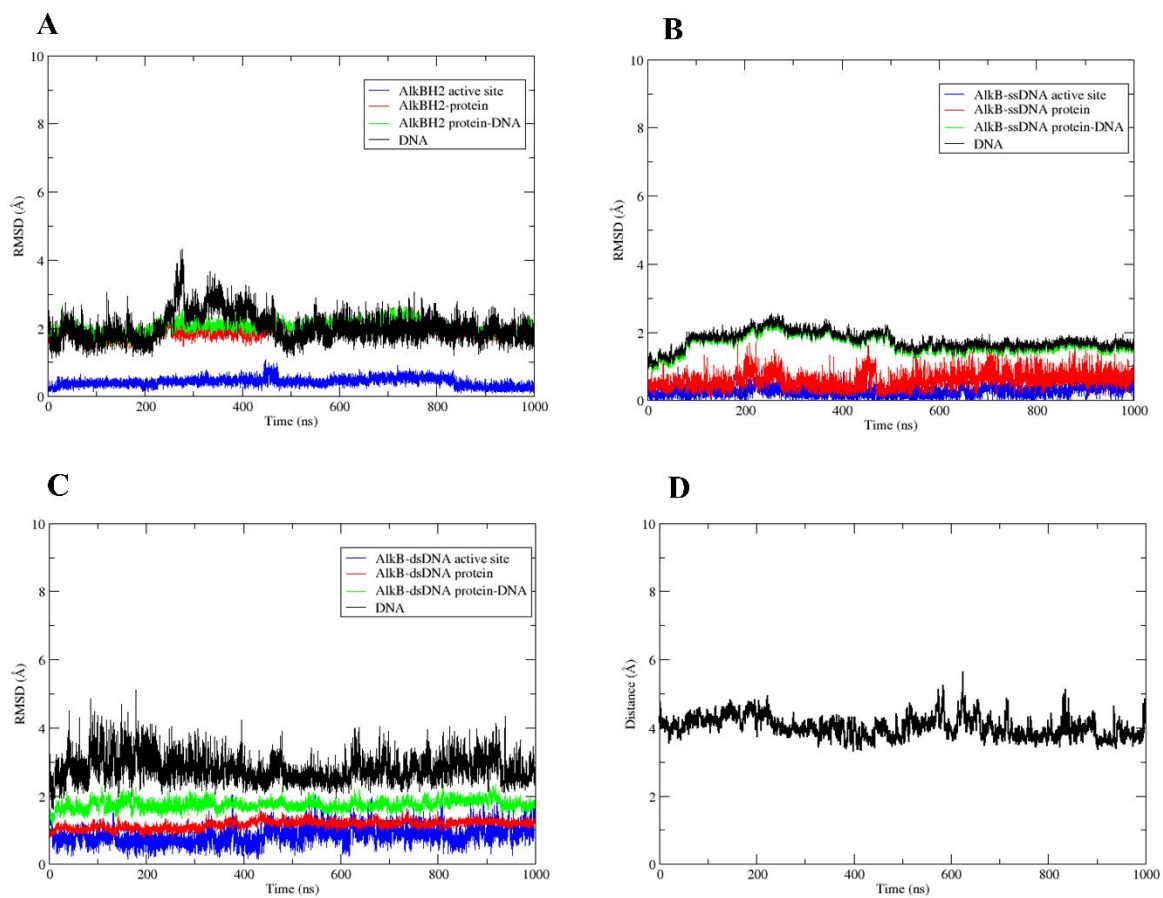


Figure S39 RMSD Plots for AlkBH2-dsDNA (A), AlkB-ssDNA (B), AlkB-dsDNA (C) and plot of the distance between the proximal oxygen (O_p) and the carbon of the methyl-group of m_3C (D) at the ferryl intermediate stage of the AlkBH2-dsDNA complex reaction.

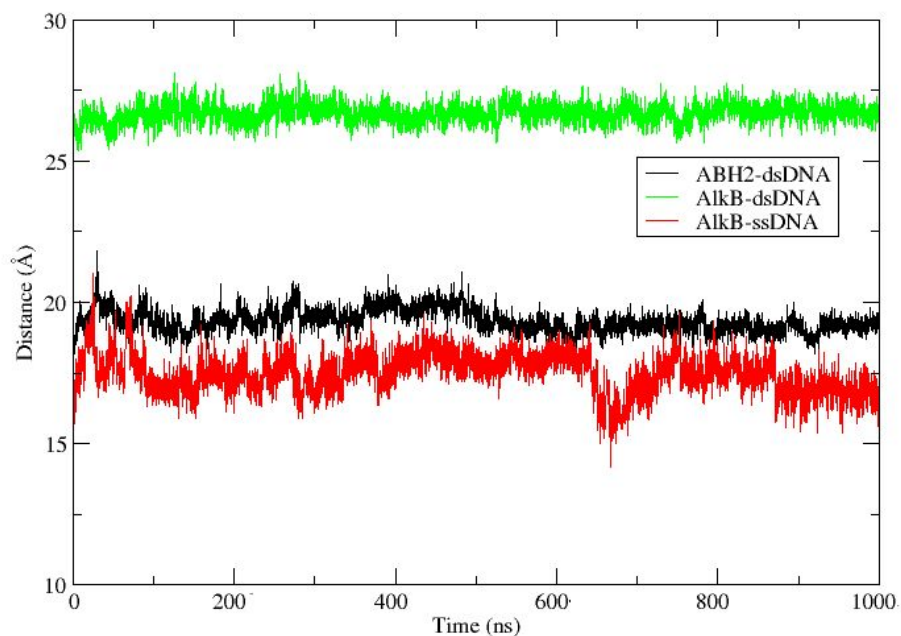


Figure S40 The distance between the center of masses of the protein and the DNA in the AlkBH2-dsDNA, AlkB-ssDNA and AlkB-dsDNA complexes during the MD simulations of the ferryl complex.

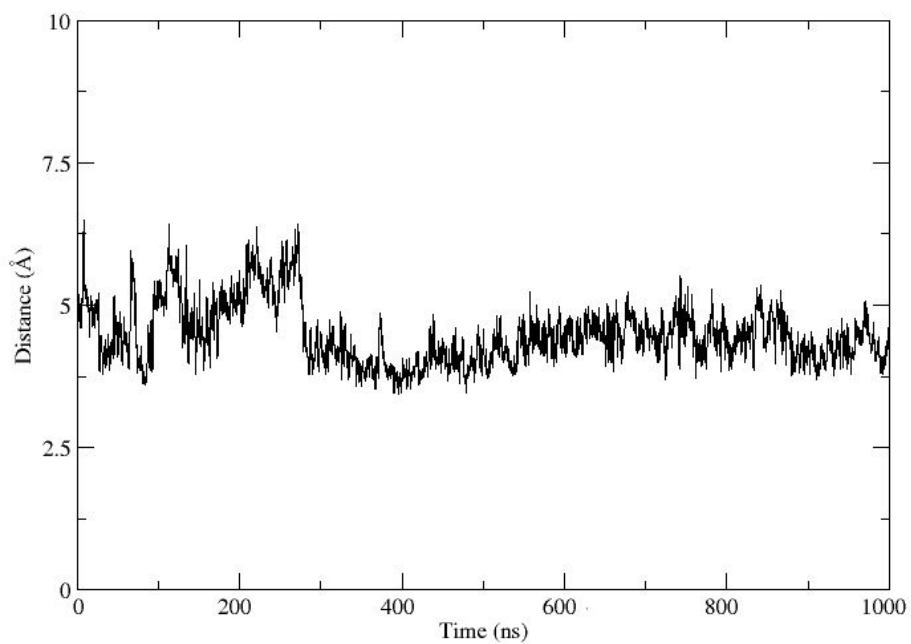


Figure S41 Distance between proximal oxygen (O_p) and the methyl carbon of m_3C DNA substrate in the AlkB-ssDNA ferryl complex MD simulations.

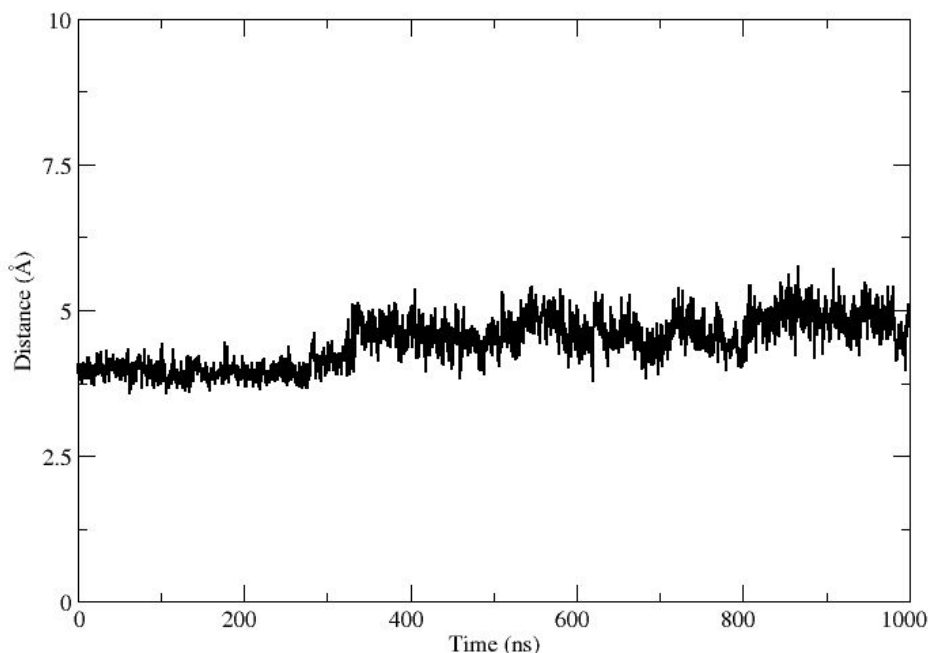


Figure S42 Distance between the proximal oxygen (O_p) and the methyl carbon of m_3C DNA substrate in the AlkB-dsDNA ferryl complex MD simulations.

Dynamic cross correlation analysis (DCCA) of AlkBH2-dsDNA (Figure 9A) shows that residues 95-101 ($\beta 3$) and 103-108 ($\beta 4$), belonging to a crystallographically observed β -hairpin,^{10,11} have a strong positive correlation with residues 123-128; this aids in substrate recognition. Residues 166-175, located on the first strand of the double-stranded β -helix (DSBH) core fold, which includes the coordinating HXD motif, have a strong positive correlation with the Fe center, the oxo group of the $Fe(IV)=O$ species, succinate, and DNA. This observation implies that these residues are important for the proper orientation of the reactive groups. Residues 151-173 (belonging to $\beta 8$) and 178-190 (belonging to $\beta 8$ and the loop connecting $\beta 8$ - $\beta 9$) have a positive correlation with residues 234-255 ($\beta 13$ - $\beta 14$) and 168-179 ($\beta 12$ and $\alpha 5$), respectively. Moreover, residues belonging to $\beta 9$ (aa 182-188) and $\beta 10$ (aa 193-202) have a positive correlation with residues belonging to $\beta 14$ (aa 242-255) and $\beta 13$ (aa 231-238), respectively.

DCCA calculations with AlkB-ssDNA (Figure S35) reveals that residues 122-136 located on the first strand of the DSBH, which include the coordinating HXD motif, have a strong positive correlation with the Fe center, the oxo group of the $Fe(IV)=O$ species, succinate, and residues belonging to $\alpha 3$ and $\beta 11$ (aa 183-192). Residues 117-123 (in $\beta 5$) and 143-150 (in $\beta 7$) have a positive correlation with residues 203-209, which belong to $\beta 12$ and the loop connecting $\beta 11$ and $\beta 12$. Residues 142-157, belonging to $\beta 7$ - $\beta 8$ have a positive correlation with residues 165-178 (in $\beta 9$) and 185-192 (in $\alpha 3$ and $\beta 9$).

With AlkB-dsDNA (Figure S36), DCCA shows that residues 50-57 and 79-89, which belong to the nucleotide recognition lid, have a positive correlation with the DNA substrate. Residues 114-124 (in $\beta 5$) and 121-136 (in $\beta 5$ and $\beta 6$) have a positive correlation with residues 203-211 (in $\beta 12$) and 180-192 (in $\beta 10$ and $\beta 11$), respectively. Residues 129-136 located on the first strand of the DSBH, which includes the coordinating HXD motif, have a positive correlation with residues that belong to $\beta 8$ (aa 158-162). Figures S15 and S16 contain the annotated secondary structures of AlkBH2-dsDNA and AlkBs, respectively.

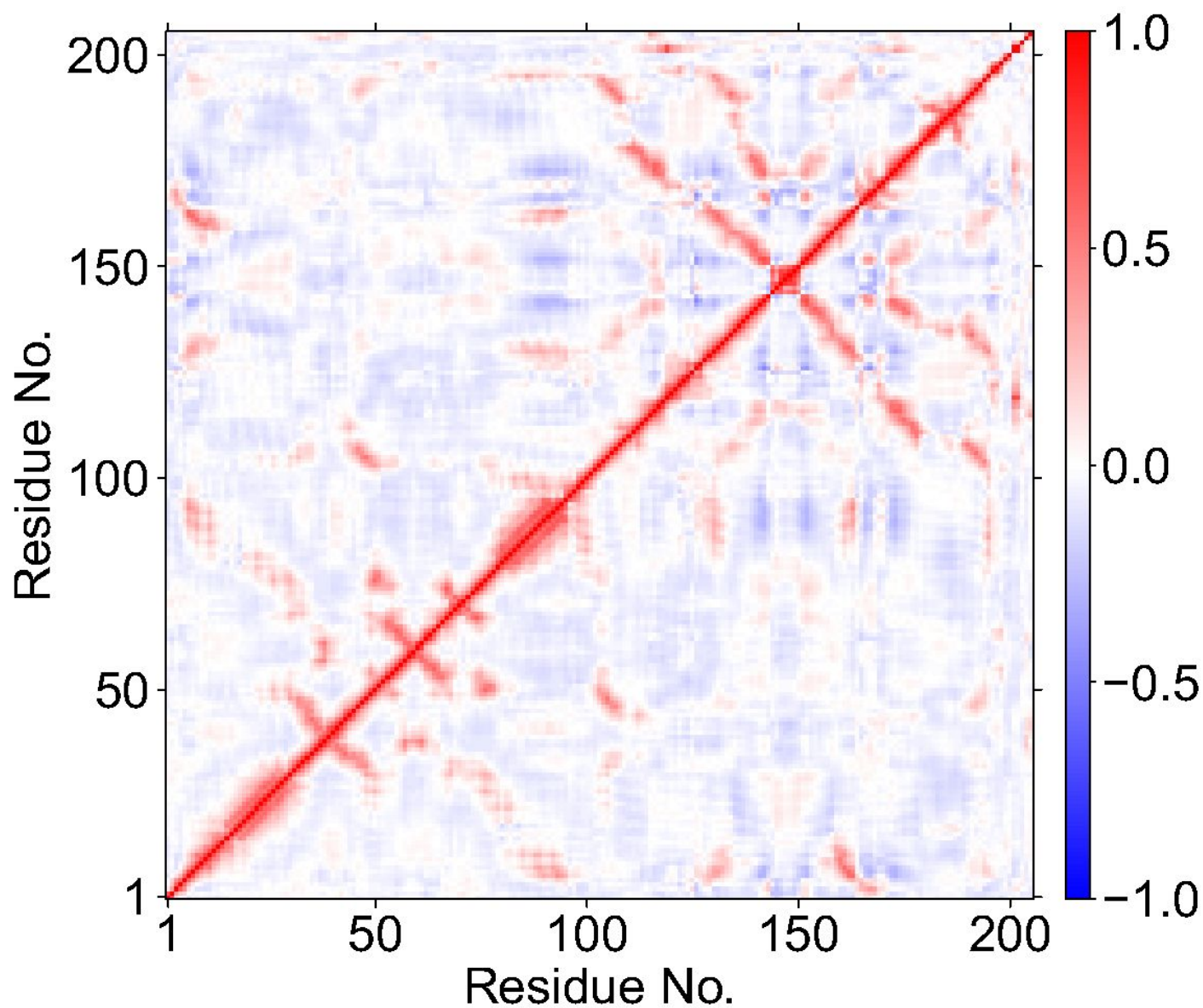


Figure S43 Dynamic cross correlation for the ferryl complex of AlkB-ssDNA. Residue numbers 1-200 (protein), 201 (Fe), 202 (O), 203 (succinate), 204-206 (DNA), and 205 (m₃C substrate).

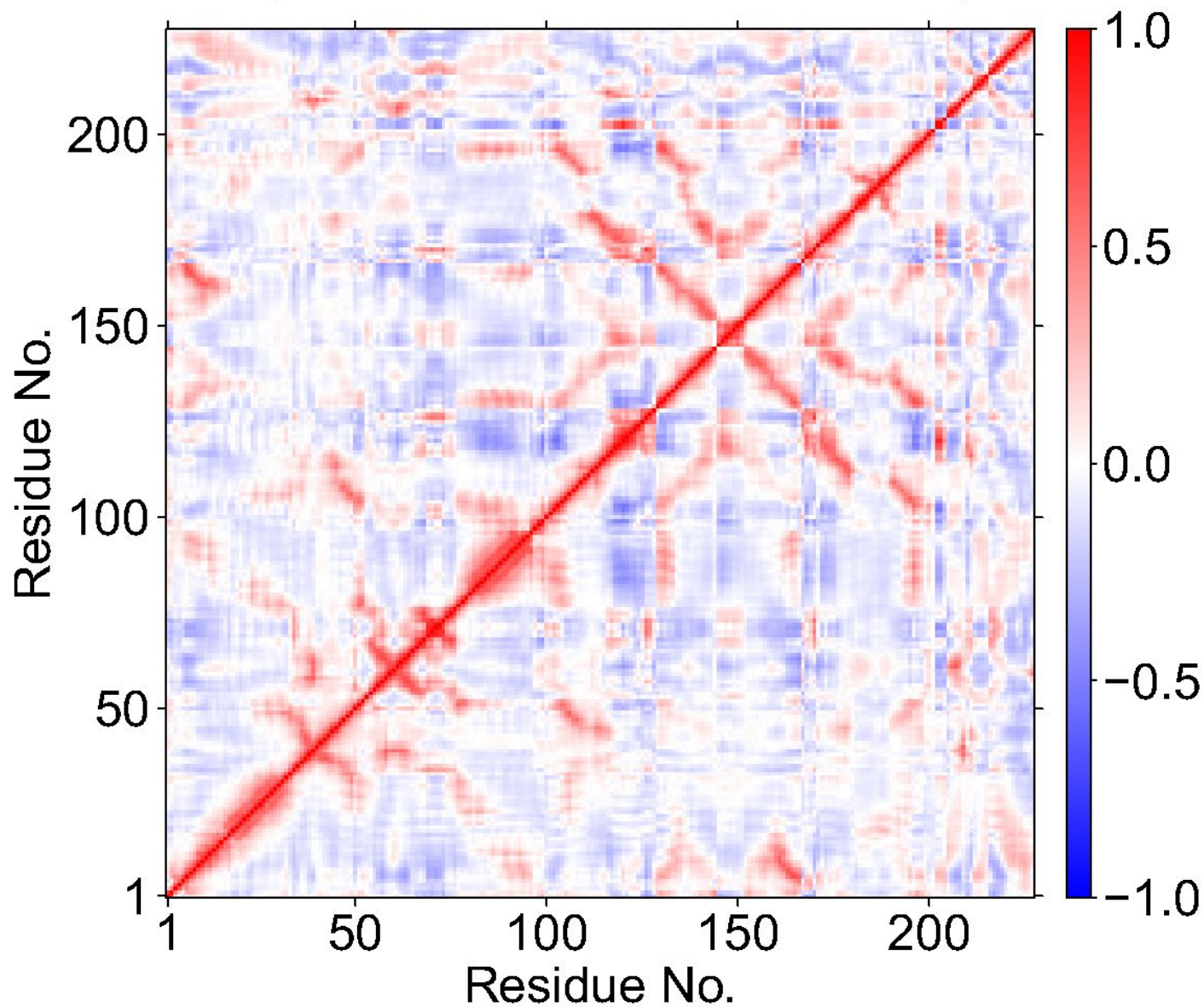


Figure S44 Dynamic cross correlation for the ferryl complex of AlkB-dsDNA. Residue numbers 1-201 (protein), 202 (Fe), 203 (O), 204 (succinate), 205-229 (DNA), and 211 (m_3C substrate).

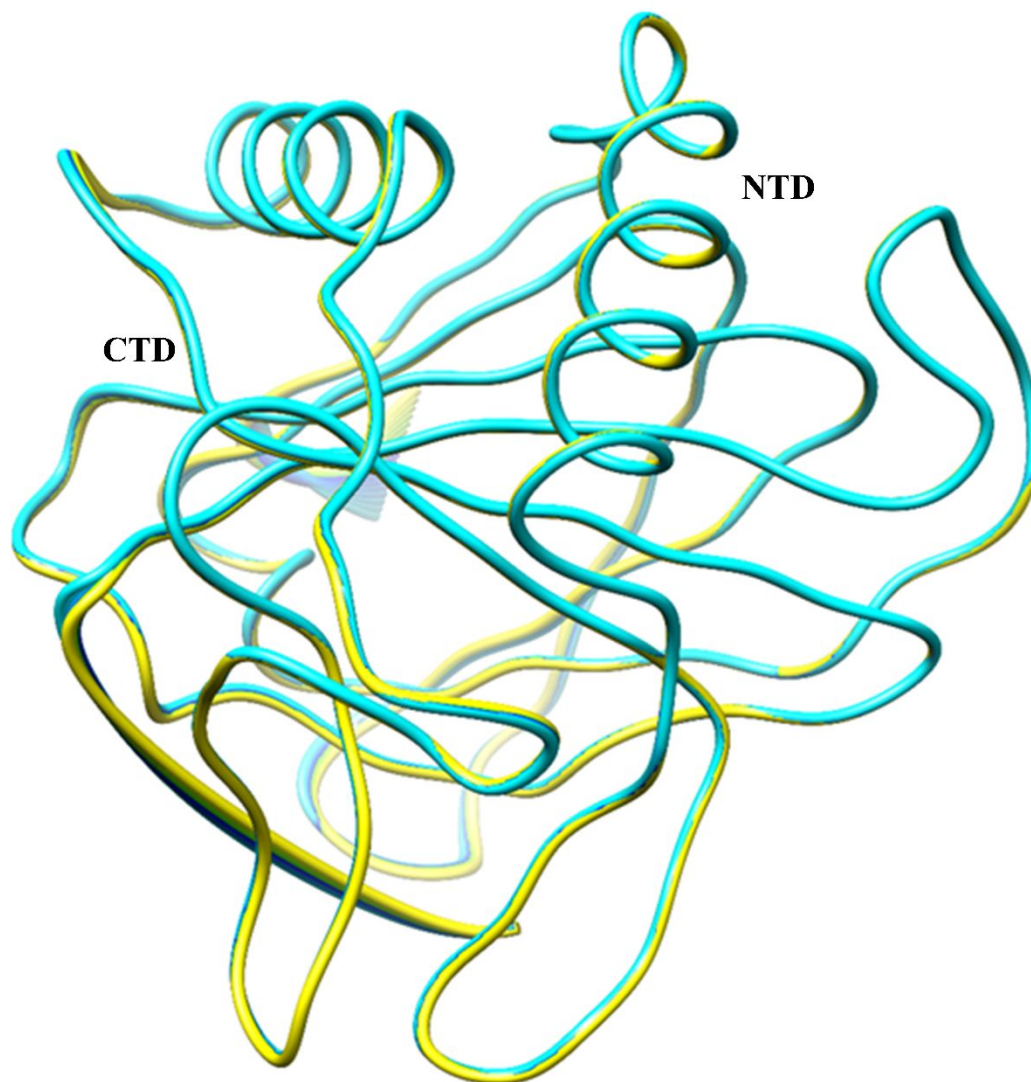


Figure S45 PCA for the AlkB-ssDNA ferryl MD simulation. Yellow to blue coloring represents the main direction of motion of protein residues. NTD and CTD are N-terminal Domain and C-terminal Domain, respectively.

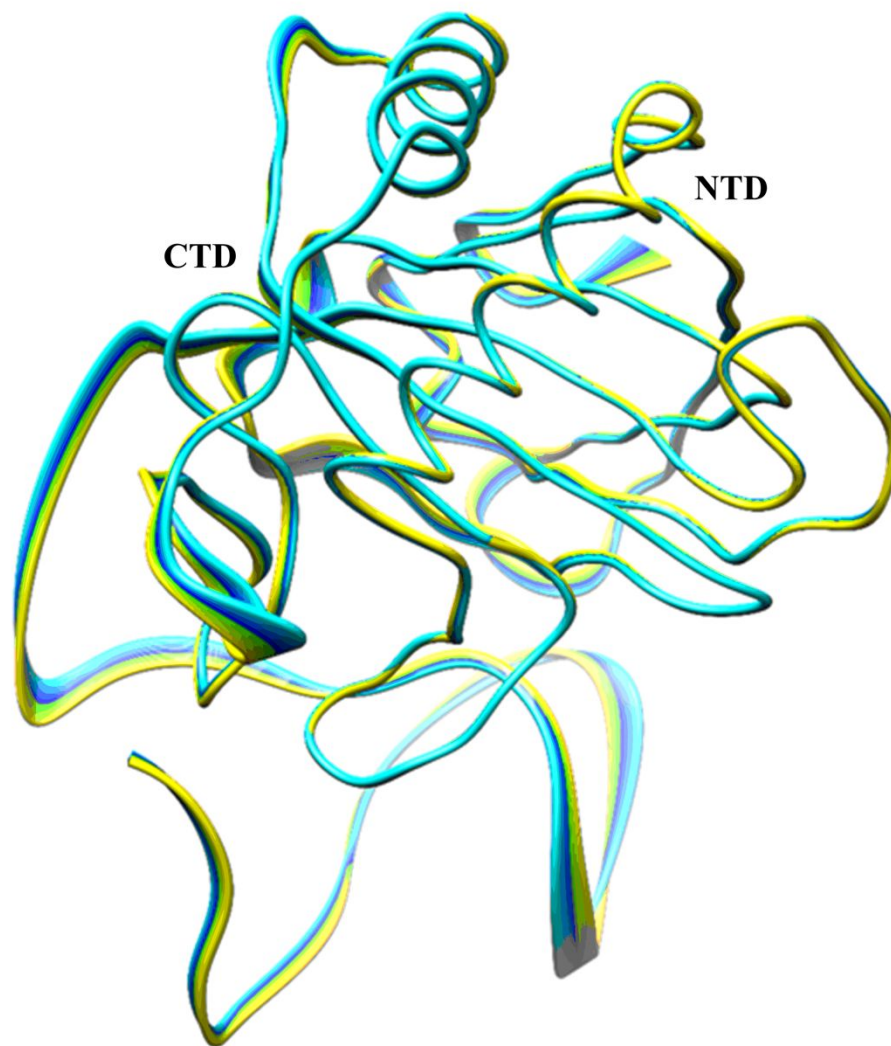


Figure S46 PCA for the AlkB-dsDNA ferryl MD simulation. Yellow to blue coloring represents the main direction of motion of protein residues. NTD and CTD are N-terminal Domain and C-terminal Domain, respectively.

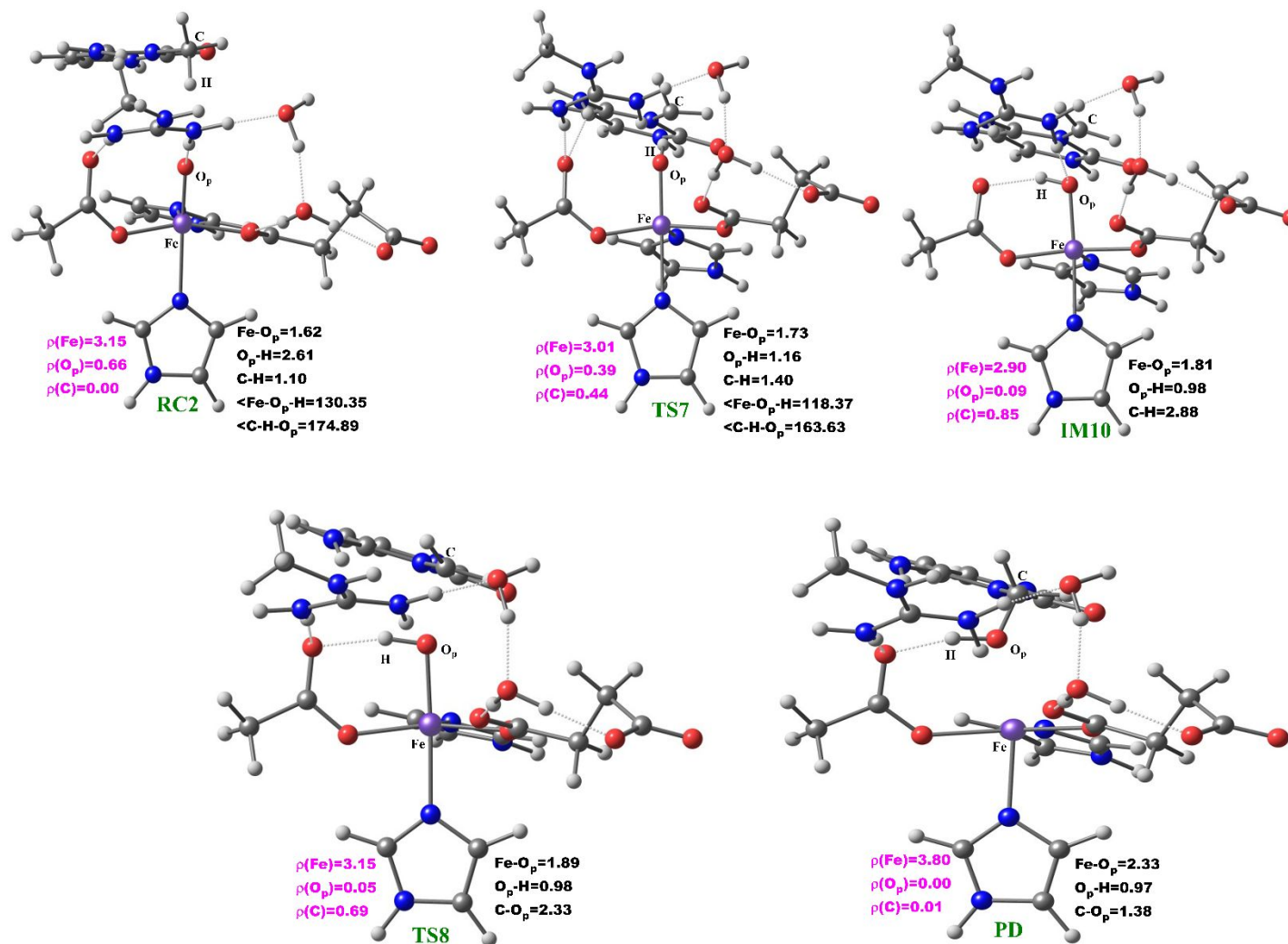


Figure S47 The reaction state geometries of the hydrogen atom abstraction and rebound hydroxylation steps stationary points in AlkB-ssDNA. Distances (Å) and spin densities are in black and pink, respectively.

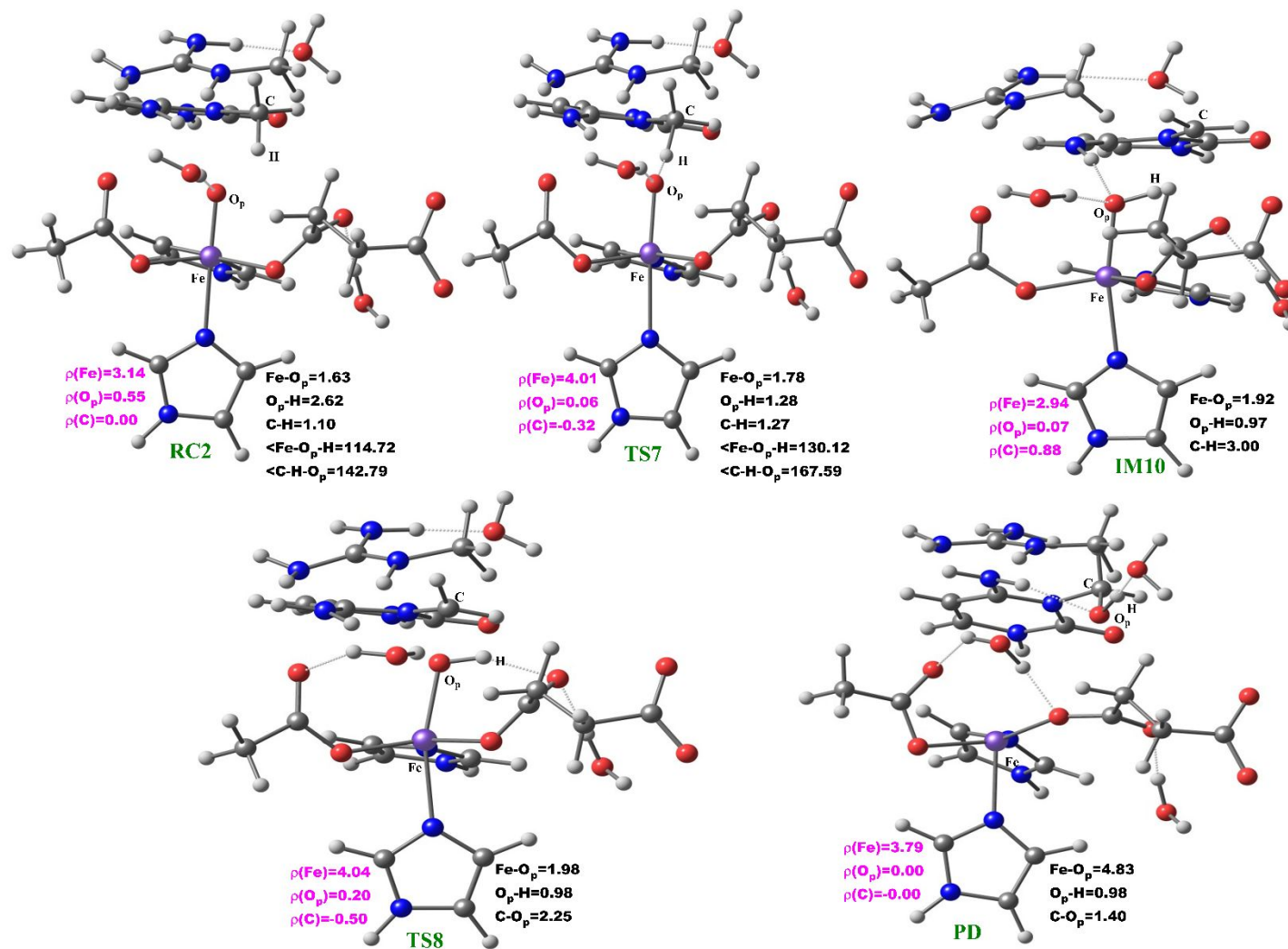


Figure S48 The reaction state geometries of the hydrogen atom abstraction and rebound hydroxylation steps stationary points in AlkB-dsDNA. Distances (\AA) and spin densities are in black and pink, respectively.

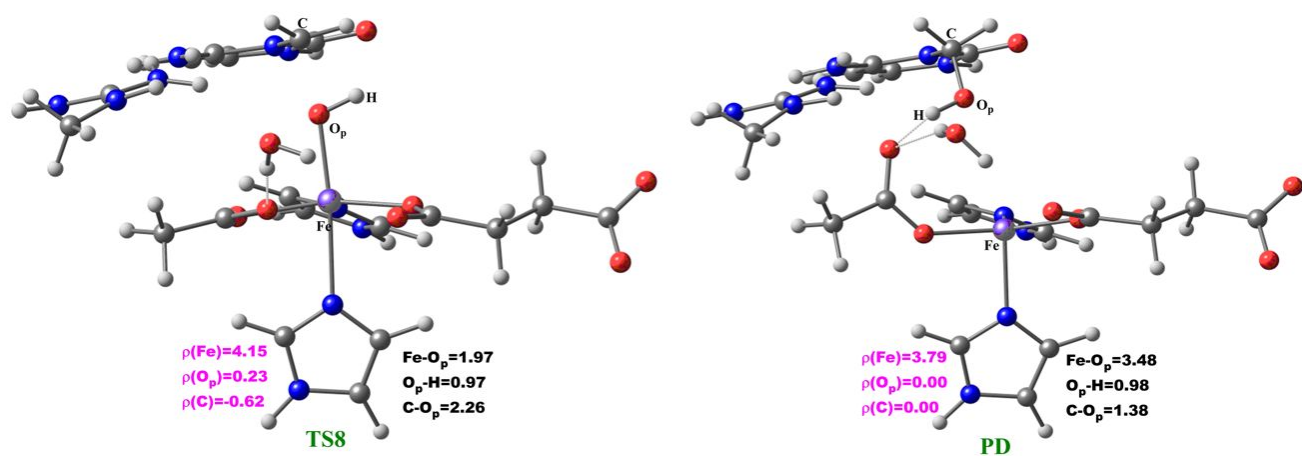


Figure S49 Optimized geometries of the rebound hydroxylation stationary points in AlkBH2-dsDNA. Distances and angles are in Å and degrees, respectively.

Table S1. Calculated activation barriers (in kcal/mol) at B3LYP/def2-TZVP (BS2) for all the multiple snapshots with and without ZPE in the AlkB-ssDNA complex.

Snapshot	Barrier (BS2)	Barrier (BS2+ZPE)
1.	26.6	23.6
2.	27.2	24.1
3.	31.3	26.7
4.	25.6	22.1
5.	24.8	21.0
Boltzmann weighted average	25.6	21.9

Table S2. Selected distances and angles for the different snapshots RC2 and TS7 for HAT step in the AlkB-ssDNA complex, calculated at B3LYP/def2-TZVP.

	d(Fe–O _p) (Å)	d(O _p –H) (Å)	d(C–H) (Å)	<(Fe–O _p –H) (deg)	<(C–H _p –O) (deg)	Barrier with ZPE (kcal/mol)	C _{substrate} spin density in TS7
Snapshot 1							
RC2	1.623	2.472	1.099	137.46	175.36	23.6	-0.356
TS7	1.775	1.254	1.293	140.45	169.59		
Snapshot 2							
RC2	1.622	2.468	1.101	123.22	142.43	24.1	0.418
TS7	1.735	1.191	1.377	121.88	165.21		
Snapshot 3							
RC2	1.626	3.344	1.101	125.10	144.26	26.7	0.465
TS7	1.726	1.161	1.404	120.04	173.05		
Snapshot 4							
RC2	1.627	2.605	1.103	130.35	174.89	22.1	0.439
TS7	1.729	1.163	1.400	118.37	163.63		
Snapshot 5							
RC2	1.621	2.831	1.103	128.44	172.09	21.0	-0.366
TS7	1.749	1.232	1.295	145.55	168.20		

Table S3. Calculated activation barriers (in kcal/mol) at B3LYP/def2-TZVP (BS2) for all the multiple snapshots with and without ZPE in the AlkB-dsDNA complex.

Snapshot	Barrier (BS2)	Barrier (BS2+ZPE)
1.	26.2	23.6
2.	24.1	21.5
3.	25.6	22.1
4.	27.4	24.9
5.	29.0	25.3
Boltzmann weighted average	25.1	22.3

Table S4. Selected distances and angles for the different snapshots RC2 and TS7 for HAT step in the AlkB-dsDNA complex, calculated at B3LYP/def2-TZVP.

	d(Fe–O _p) (Å)	d(O _p –H) (Å)	d(C–H) (Å)	<(Fe–O _p – H) (deg)	<(C–H _p – O) (deg)	Barrier with ZPE (kcal/mol)	C _{substrate} spin density in TS7
Snapshot 1							
RC2	1.611	3.258	1.103	126.24	153.66	23.6	-0.342
TS7	1.748	1.269	1.279	139.91	175.39		
Snapshot 2							
RC2	1.622	2.603	1.103	127.49	175.45	21.5	-0.324
TS7	1.772	1.296	1.263	129.88	168.70		
Snapshot 3							
RC2	1.633	2.620	1.101	114.72	142.79	22.1	-0.330
TS7	1.781	1.279	1.269	130.12	167.59		
Snapshot 4							
RC2	1.615	3.292	1.099	118.94	144.01	24.9	-0.314
TS7	1.783	1.306	1.273	138.81	165.12		
Snapshot 5							
RC2	1.627	2.874	1.099	115.41	154.39	25.3	-0.323
TS7	1.772	1.309	1.275	133.70	168.83		

Table S5. Calculated pKa values of the ionisable side chains of AlkBH2-dsDNA, AlkB-ssDNA and AlkB-dsDNA, done using Propka software. The yellow highlighted ones are the iron-coordinating residues.

AlkBH2-dsDNA			AlkB-ssDNA			AlkB-dsDNA		
Residues	pKa	pK model	Residues	pKa	pK model	Residues	pKa	pK model
ASP 66	3.28	3.80	ASP 36	3.05	3.80	ASP 36	3.03	3.80
ASP 79	1.92	3.80	ASP 39	4.20	3.80	ASP 39	4.21	3.80
ASP 117	3.43	3.80	ASP 82	1.70	3.80	ASP 82	1.78	3.80
ASP 143	3.72	3.80	ASP 111	3.94	3.80	ASP 111	3.98	3.80
ASP 163	2.97	3.80	ASP 115	4.16	3.80	ASP 115	4.11	3.80
ASP 166	4.37	3.80	ASP 133	-2.93	3.80	ASP 133	-2.79	3.80
ASP 173	-2.44	3.80	ASP 135	5.28	3.80	ASP 135	6.83	3.80
ASP 174	4.97	3.80	ASP 138	1.31	3.80	ASP 138	1.66	3.80
ASP 194	3.31	3.80	ASP 163	3.35	3.80	ASP 163	3.18	3.80
ASP 201	3.40	3.80	ASP 174	4.03	3.80	ASP 174	3.98	3.80
GLU 63	4.26	4.50	ASP 202	2.87	3.80	ASP 202	3.75	3.80
GLU 77	3.70	4.50	GLU 31	4.51	4.50	GLU 31	4.54	4.50
GLU 80	4.61	4.50	GLU 136	3.89	4.50	GLU 136	3.87	4.50
GLU 84	4.89	4.50	GLU 171	3.81	4.50	GLU 171	4.65	4.50
GLU 86	3.61	4.50	GLU 181	4.67	4.50	GLU 181	4.63	4.50
GLU 88	3.88	4.50	HIS 66	6.35	6.50	HIS 66	6.42	6.50
GLU 90	4.55	4.50	HIS 72	6.11	6.50	HIS 72	5.52	6.50
GLU 139	4.77	4.50	HIS 97	6.49	6.50	HIS 97	5.91	6.50
GLU 170	5.39	4.50	HIS 131	-1.92	6.50	HIS 131	-1.92	6.50
GLU 175	8.44	4.50	HIS 172	4.58	6.50	HIS 172	4.34	6.50
GLU 177	4.48	4.50	HIS 187	0.85	6.50	HIS 187	0.72	6.50
HIS 55	6.05	6.50	HIS 197	5.38	6.50	HIS 197	5.30	6.50
HIS 59	5.96	6.50	CYS 64	9.22	9.00	CYS 64	9.25	9.00
HIS 106	4.51	6.50	CYS 100	13.18	9.00	CYS 100	13.07	9.00
HIS 144	5.65	6.50	CYS 117	18.79	9.00	CYS 117	18.84	9.00
HIS 167	3.68	6.50	CYS 203	11.44	9.00	CYS 203	10.66	9.00
HIS 171	-2.32	6.50	TYR 55	10.20	10.00	TYR 55	10.34	10.00
HIS 199	5.61	6.50	TYR 76	12.92	10.00	TYR 76	15.62	10.00
HIS 220	6.36	6.50	TYR 78	15.22	10.00	TYR 78	16.21	10.00
HIS 228	6.13	6.50	TYR 109	11.36	10.00	TYR 109	11.40	10.00
HIS 233	5.75	6.50	TYR 122	12.54	10.00	TYR 122	12.52	10.00
HIS 236	0.57	6.50	TYR 186	10.12	10.00	TYR 186	11.44	10.00
CYS 169	13.72	9.00	TYR 205	11.44	10.00	TYR 205	12.44	10.00
TYR 69	9.89	10.00	LYS 87	10.37	10.50	LYS 87	10.38	10.50
TYR 91	13.29	10.00	LYS 127	10.17	10.50	LYS 127	9.54	10.50
TYR 115	11.08	10.00	LYS 134	10.33	10.50	LYS 134	9.21	10.50
TYR 122	16.56	10.00	LYS 160	10.61	10.50	LYS 160	10.67	10.50
TYR 161	11.60	10.00	LYS 166	10.25	10.50	LYS 166	10.14	10.50
TYR 235	11.21	10.00	LYS 193	10.27	10.50	LYS 193	10.33	10.50
LYS 75	11.50	10.50	LYS 214	10.53	10.50	LYS 214	10.56	10.50

LYS 87	11.32	10.50	ARG 23	12.35	12.50	ARG 23	12.47	12.50
LYS 104	10.18	10.50	ARG 24	13.82	12.50	ARG 24	12.65	12.50
LYS 111	10.13	10.50	ARG 35	12.41	12.50	ARG 35	12.40	12.50
LYS 132	9.92	10.50	ARG 47	12.73	12.50	ARG 47	12.66	12.50
LYS 162	11.33	10.50	ARG 73	12.41	12.50	ARG 73	12.41	12.50
LYS 200	10.08	10.50	ARG 102	12.22	12.50	ARG 102	12.04	12.50
LYS 242	10.02	10.50	ARG 121	12.28	12.50	ARG 121	12.15	12.50
LYS 243	10.18	10.50	ARG 140	14.01	12.50	ARG 140	14.08	12.50
LYS 255	10.28	10.50	ARG 161	12.56	12.50	ARG 161	9.67	12.50
ARG 58	12.20	12.50	ARG 167	12.23	12.50	ARG 167	11.43	12.50
ARG 61	12.49	12.50	ARG 183	12.17	12.50	ARG 183	12.37	12.50
ARG 98	12.20	12.50	ARG 204	10.43	12.50	ARG 204	10.37	12.50
ARG 110	9.61	12.50	ARG 210	13.09	12.50	ARG 210	12.86	12.50
ARG 140	13.36	12.50						
ARG 142	12.53	12.50						
ARG 160	13.99	12.50						
ARG 172	12.90	12.50						
ARG 176	12.40	12.50						
ARG 193	10.55	12.50						
ARG 198	11.52	12.50						
ARG 203	13.06	12.50						
ARG 209	12.67	12.50						
ARG 210	12.42	12.50						
ARG 215	11.95	12.50						
ARG 241	12.34	12.50						
ARG 248	9.14	12.50						
ARG 254	11.60	12.50						

Dioxygen activation step reaction states cartesian coordinates for AlkBH2-dsDNA via "off-line" Fe(III)-superoxo complex

RC1

QM/MM (BS1) = -3428.050920 a.u.

QM/MM (BS2+ZPE) = -3430.055821 a.u.

6	35.034000670	35.287516737	30.406645110
7	35.821561871	34.925606648	31.473095110
1	36.553334286	34.199392415	31.464118374
6	35.447607248	35.644997988	32.538496132
1	35.903135576	35.554584948	33.520444235
7	34.442880118	36.461713919	32.221215069
6	34.172002941	36.244116631	30.886910178
1	33.369134589	36.764262364	30.374786454
6	29.304433005	38.355113365	31.673558766
1	28.870761713	37.641242709	32.388046341
1	28.831623859	39.337546432	31.820975424
6	30.804472962	38.505349246	31.895490216
8	31.373756464	39.568148262	31.588446675
8	31.416967846	37.509569492	32.440548858
6	32.325054224	33.056485971	34.489161986
7	31.265987623	33.375302029	33.671461474
1	30.520675118	32.760388445	33.318334759
6	31.347204954	34.676592620	33.356268015
1	30.637743361	35.204117318	32.724816161
7	32.408441446	35.226024430	33.934444564
6	33.033355914	34.224737788	34.643448942
1	33.954028784	34.405889892	35.191208996
6	29.317154511	44.311490844	33.742325652
1	29.581742892	45.258307123	33.239546839
1	28.631002752	43.756162952	33.088128553
7	30.501276544	43.511944836	34.020546761
1	31.121765497	43.809816889	34.775431421
6	30.867811848	42.376611357	33.379247384
7	30.173291109	41.907976870	32.338179265
1	29.725999309	42.559805774	31.699605203
1	30.552343165	41.055768248	31.875291854
7	31.916709017	41.695980061	33.842421720
1	32.430218233	42.029592655	34.658211871
1	32.279191268	40.861619598	33.368301082
26	33.003121451	37.241978544	33.567939439
6	34.423500864	39.507940019	34.636705557
8	34.842948104	40.643046835	34.858740695
8	33.588754372	39.182148252	33.716743435
6	34.896635263	38.293566230	35.476329905
8	34.648565922	37.177527639	35.004553062
6	35.701484214	38.496105832	36.721215911
6	35.740506099	37.258464055	37.608060163
6	36.539382798	37.379264050	38.915135863
8	36.092277421	36.720979062	39.889491046
8	37.588481510	38.075768267	38.916505951
1	36.189095458	36.423032998	37.041562006
1	34.713751399	36.953582420	37.856543384
1	35.292286735	39.370973294	37.250396039
1	36.722558090	38.800370495	36.420840696
8	32.031130537	37.584369268	35.419284846
8	32.534582623	38.313925584	36.322990478
8	36.795645506	38.982803203	29.772603356
6	35.912511158	38.759292576	28.964223338
7	34.640022689	39.333122040	29.109937654

6	34.447267177	40.243994854	30.245143071
6	33.591872046	39.086001641	28.254181624
7	32.407566007	39.581178511	28.542662950
6	33.851540888	38.318165775	27.078945990
6	35.078119521	37.757642849	26.912848586
7	36.068076103	37.925796165	27.858907761
1	33.992064489	41.174739364	29.879567441
1	35.425631147	40.460556209	30.678704527
1	31.559792600	39.419431076	27.961262453
1	35.307809144	37.148058223	26.034767605
1	33.053906666	38.149983053	26.359554730
1	33.800936795	39.786772524	31.008804633
1	32.203305198	39.971276940	27.859187748
1	35.048324503	34.752780105	29.456951006
1	29.055490876	38.010764769	30.669806215
1	32.532002789	32.036640860	34.813438973
1	28.774296358	44.539172583	34.659676935
1	36.918719064	37.401704156	27.817596566

TS1

QM/MM (BS1) = -3428.034641 a.u.

QM/MM (BS2+ZPE) = -3430.036944 a.u.

6	35.013937301	35.291708826	30.389086490
7	35.821311354	34.961074065	31.451486395
1	36.566986610	34.249125197	31.443496178
6	35.439930897	35.683142888	32.513098323
1	35.907217083	35.630015858	33.492150948
7	34.408436389	36.465822303	32.196538047
6	34.130865702	36.229446403	30.868301088
1	33.312027273	36.725903776	30.359374146
6	29.286856536	38.299409357	31.745986700
1	28.864795452	37.554311503	32.435252539
1	28.793705579	39.266075742	31.927256674
6	30.783884823	38.474516649	33.4921346119
8	31.322851158	39.564971410	31.709691988
8	31.420603256	37.479176700	32.492244501
6	32.313355391	33.010437284	34.497713909
7	31.239760302	33.331526222	33.699250487
1	30.483435947	32.720246165	33.364188899
6	31.322143362	34.630829890	33.376528524
1	30.604441326	35.160755359	32.756570971
7	32.397888175	35.174652056	33.932182897
6	33.031959251	34.173903270	34.632238529
1	33.966583890	34.353394694	35.155888082
6	29.279641882	44.341950387	33.723367401
1	29.552272757	45.291608295	33.230910534
1	28.579382221	43.804877871	33.069165671
7	30.455281876	43.524230945	33.978660112
1	31.094326074	43.812747615	34.721415706
6	30.780952530	42.377264161	33.340532220
7	30.058896233	41.907197344	32.320268552
1	29.594725578	42.553118376	31.688964867
1	30.425255464	41.043094257	31.869591752
7	31.827960325	41.678315341	33.784752089
1	32.354035156	41.998860099	34.596489388
1	32.138947311	40.837548341	33.287376551
26	33.015240033	37.171407852	33.624981957
6	34.388602460	39.598071521	34.540070356
8	34.916162157	40.640253722	34.865915703
8	33.705230216	39.229342777	33.571321135
6	34.482086273	38.177501456	35.690982729

8	34.614586086	37.157945276	34.912616326	1	28.631088860	43.762296888	33.055310176
6	35.482152235	38.446004838	36.805814150	7	30.489286081	43.495438591	34.001925278
6	35.639762520	37.194574364	37.672614781	1	31.092770357	43.778379019	34.774902439
6	36.474596162	37.336328111	38.955706168	6	30.799696692	42.299142438	33.437738779
8	36.047995059	36.690328518	39.948982290	7	30.147186325	41.829097852	32.374199789
8	37.522775301	38.032489464	38.927265505	1	29.794955232	42.481927340	31.675807748
1	36.119311145	36.407229321	37.064550423	1	30.534468409	40.939083379	31.968312546
1	34.647086305	36.819394357	37.958971948	7	31.755533105	41.571094743	34.013089362
1	35.118966988	39.299304549	37.396917329	1	32.252177516	41.943199744	34.821361545
1	36.442613070	38.742150742	36.360825657	1	32.094526321	40.678665539	33.633252453
8	32.228306272	37.778830244	35.356762776	26	33.098314188	37.208230783	33.439869681
8	33.157925143	38.368328423	36.178579182	6	35.383597217	41.013078276	33.823025161
8	36.789627893	38.999192706	29.767995387	8	34.811322402	41.886446669	34.056064981
6	35.905812684	38.765420375	28.963844478	8	35.976193369	40.161844489	33.307557905
7	34.630656146	39.336279783	29.107770017	6	34.828310098	38.111683564	35.655628264
6	34.435042378	40.252023918	30.237988103	8	34.723985396	37.056969748	35.034159254
6	33.580793477	39.076277813	28.258850152	6	35.757558153	38.326483791	36.827796972
7	32.396189839	39.574347568	28.544204031	6	35.755343271	37.107009489	37.747488547
6	33.837390202	38.293602928	27.093360455	6	36.542970673	37.260313551	39.054453056
6	35.067042794	37.739682648	26.926277131	8	36.065790915	36.665448477	40.054904249
7	36.061290765	37.923778407	27.864469827	8	37.606871033	37.933422048	39.034308723
1	34.002058345	41.190889034	29.865558769	1	36.192003133	36.253194968	37.200556776
1	35.410611398	40.451591142	30.686408231	1	34.723574680	36.825011346	38.002584842
1	31.541958009	39.396946864	27.977158064	1	35.455951437	39.239221468	37.361884658
1	35.295333304	37.123645044	26.052249748	1	36.774400955	38.504803971	36.437843013
1	33.037772570	38.114549197	26.379001570	8	33.206890348	39.023009826	34.244508125
1	33.771995176	39.803641329	30.992709035	8	34.113367562	39.176240956	35.386024918
1	32.203975909	40.000942802	29.445617987	8	36.763502645	38.948994751	29.769611409
1	35.031337802	34.750672736	29.443018578	6	35.880169564	38.719837189	28.961985791
1	29.046381116	37.985285387	30.730326805	7	34.601527208	39.273496760	29.120126649
1	32.528769584	31.990936784	34.817530704	6	34.392410981	40.147728040	30.278880380
1	28.750875687	44.561366171	34.650907346	6	33.560347243	39.049498777	28.250075314
1	36.913661151	37.402374591	27.824780094	7	32.377708975	39.546564545	28.540202387

IMI

QM/MM (BS1) = -3428.111730 a.u.

QM/MM (BS2+ZPE) = -3430.110558 a.u.

6	35.074123884	35.248243911	30.278106189
7	35.861421904	34.895308880	31.347486703
1	36.581490559	34.159776222	31.355168002
6	35.494730900	35.637813830	32.402361845
1	35.949049339	35.561167834	33.386342058
7	34.501776376	36.460033934	32.075352298
6	34.225973956	36.222758328	30.747876264
1	33.416920512	36.731942133	30.233352298
6	29.266980348	38.378906343	31.650593388
1	28.782893853	37.695479461	32.363727307
1	28.828295213	39.380743711	31.768201000
6	30.769137183	38.443238580	31.923396415
8	31.379257093	39.526598561	31.710818009
8	31.325385377	37.403192001	32.386056307
6	32.324683599	33.084907763	34.528435024
7	31.247535218	33.409216094	33.736735874
1	30.509663098	32.790673714	33.376402712
6	31.304977064	34.722768225	33.458522898
1	30.589948982	35.256462293	32.838192984
7	32.363994007	35.278208980	34.036022465
6	33.016154732	34.262252359	34.700961005
1	33.950377800	34.443949924	35.224920392
6	29.316842465	44.308844190	33.717429360
1	29.594050152	45.254447267	33.219276360

1	28.631088860	43.762296888	33.055310176
7	30.489286081	43.495438591	34.001925278
1	31.092770357	43.778379019	34.774902439
6	30.799696692	42.299142438	33.437738779
7	30.147186325	41.829097852	32.374199789
1	29.794955232	42.481927340	31.675807748
1	30.534468409	40.939083379	31.968312546
7	31.755533105	41.571094743	34.013089362
1	32.252177516	41.943199744	34.821361545
1	32.094526321	40.678665539	33.633252453
26	33.098314188	37.208230783	33.439869681
6	35.383597217	41.013078276	33.823025161
8	34.811322402	41.886446669	34.056064981
8	35.976193369	40.161844489	33.307557905
6	34.828310098	38.111683564	35.655628264
8	34.723985396	37.056969748	35.034159254
6	35.757558153	38.326483791	36.827796972
6	35.755343271	37.107009489	37.747488547
6	36.542970673	37.260313551	39.054453056
8	36.065790915	36.665448477	40.054904249
8	37.606871033	37.933422048	39.034308723
1	36.192003133	36.253194968	37.200556776
1	34.723574680	36.825011346	38.002584842
1	35.455951437	39.239221468	37.361884658
1	36.774400955	38.504803971	36.437843013
8	33.206890348	39.023009826	34.244508125
8	34.113367562	39.176240956	35.386024918
8	36.763502645	38.948994751	29.769611409
6	35.880169564	38.719837189	28.961985791
7	34.601527208	39.273496760	29.120126649
6	34.392410981	40.147728040	30.278880380
6	33.560347243	39.049498777	28.250075314
7	32.377708975	39.546564545	28.540202387
6	33.829630013	38.304869048	27.061633803
6	35.057273663	37.746129836	26.895057584
7	36.044616845	37.903607271	27.846397366
1	34.042825848	41.129639291	29.928262627
1	35.347810224	40.252120032	30.796668073
1	31.533975767	39.397869993	27.948808843
1	35.291626354	37.148626084	26.010069114
1	33.036730212	38.147899180	26.334371385
1	33.647027339	39.714400105	30.964398245
1	32.164212985	39.899742177	29.470401273
1	35.062330470	34.690153819	29.341909793
1	29.026462890	38.020079019	30.649862843
1	32.534990608	32.061377446	34.838634923
1	28.776862058	44.539895418	34.635636201
1	36.895730519	37.380278383	27.805107178

TS2

QM/MM (BS1) = -3428.102605 a.u.

QM/MM (BS2+ZPE) = -3430.111891 a.u.

6	35.059649214	35.270838441	30.297040389
7	35.845856489	34.931374050	31.372697782
1	36.569532206	34.197851361	31.385115085
6	35.475845729	35.682552559	32.418483188
1	35.922248591	35.618830458	33.406979674
7	34.478657744	36.497278588	32.077149860
6	34.204111760	36.245076987	30.751319504
1	33.392375208	36.745414679	30.232904440
6	29.308713133	38.333098273	31.627712865

1	28.851025752	37.629613044	32.338530236
1	28.866964327	39.328801392	31.778663189
6	30.818607312	38.412507617	31.848997666
8	31.408104296	39.495026904	31.607371847
8	31.399986997	37.372927142	32.298483859
6	32.319605995	33.152177754	34.524319750
7	31.258742858	33.466339322	33.705740200
1	30.537870262	32.838124509	33.326765045
6	31.301583440	34.780450741	33.436236217
1	30.600364217	35.304955307	32.793858726
7	32.335321792	35.349784775	34.047787351
6	32.985479115	34.339592503	34.726182524
1	33.898471682	34.539396910	35.279342769
6	29.321522271	44.261162923	33.724928532
1	29.602320235	45.199171142	33.214144167
1	28.636073874	43.706970756	33.068562833
7	30.491066339	43.447717567	34.025043323
1	31.088414424	43.735418711	34.801253911
6	30.818401447	42.253353255	33.463479267
7	30.180898424	41.785161556	32.388745892
1	29.825263732	42.441837396	31.695088781
1	30.575634340	40.909151706	31.967699600
7	31.770830873	41.532886580	34.051891681
1	32.255138580	41.921265410	34.860603404
1	32.121168205	40.623935594	33.708339238
26	33.112423525	37.264876869	33.455136751
6	35.373338804	41.008497432	33.811017579
8	34.818227975	41.889085126	34.340323635
8	35.951335252	40.157609383	33.278346760
6	34.803018479	38.144079796	35.653992255
8	34.636803249	37.067170809	35.046614356
6	35.801387486	38.283580248	36.793310951
6	35.779915125	37.062957129	37.710967410
6	36.560019737	37.216046525	39.023907659
8	36.074879492	36.624337691	40.023009255
8	37.624237921	37.888936271	39.011676235
1	36.208207626	36.199882032	37.171536834
1	34.743098733	36.795292074	37.962256710
1	35.570768654	39.204864334	37.347080993
1	36.805601474	38.419961571	36.356297180
8	33.058457601	38.965817555	34.075505761
8	34.150992758	39.222331691	35.406155191
8	36.782594000	38.952908281	29.761261559
6	35.898264299	38.726473591	28.953953452
7	34.621604791	39.283426798	29.111718441
6	34.418394711	40.170023691	30.262715931
6	33.576949999	39.053689189	28.246693797
7	32.393251847	39.542597711	28.544470540
6	33.844783141	38.311404964	27.056143837
6	35.072078804	37.752840465	26.887621855
7	36.059787044	37.908380264	27.839163946
1	34.052998794	41.142405846	29.902678998
1	35.378783577	40.291891713	30.766799383
1	31.549911008	39.399800114	27.950994133
1	35.305981652	37.155758271	26.002246419
1	33.050098664	38.153158720	26.331073669
1	33.686873650	39.738600857	30.962552652
1	32.178287375	39.882387021	29.480181591
1	35.060429406	34.711335213	29.361613824
1	29.047531183	37.994795777	30.625015140
1	32.528679211	32.129151754	34.837007306
1	28.779197142	44.507337957	34.637807839

1	36.910053876	37.383694767	27.797643557
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IM2

QM/MM (BS1) = -3428.108480 a.u.

QM/MM (BS2+ZPE) = -3430.118173 a.u.

6	35.050210126	35.287806377	30.322082924
7	35.835804936	34.957775354	31.402031400
1	36.563620254	34.227519196	31.417041406
6	35.462043669	35.712256236	32.443128507
1	35.906202381	35.660818440	33.433394514
7	34.459323560	36.519323869	32.093086737
6	34.187447382	36.258916417	30.767089611
1	33.377912534	36.755040180	30.242042934
6	29.325314382	38.297840844	31.605171195
1	28.883859533	37.586027678	32.317578686
1	28.882788103	39.290851980	31.772220456
6	30.838578732	38.391899947	31.787831518
8	31.416451130	39.456769331	31.490080239
8	31.437384816	37.362142505	32.268060903
6	32.332957360	33.197704085	30.242042934
7	31.278768698	33.504658359	33.697134180
1	30.565754633	32.871229562	33.311040188
6	31.317175589	34.815329644	33.420873498
1	30.619136007	35.331051631	32.769075937
7	32.343310490	35.393161651	34.040551635
6	32.991725841	34.388894233	34.732480400
1	33.895926212	34.599412838	35.295207852
6	29.312098153	44.231420304	33.732243439
1	29.589503631	45.164193331	33.209822725
1	28.625741053	43.668736991	33.083934506
7	30.483624964	43.424411431	34.040939987
1	31.076605219	43.719869319	34.817531726
6	30.831290982	42.234061564	33.481127958
7	30.198917317	41.762312344	32.400209872
1	29.847478222	42.421124710	31.705513303
1	30.602765051	40.904343099	31.966776033
7	31.788600513	41.526902733	34.069138351
1	32.259105060	41.923772218	34.882523391
1	32.157669677	40.606190481	33.742916283
26	33.107051228	37.326596716	33.453007850
6	35.369850197	41.015625550	33.795874352
8	34.824273052	41.904675206	34.321024769
8	35.946771993	40.168201744	33.255953577
6	34.784257134	38.218331333	35.663452033
8	34.510619134	37.147974603	35.023040356
6	35.850444350	38.213514815	36.757318357
6	35.795948121	36.995033795	37.674321865
6	36.569434922	37.149910354	38.993259798
8	36.074399628	36.573281602	39.997064515
8	37.637710171	37.816189740	38.983796363
1	36.209357914	36.115275808	37.149798714
1	34.753637552	36.752368285	37.926940870
1	35.717642668	39.138898400	37.335653431
1	36.838843446	38.291210581	36.272633670
8	32.970574775	39.056983264	33.801118303
8	34.230083298	39.323474239	35.470004617
8	36.793116563	38.953220575	29.756011517
6	35.910507978	38.730016755	28.945951472
7	34.634559569	39.288592557	29.100827761
6	34.433091778	40.180947449	30.248810412
6	33.590685937	39.056172406	28.234989809
7	32.405512212	39.540281306	28.532544515

6	33.860613759	38.314869578	27.044065181
6	35.087991953	37.756608853	26.877223448
7	36.073561380	37.911802205	27.831129819
1	34.040141501	41.141173419	29.886028049
1	35.399300806	40.328923114	30.734301010
1	31.563853162	39.400692899	27.935989191
1	35.323581823	37.159077313	25.992631554
1	33.066396884	38.155552575	26.318707495
1	33.726196822	39.741182221	30.967617937
1	32.185941389	39.871295714	29.470893646
1	35.060760084	34.729899830	29.385762304
1	29.054713785	37.970896963	30.601203894
1	32.534405587	32.174040426	34.842801363
1	28.772992708	44.487962243	34.644174836
1	36.923783592	37.386964685	27.790629587

IM3

QM/MM (BS1) = -3428.112549 a.u.

QM/MM (BS2+ZPE) = -3430.125638 a.u.

6	35.016539773	35.289167431	30.603818373
7	35.774435605	34.892424091	31.679722823
1	36.514053549	34.175014198	31.658772479
6	35.342076800	35.551267023	32.764652862
1	35.752563424	35.420350746	33.760868441
7	34.330919579	36.360904076	32.449485815
6	34.116187119	36.204549079	31.096580713
1	33.311223130	36.724917310	30.589214489
6	29.473444762	38.308792908	31.697549789
1	29.058816136	37.546217948	32.374052519
1	28.981047359	39.266089326	31.920921723
6	30.973883713	38.472663814	31.957541678
8	31.466408267	39.626875977	31.894499983
8	31.660093633	37.442599899	32.266271766
6	32.233690762	33.001335097	34.503824620
7	31.198097378	33.318779024	33.655405061
1	30.479612324	32.700449702	33.257780848
6	31.257919035	34.634366811	33.384881772
1	30.566993421	35.161980960	32.733626163
7	32.279342433	35.184726760	34.022905103
6	32.904300759	34.180626959	34.722622929
1	33.794297393	34.379582819	35.309786950
6	29.341735656	44.399789185	33.713971944
1	29.633824681	45.362644583	33.260711738
1	28.660481878	43.888472594	33.021196833
7	30.506937148	43.569097699	33.975295449
1	31.136321374	43.840983053	34.731752713
6	30.787237992	42.385539546	33.382369783
7	30.058185448	41.912145432	32.365511984
1	29.667976838	42.559299923	31.684666767
1	30.437624628	41.033523224	31.953539812
7	31.791548612	41.649571978	33.857252954
1	32.356021719	41.972329602	34.642474028
1	32.029506842	40.776166632	33.373679576
26	32.950872410	37.168676779	33.807342554
6	35.597482300	41.118134560	33.806080890
8	34.870261857	41.740567329	34.478656987
8	36.329962108	40.536932536	33.124692050
6	34.812448978	37.885503238	35.369058580
8	34.383887036	36.691900010	35.315853549
6	35.759894492	38.282150876	36.495820662

6	35.786365287	37.215272238	37.589222659
6	36.575082196	37.456970443	38.882193865
8	36.134214327	36.832544327	39.885290431
8	37.605667102	38.179949917	38.870281583
1	36.196252268	36.284572104	37.158772041
1	34.755418800	36.972024697	37.880075351
1	35.417791153	39.254867895	36.884853530
1	36.765772948	38.462220406	36.078390598
8	31.892409685	37.811356907	34.844651583
8	34.398662908	38.712689878	34.507225875
8	36.820796200	38.975234709	29.731106001
6	35.938920987	38.719759712	28.932074555
7	34.658797252	39.280776339	29.071001046
6	34.446988179	40.173388766	30.214968977
6	33.627091946	39.050463039	28.193334511
7	32.455414267	39.597084287	28.438190301
6	33.887835351	38.247993861	27.042921465
6	35.111149416	37.674682589	26.899943419
7	36.097952445	37.862828776	27.845873163
1	34.161563978	41.171598465	29.851609731
1	35.385469716	40.236548013	30.770279179
1	31.603877515	39.428436969	27.864417423
1	35.341954984	37.043430398	26.037535493
1	33.097532763	38.076766142	26.316926719
1	33.658942140	39.774061522	30.872386707
1	32.269988357	40.075933462	29.312625828
1	35.079698380	34.801521944	29.631049030
1	29.201787658	38.019668134	30.682327348
1	32.467897743	31.983312293	34.815022277
1	28.786965454	44.593449584	34.632009516
1	36.952888335	37.345171531	27.812886751

**Ferryl flip mechanism reaction states coordinate
AlkBH2-dsDNA**

IM3'

QM/MM (BS1) = -3580.810509 a.u.

QM/MM (BS2+ZPE) = -3582.962240 a.u.

6	35.039985247	35.175720984	30.678143212
7	35.773272511	34.730309810	31.750960056
1	36.511646835	34.012721452	31.714822483
6	35.321051054	35.344521224	32.853741588
1	35.710936172	35.169537918	33.851748622
7	34.322702107	36.173499864	32.551455762
6	34.134991343	36.076058747	31.189571693
1	33.343908990	36.623591753	30.687663138
6	29.537182394	38.250299222	31.749361845
1	29.076941584	37.499445961	32.409344736
1	29.082857823	39.224801690	31.975845723
6	31.039112069	38.332391277	32.041515773
8	31.594182379	39.458774780	32.016864358
8	31.664072268	37.259459803	32.332532372
6	32.197092217	32.815714408	34.506143173
7	31.145030875	33.147117491	33.683303132
1	30.413110000	32.542307769	33.290828374
6	31.201793920	34.467886600	33.434224074
1	30.497065690	35.008370758	32.808754409
7	32.237977055	35.003360566	34.060425913
6	32.873767687	33.987101801	34.729164560
1	33.772469768	34.174713721	35.303007358
6	29.284807795	44.248030204	33.712370479

1	29.522638476	45.170557423	33.155054880	1	36.523593742	34.152206061	31.600465703
1	28.593848191	43.650655893	33.102673693	6	35.338743603	35.518817382	32.705136112
7	30.490180549	43.481404916	33.997393023	1	35.773431608	35.425375512	33.696186677
1	31.133905469	43.836965597	34.705338740	7	34.313054185	36.302897941	32.388442700
6	30.833655166	42.295346586	33.444991667	6	34.090165722	36.142208613	31.041095415
7	30.092025555	41.715307873	32.492971929	1	33.278694848	36.657594878	30.536008325
1	29.666838848	42.316038120	31.784460373	6	29.293842538	38.188134061	31.748126672
1	30.533510736	40.861756015	32.094660679	1	28.855163214	37.394267104	32.372716849
7	31.913475459	41.661387458	33.899067567	1	28.781327070	39.131099634	31.983900283
1	32.502868030	42.077763374	34.619736663	6	30.775188933	38.344735304	32.076766376
1	32.217248923	40.803467268	33.434358585	8	31.217694653	39.526162407	32.181610026
26	32.930468277	36.963911097	33.908454812	8	31.488032381	37.317333342	32.276424142
6	35.817930535	41.869189924	33.151483791	6	32.346082167	33.088437333	30.57820290
8	34.986484040	42.034603863	33.954728986	7	31.303585079	33.418899265	33.744473085
8	36.618140550	41.865168801	32.306544117	1	30.588131649	32.803145157	33.336460133
6	34.754883029	37.532057631	35.572583161	6	31.356784305	34.737205381	33.495186007
8	34.332377028	36.346993096	35.523030045	1	30.674817148	35.272109551	32.841967637
6	35.674142901	37.990161983	36.689156073	7	32.380820156	35.286836718	34.134110585
6	35.883701161	36.892016917	37.727740176	6	33.014612905	34.269414651	34.811483341
6	36.586184282	37.265080110	39.037218288	1	33.914903852	34.450205196	35.391324702
8	36.068715079	36.782430903	40.081724011	6	29.489875800	44.530378996	33.809017083
8	37.630268118	37.966261809	38.998743974	1	29.919715796	45.527413207	33.625938614
1	36.471595944	36.072600516	37.274962812	1	28.935269367	44.240607900	32.907803230
1	34.908752549	36.465757029	37.990870017	7	30.566417586	43.590884471	34.085487885
1	35.203996633	38.883393039	37.136487382	1	31.200809353	43.821075415	34.853274871
1	36.610594477	38.361619329	36.242854358	6	30.653609285	42.316973309	33.638603255
8	31.846932134	37.583158939	34.931887601	7	29.881449385	41.846521034	32.656850122
8	34.353340411	38.344997729	34.672540837	1	29.583118753	42.492605185	31.923581585
8	35.752264005	38.851368692	29.225891290	1	30.207386809	40.929965703	32.283774674
6	35.224917725	38.444464493	28.197385982	7	31.518732605	41.494819018	34.237460484
7	33.912700364	38.814845815	27.852487360	1	32.147994343	41.845956974	34.957927488
6	33.211567497	39.759268356	28.737269524	1	31.643314360	40.550385687	33.870339884
6	33.236059810	38.312982955	26.759350919	26	33.051720867	37.270655119	33.732996204
7	31.984572502	38.644525535	26.536163387	6	36.877131400	41.459820415	32.854971295
6	33.955430458	37.456551668	25.876480175	8	35.997017261	41.841666283	33.510159226
6	35.238641757	37.142571740	26.154389313	8	37.829960583	41.115250491	32.277976574
7	35.861903387	37.589016958	27.301331850	6	35.033298050	38.489423080	35.527482956
1	32.750547965	40.547501766	28.131676397	8	34.629121045	37.384663918	34.997859166
1	33.928206966	40.204631920	29.428448863	6	35.919659221	38.409597565	36.762784536
1	31.483589711	38.283889779	25.717145884	6	35.773574168	37.164450685	37.625874000
1	35.803273781	36.516595875	25.468390757	6	36.567046084	37.214835137	38.941963552
1	33.475978053	37.043538340	24.996437317	8	36.067822193	36.605490012	39.925479745
1	32.420157870	39.241680296	29.296461860	8	37.661036029	37.838741591	38.949644332
1	31.397181903	39.219567889	27.168347268	1	36.120907641	36.278520925	37.063557105
8	36.635429961	39.829297557	34.269291538	1	34.715422430	36.984402571	37.869605479
1	37.089331863	39.403757539	33.528585781	1	35.702888899	39.312208357	37.351602463
1	33.570942578	39.571619495	31.798870256	1	36.967221027	38.522424050	36.433659719
8	34.508032468	39.843419715	31.798865520	8	32.071445361	38.030331871	34.777142367
1	35.739658775	39.430923700	34.233097296	8	34.766087558	39.623607519	35.079783794
1	34.909517972	39.375865580	31.048106876	8	35.834728124	38.957944742	28.865848573
1	35.122270092	34.722361251	29.690336816	6	35.238868954	38.439265687	27.930090838
1	29.269618259	37.984145815	30.726796875	7	33.896170972	38.743158671	27.657840367
1	32.459455752	31.799692354	34.800985295	6	33.197965721	39.686563821	28.549558468
1	28.766739733	44.513030206	34.634025407	6	33.182865240	38.180985188	26.618428462
1	36.749251325	37.195796234	27.542088152	7	31.923346175	38.502353881	26.426406581
				6	33.869832530	37.263557969	25.770044167
				6	35.163009871	36.962194917	26.020876025
				7	35.838787374	37.504977112	27.092865246
				1	32.728448105	40.475096237	27.951096502
				1	33.909166253	40.134434647	29.244339578
				1	31.398930072	38.118948665	25.633146018
				1	35.693633584	36.269985630	25.374303555

IM4

QM/MM (BS1) = -3580.818612 a.u.

QM/MM (BS2+ZPE) = -3582.964722 a.u.

6	35.004749736	35.239871729	30.548858204
7	35.774438193	34.859127132	31.621226528

1	36.523593742	34.152206061	31.600465703
6	35.338743603	35.518817382	32.705136112
1	35.773431608	35.425375512	33.696186677
7	34.313054185	36.302897941	32.388442700
6	34.090165722	36.142208613	31.041095415
1	33.278694848	36.657594878	30.536008325
6	29.293842538	38.188134061	31.748126672
1	28.855163214	37.394267104	32.372716849
1	28.781327070	39.131099634	31.983900283
6	30.775188933	38.344735304	32.076766376
8	31.217694653	39.526162407	32.181610026
8	31.488032381	37.317333342	32.276424142
6	32.346082167	33.088437333	30.57820290
7	31.303585079	33.418899265	33.744473085
1	30.588131649	32.803145157	33.336460133
6	31.356784305	34.737205381	33.495186007
1	30.674817148	35.272109551	32.841967637
7	32.380820156	35.286836718	34.134110585
6	33.014612905	34.269414651	34.811483341
1	33.914903852	34.450205196	35.391324702
6	29.489875800	44.530378996	33.809017083
1	29.919715796	45.527413207	33.625938614
1	28.935269367	44.240607900	32.907803230
7	30.566417586	43.590884471	34.085487885
1	31.200809353	43.821075415	34.853274871
6	30.653609285	42.316973309	33.638603255
7	29.881449385	41.846521034	32.656850122
1	29.583118753	42.492605185	31.923581585
1	30.207386809	40.929965703	32.283774674
7	31.518732605	41.494819018	34.237460484
1	32.147994343	41.845956974	34.957927488
1	31.643314360	40.550385687	33.870339884
26	33.051720867	37.270655119	33.732996204
6	36.877131400	41.459820415	32.854971295
8	35.997017261	41.841666283	33.510159226
8	37.829960583	41.115250491	32.277976574
6	35.033298050	38.489423080	35.527482956
8	34.629121045	37.384663918	34.997859166
6	35.919659221	38.409597565	36.762784536
6	35.773574168	37.164450685	37.625874000
6	36.567046084	37.214835137	38.941963552
8	36.067822193	36.605490012	39.925479745
8	37.661036029	37.838741591	38.949644332
1	36.120907641	36.278520925	37.063557105
1	34.715422430	36.984402571	37.869605479
1	35.702888899	39.312208357	37.351602463
1	36.967221027	38.522424050	36.433659719
8	32.071445361	38.030331871	34.777142367
8	34.766087558	39.623607519	35.079783794
8	35.834728124	38.957944742	28.865848573
6	35.238868954	38.439265687	27.930090838
7	33.896170972	38.743158671	27.657840367
6	33.197965721	39.686563821	28.549558468
6	33.182865240	38.180985188	26.618428462
7	31.923346175	38.502353881	26.426406581
6	33.869832530	37.263557969	25.770044167
6	35.163009871	36.962194917	26.020876025
7	35.838787374	37.504977112	27.092865246
1	32.728448105	40.475096237	27.951096502
1	33.909166253	40.134434647	29.244339578
1	31.398930072	38.118948665	25.633146018
1	35.693633584	36.269985630	25.374303555

1	33.349427648	36.773125289	24.954770573
1	32.410652846	39.156850944	29.103724753
1	31.352841014	39.097566407	27.056764906
8	33.721201590	39.065716954	32.835876146
1	32.854969676	39.463179430	32.549599334
1	34.821767250	39.909247561	31.604780979
8	35.290608005	40.579206347	31.069652656
1	34.084766802	39.496916649	33.686552572
1	35.557863619	40.082130440	30.277585235
1	35.074715435	34.750579178	29.577382566
1	29.080678898	37.933632735	30.709927429
1	32.553583489	32.058931848	34.869588987
1	28.792407354	44.597570970	34.643936436
1	36.726192839	37.127596590	27.357568834

TS3

QM/MM (BS1) = -3580.806149 a.u.

QM/MM (BS2+ZPE) = -3582.951774 a.u.

6	35.014830483	35.227739001	30.497666851
7	35.776543334	34.845958937	31.575616640
1	36.524686853	34.138045531	31.562784462
6	35.335436229	35.504458274	32.656432156
1	35.763414711	35.412564358	33.650345365
7	34.312129453	36.288771808	32.331173990
6	34.098094967	36.130830556	30.982842573
1	33.291110325	36.648343505	30.472982701
6	29.288144982	38.181379081	31.739214512
1	28.856835578	37.385627846	32.366071917
1	28.776102895	39.123794400	31.978756526
6	30.773168391	38.339735490	32.044920489
8	31.223330100	39.518389328	32.117591813
8	31.482527737	37.309907143	32.253996923
6	32.353845801	33.127122974	34.579032243
7	31.310498283	33.453602470	33.744861279
1	30.600807572	32.833710927	33.332844011
6	31.355222089	34.772789630	33.500389836
1	30.672410413	35.302749379	32.844154594
7	32.373296398	35.330833525	34.143548890
6	33.012213303	34.313285551	34.819016708
1	33.909743088	34.500096238	35.401497203
6	29.488716913	44.512114586	33.806475249
1	29.921896255	45.506990786	33.618687452
1	28.932772349	44.220189819	32.906718755
7	30.561424624	43.569422031	34.087636482
1	31.194406870	43.799296353	34.856663436
6	30.654147141	42.296532367	33.636954571
7	29.892269086	41.828265266	32.646535875
1	29.591701971	42.478671604	31.918133234
1	30.226835322	40.917724997	32.263810695
7	31.513888886	41.474108031	34.242732545
1	32.138811429	41.825719278	34.966508493
1	31.649027018	40.529227075	33.880319971
26	33.091392063	37.297106187	33.650557374
6	36.859998508	41.438651542	32.881413409
8	35.980007504	41.780884490	33.559814171
8	37.818292277	41.135839815	32.290589328
6	34.990078350	38.427115809	35.530641832
8	34.674706807	37.321480350	34.958575830
6	35.915014367	38.384008162	36.737076518
6	35.776959834	37.153270916	37.626127486
6	36.569837832	37.223814397	38.941942660

8	36.073699072	36.614551680	39.927028768
8	37.656757128	37.859168796	38.947906757
1	36.124484906	36.257922600	37.079218190
1	34.720298788	36.975030900	37.877722931
1	35.721960929	39.298647803	37.313993672
1	36.954051250	38.472150819	36.374646258
8	32.254083702	38.255964710	34.653758013
8	34.587565480	39.548572519	35.138338908
8	35.830176507	38.944202622	28.891150791
6	35.238878304	38.435498072	27.947315711
7	33.897421217	38.743346359	27.671463078
6	33.200040196	39.686552497	28.564436451
6	33.186148007	38.186121907	36.628071162
7	31.927096449	38.508230225	26.434086218
6	33.874665527	37.272954754	25.776136998
6	35.168204211	36.972616486	26.025894694
7	35.841848728	37.509381386	27.102370280
1	32.730164867	40.474684024	27.965674547
1	33.912591305	40.134511595	29.258252373
1	31.404378623	38.126187630	25.639083742
1	35.700721680	36.285492931	25.375063485
1	33.355553986	36.786472356	24.957682476
1	32.413030297	39.157885930	29.120028386
1	31.354609482	39.100021001	27.065895447
8	33.728877999	39.083385859	32.847812283
1	32.855934927	39.429913342	32.516926841
1	34.820990841	39.961005557	31.686488825
8	35.290412220	40.592295732	31.103027886
1	33.889540424	39.383211794	33.912739470
1	35.544457295	40.050159498	30.336926706
1	35.081988802	34.729270035	29.530668524
1	29.072528235	37.926884619	30.701520284
1	32.557988402	32.096931760	34.870749875
1	28.791573862	44.586554230	34.641051568
1	36.729431177	37.130523470	27.364356104

IM5

QM/MM (BS1) = -3580.810798 a.u.

QM/MM (BS2+ZPE) = -3582.957150 a.u.

6	35.013101238	35.240445516	30.454990744
7	35.774571461	34.852198455	31.530269515
1	36.519114801	34.140567701	31.516962306
6	35.338705581	35.513457187	32.612582884
1	35.768722703	35.408073670	33.604177010
7	34.322404371	36.307648646	32.292160873
6	34.105683834	36.152473381	30.944238442
1	33.299987623	36.676533365	30.437585305
6	29.214366175	38.202131646	31.711214828
1	28.765821388	37.420055356	32.343505048
1	28.701787464	39.150813407	31.923263740
6	30.693111769	38.349201677	32.053064633
8	31.145671852	39.521579526	32.171624758
8	31.388935358	37.308018113	32.245574966
6	32.377869352	33.140589820	34.560678858
7	31.338358946	33.464329253	33.720871404
1	30.620199701	32.845558872	33.323651524
6	31.399468033	34.777014788	33.449095325
1	30.723344665	35.308771257	32.786653560
7	32.426947854	35.332981857	34.078812013
6	33.053223212	34.322307801	34.775664624
1	33.954788106	34.508216659	35.351922122

6	29.472208281	44.516619028	33.804899502	7	35.781826201	34.826401832	31.491120247
1	29.899658782	45.512873602	33.611056192	1	36.527724801	34.116784121	31.477231101
1	28.907736518	44.220899017	32.911928299	6	35.345355387	35.479988689	32.576787080
7	30.550085387	43.577655130	34.074288711	1	35.773798534	35.372849860	33.568254902
1	31.192052507	43.808202528	34.834885802	7	34.332757782	36.278284817	32.256437038
6	30.634293358	42.303955586	33.621292401	6	34.118750374	36.135451517	30.907648280
7	29.856475553	41.838116424	32.643744375	1	33.316940086	36.667232212	30.402949035
1	29.562484100	42.485733987	31.910079839	6	29.183161000	38.199057729	31.701073776
1	30.176814350	40.914317233	32.272805099	1	28.726499687	37.421593806	32.333555949
7	31.502237197	41.479572824	34.213108102	1	28.674363637	39.151462771	31.905944007
1	32.128192133	41.833046366	34.934000992	6	30.662030136	38.339100122	32.043252782
1	31.648889570	40.545715656	33.820759346	8	31.117106546	39.510389935	32.171559267
26	33.052837389	37.314187928	33.608213711	8	31.350631741	37.292024524	32.2203049536
6	36.809234307	41.441700587	32.884758555	6	32.386494164	33.166107181	34.549234002
8	35.938033165	41.757657167	33.589360581	7	31.339190464	33.485096359	33.717408018
8	37.771243133	41.186094233	32.279028694	1	30.616919791	32.863146639	33.331067541
6	35.103434832	38.339571720	35.592817338	6	31.398963389	34.795918502	33.436950569
8	34.780011831	37.278021235	35.035153313	1	30.716374813	35.324009737	32.778609007
6	35.960640591	38.376710956	36.831729505	7	32.433885627	35.355919574	34.051881955
6	35.828992605	37.140350445	37.708280476	6	33.064444521	34.348775337	34.750527895
6	36.596926268	37.229451257	39.032989500	1	33.970142882	34.537734843	35.319684120
8	36.089483836	36.626946064	40.014191850	6	29.466511286	44.514537530	33.804326657
8	37.678371706	37.874399883	39.042212493	1	29.896186654	45.509092921	33.606292459
1	36.207100841	36.257284355	37.162449765	1	28.897708419	44.218838220	32.914028513
1	34.771018141	36.941364141	37.935611540	7	30.541740310	43.572010073	34.071373786
1	35.696178773	39.287289628	37.387544764	1	31.183148867	43.799249600	34.833370408
1	37.009988545	38.516034118	36.517964592	6	30.622634768	42.298587495	33.616971256
8	32.201763789	38.093726210	34.753136141	7	29.841887904	41.835134055	32.640304125
8	34.735790843	39.512808958	35.163612265	1	29.551707045	42.483903336	31.906303689
8	35.845180952	38.935650398	28.909336687	1	30.155800378	40.907846559	32.271332208
6	35.249356120	38.434474050	27.964726934	7	31.490425945	41.472172195	34.206155755
7	33.906066730	38.742272585	27.698843127	1	32.114614837	41.825765734	34.928735192
6	33.208582630	39.668575150	28.610391473	1	31.636362151	40.540015559	33.806630298
6	33.195079032	38.201629922	26.646689120	26	33.072695130	37.332239323	33.529297921
7	31.937752899	38.530356226	26.453754164	6	36.725724803	41.345700896	32.979124596
6	33.881781616	37.297013036	25.783614156	8	35.843271146	41.562476520	33.708508728
6	35.175277353	36.991927069	26.027698564	8	37.700374409	41.186964841	32.360439280
7	35.850242104	37.517127752	27.108833190	6	35.117985058	38.200871606	35.678190138
1	32.758852582	40.482402498	28.030588874	8	34.861293996	37.207770759	34.986967306
1	33.917421858	40.080228767	29.330447179	6	36.210644079	38.218041100	36.714165614
1	31.413821442	38.153109856	25.657205787	6	35.957708906	37.085502710	37.716275307
1	35.707729363	36.312476372	25.368325265	6	36.681520394	37.223790272	39.058986608
1	33.361314445	36.822792156	24.959008938	8	36.157468688	36.614075526	40.026361598
1	32.406452549	39.133337292	29.137193224	8	37.734780868	37.909808561	39.094997051
1	31.367266629	39.121832132	27.087960429	1	36.260753429	36.121503685	37.271629800
8	33.705142452	38.969085558	32.876142872	1	34.882236091	37.001550655	37.936741117
1	32.873474866	39.393022888	32.558821619	1	36.195982811	39.188252661	37.224441117
1	34.787168488	39.769018326	31.774568076	1	37.194672288	38.110575303	36.232272014
8	35.283004887	40.417335800	31.222257437	8	32.241971158	38.155656532	34.699040097
1	34.218171016	39.408571751	34.276055635	8	34.405296679	39.298465729	35.635990999
1	35.545206070	39.905144564	30.439066043	8	35.855314844	38.942478214	28.933647878
1	35.071795086	34.733194202	29.492016984	6	35.258066621	38.443945746	27.988415664
1	29.016439606	37.928179494	30.674951051	7	33.912917474	38.748027858	27.725658162
1	32.570191240	32.110785504	34.861648423	6	33.209064726	39.661202821	28.645586951
1	28.782296094	44.590366936	34.645524116	6	33.204962772	38.216669409	26.666686877
1	36.737704752	37.135536530	27.367233420	7	31.947535693	38.545345950	26.473760896
				6	33.894360906	37.321787236	25.795694495
				6	35.187611999	37.015948774	26.039358461
				7	35.859837235	37.532270445	27.126333161
				1	32.755707740	40.478460672	28.073696018
				1	33.913275346	40.070149756	29.371135892
				1	31.425216930	38.171366508	25.674632065

TS4

QM/MM (BS1) = -3580.795662 a.u.

QM/MM (BS2+ZPE) = -3582.946226 a.u.

6	35.023800038	35.223205281	30.415980315
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1	35.722522978	36.344320941	25.373706654	6	36.652164043	37.033470065	39.053573389
1	33.376924364	36.856755726	24.964200638	8	36.164436666	36.456688740	40.060351425
1	32.410106471	39.115719478	29.166493604	8	37.685628525	37.750520505	39.039378305
1	31.375141803	39.132601391	27.110208400	1	36.397742655	35.966288478	37.212454628
8	33.694256995	38.867091284	32.729613877	1	34.893162606	36.467058185	38.005268946
1	32.866291275	39.352195942	32.506358970	1	35.747133885	38.944169078	37.406259768
1	34.776616571	39.771219364	31.764625212	1	36.683559981	38.097397599	36.143659347
8	35.260765467	40.443875653	31.228796766	8	31.831136690	37.833722784	34.747707126
1	33.577084854	39.100226073	35.101372829	8	33.519284183	38.516297992	36.432249546
1	35.545121142	39.947272444	30.442966492	8	35.827574161	38.879952540	29.075258986
1	35.074354637	34.713207204	29.453996159	6	35.246123826	38.432663798	28.094086159
1	28.992842545	37.920389423	30.664642308	7	33.908822346	38.758273180	27.816104778
1	32.578833414	32.138079694	34.856206999	6	33.197352261	39.649633186	28.751144715
1	28.780106734	44.591388873	34.647540736	6	33.215084631	38.267120364	26.727782861
1	36.747301752	37.148352038	27.381256453	7	31.962263209	38.606253579	26.526330168

IM6

QM/MM (BS1) = -3580.796277 a.u.

QM/MM (BS2+ZPE) = -3582.948764 a.u.

6	34.977870178	35.238519877	30.446338188	1	33.894099127	40.027218849	29.500720859
7	35.760876655	34.892564583	31.522028987	1	31.446755931	38.247840870	25.715260987
1	36.520622491	34.195773668	31.512478481	1	35.753173295	36.452379025	25.392284638
6	35.324258243	35.566861850	32.595174693	1	33.410991806	36.980463910	24.972435562
1	35.760875618	35.507222717	33.587528432	1	32.381220415	39.101117621	29.241556222
7	34.284757654	36.327953113	32.263666002	1	31.385232393	39.183823167	27.167202542
6	34.052988925	36.137944762	30.922459697	8	33.472042901	38.890436018	32.975628296
1	33.226202126	36.625537283	30.414656213	1	32.685881230	39.190922545	32.424289056
6	29.203055000	38.152491295	31.608152664	1	34.681258868	39.679139268	31.987767854
1	28.748390046	37.395862732	32.264947865	8	35.212523875	40.291223934	31.430961123
1	28.737633730	39.126860025	31.812143217	1	32.423883087	38.212926830	35.525603344
6	30.696135265	38.247908118	31.868422345	1	35.466164769	39.754428999	30.660508624
8	31.223918318	39.395099755	31.826629757	1	35.043163014	34.726934088	29.486086060
8	31.349326785	37.195240678	32.136100137	1	28.981626136	37.869948692	30.578975195
6	32.345507301	33.077569816	34.486278679	1	32.557450824	32.057636804	34.807029028
7	31.277678112	33.382060045	33.674383913	1	28.771563401	44.506356725	34.642701569
1	30.538789358	32.757900973	33.325284941	1	36.749336676	37.173504817	27.437601892

TS5

QM/MM (BS1) = -3580.776832 a.u.

QM/MM (BS2+ZPE) = -3582.933015 a.u.

6	35.053840208	35.243862678	30.364342956	6	33.034099159	34.631115075	34.637505488
7	35.769485956	34.883502936	31.481294182	6	33.034099159	34.631115075	34.637505488
1	36.501300594	34.156552125	31.516964539	6	33.034099159	34.631115075	34.637505488
6	35.321180845	35.599128533	32.520809383	6	33.034099159	34.631115075	34.637505488
1	35.715438512	35.542493809	33.529931579	6	33.034099159	34.631115075	34.637505488
7	34.337740996	36.403659698	32.123348568	6	33.034099159	34.631115075	34.637505488
6	34.157197774	36.199926748	30.776182791	6	33.034099159	34.631115075	34.637505488
1	33.382272187	36.715034132	30.217256563	6	33.034099159	34.631115075	34.637505488
6	29.309216185	38.287356203	31.333403101	6	33.034099159	34.631115075	34.637505488
1	28.854557322	37.617364803	32.077861117	6	33.034099159	34.631115075	34.637505488
1	28.878173783	39.291927088	31.438065111	6	33.034099159	34.631115075	34.637505488
6	30.800618530	38.354709190	31.555703044	6	33.034099159	34.631115075	34.637505488
8	31.373610020	39.473961458	31.413694413	6	33.034099159	34.631115075	34.637505488
8	31.425028829	37.317505970	31.930990628	6	33.034099159	34.631115075	34.637505488
6	32.389782572	33.425359445	34.458020112	6	33.034099159	34.631115075	34.637505488
7	31.339137588	33.700204493	33.613399754	6	33.034099159	34.631115075	34.637505488
1	30.638520659	33.046005684	33.238128221	6	33.034099159	34.631115075	34.637505488
6	31.365250993	35.000432623	33.297443709	6	33.034099159	34.631115075	34.637505488
1	30.673710533	35.484889823	32.617500814	6	33.034099159	34.631115075	34.637505488
7	32.382880201	35.606819034	33.904102466	6	33.034099159	34.631115075	34.637505488

1	33.919710084	34.866389428	35.219640838
6	29.356543713	44.098781143	33.912732178
1	29.783335066	45.027172698	33.492906364
1	28.693454616	43.659720662	33.155658936
7	30.399095000	43.151737693	34.283056730
1	31.053282552	43.429803499	35.016457079
6	30.626756239	41.913962643	33.738871458
7	29.942917678	41.567491618	32.622360211
1	29.720291629	42.318157846	31.966508015
1	30.372368019	40.785035908	32.112981139
7	31.463443007	41.066010961	34.308402923
1	31.922154177	41.455729123	35.131506791
1	31.669114402	39.762635580	34.192924848
26	33.073017664	37.541239518	33.275358401
6	36.818873599	40.993880133	33.384818085
8	35.816450654	40.996679904	33.976550822
8	37.858400060	40.997339216	32.862441203
6	34.325081923	38.013654744	35.951577107
8	34.451914025	37.496927977	34.769972899
6	35.585001390	38.167886919	36.787703281
6	35.752444491	36.924087604	37.676329971
6	36.563583608	37.113716874	38.968832781
8	36.116817117	36.505107797	39.976627419
8	37.602343398	37.821169239	38.935237979
1	36.242017702	36.118433335	37.098478337
1	34.760829981	36.557586517	37.976115359
1	35.444657969	39.054393164	37.422640990
1	36.463586185	38.326779781	36.147199839
8	31.840881881	38.572264551	34.333197592
8	33.231824979	38.332816698	36.450299507
8	35.878374103	38.967414654	28.896073256
6	35.280856835	38.472364549	27.947678515
7	33.945378366	38.801062717	27.667597512
6	33.262620957	39.753194814	28.561799402
6	33.225666938	38.250671196	26.625399362
7	31.973928593	38.593095237	26.424929245
6	33.899126962	37.320995449	25.779121812
6	35.189652596	37.008348979	26.025950560
7	35.870208744	37.540535447	27.100674272
1	32.785434219	40.538997539	27.966734706
1	33.990621333	40.205757670	29.236654623
1	31.442842173	38.200679589	25.640752603
1	35.714378321	36.316644558	25.373423671
1	33.373682609	36.840140317	24.961988222
1	32.479953914	39.236567861	29.133505891
1	31.411580160	39.206735959	27.045338435
8	33.545623626	38.944263875	32.400307521
1	32.644012747	39.307957979	31.910922755
1	34.864435113	40.052194857	31.724932351
8	35.473298349	40.566808751	31.163828061
1	32.209823799	38.453480684	35.274791987
1	35.598710213	39.989827296	30.388996017
1	35.121142722	34.703884582	29.419905900
1	29.055032519	37.902378452	30.345855577
1	32.569528372	32.409366252	34.809469414
1	28.740448154	44.360383276	34.772998359
1	36.757237928	37.156514275	27.356954311

IM7

QM/MM (BS1) = -3580.784869 a.u.

QM/MM (BS2+ZPE) = -3582.938244 a.u.

6	35.072401888	35.222755946	30.343779414
7	35.786889982	34.854280969	31.457672572
1	36.515633424	34.125063480	31.491288837
6	35.342490548	35.567618584	32.500742124
1	35.737766543	35.499051035	33.509511470
7	34.363692801	36.379983921	32.110256332
6	34.182636361	36.182579280	30.762317707
1	33.412741504	36.703486812	30.201659577
6	29.310048433	38.319246815	31.266916451
1	28.824310498	37.698747538	32.034081325
1	28.911125968	39.340776652	31.319045665
6	30.787031830	38.325797659	31.529479776
8	31.365581067	39.490306267	31.380017811
8	31.405248660	37.330039475	31.920615764
6	32.400426559	33.378114643	34.466389410
7	31.341625578	33.664237855	33.6637000705
1	30.629354213	33.018133887	33.270149519
6	31.378217614	34.966340411	33.323880150
1	30.671068880	35.452461142	32.661955835
7	32.411007903	35.561657630	33.914855316
6	33.059595522	34.576843201	34.636563902
1	33.955608696	34.801935258	35.207134363
6	29.372082395	44.232621298	33.920707175
1	29.780927246	45.191702250	33.555050199
1	28.723860643	43.823656081	33.135137691
7	30.436336034	43.295477881	34.231773078
1	31.103604975	43.552982950	34.960219105
6	30.579741094	42.018618255	33.736289819
7	29.794233492	41.690772888	32.655490131
1	29.699679159	42.421880725	31.946026231
1	30.154267822	40.858980967	32.196515938
7	31.386643020	41.135655137	34.256759769
1	31.878522751	41.524545635	35.064864843
1	31.623403727	39.452599012	34.245901343
26	33.135400147	37.492138563	33.322407804
6	36.806870113	40.997555983	33.361962571
8	35.818733149	40.997560677	33.976243878
8	37.832922181	41.003878043	32.812304771
6	34.307998325	38.024983010	36.006364860
8	34.459920054	37.482337142	34.841075451
6	35.550122233	38.195923206	36.863312788
6	35.756853411	36.926026065	37.704296337
6	36.566923632	37.106811000	38.996497352
8	36.114439444	36.505263666	40.005850042
8	37.610119726	37.808159893	38.961074349
1	36.265763997	36.155335706	37.096761839
1	34.776934369	36.524009918	37.996586433
1	35.367771764	39.051265774	37.529246006
1	36.429675528	38.412362813	36.240822719
8	31.735269289	38.444330966	34.422720036
8	33.204670830	38.352539785	36.479220600
8	35.868826094	38.941129563	28.900799799
6	35.286610897	38.454428594	27.938860348
7	33.953622741	38.782641803	27.644645020
6	33.259986194	39.727289159	28.535880750
6	33.244145648	38.234384634	26.594099258
7	31.991179931	38.570789226	26.388786153
6	33.929730118	37.315185109	25.747429635

6	35.219862362	37.009242484	26.003208416
7	35.887599663	37.533844006	27.089432637
1	32.802750761	40.527555843	27.944292453
1	33.974545272	40.161271078	29.237261415
1	31.467076491	38.181123579	25.598812575
1	35.755811307	36.329827618	25.347423536
1	33.415545890	36.838393625	24.920910849
1	32.457612988	39.205078957	29.073415697
1	31.424512638	39.184223955	27.004827424
8	33.587230219	38.883354430	32.581543659
1	32.307120968	39.432132357	31.738450502
1	34.826184091	40.010433866	31.758622807
8	35.408455202	40.528021048	31.173478079
1	32.160472019	38.390285474	35.351959238
1	35.562193390	39.932662363	30.418479069
1	35.131711815	34.681989022	29.399257954
1	29.053111357	37.896916422	30.295480554
1	32.580526855	32.360325306	34.812418418
1	28.741440308	44.437940954	34.785693718
1	36.773706421	37.150183002	27.349416366

TS6

QM/MM (BS1) = -3580.776499 a.u.

QM/MM (BS2+ZPE) = -3582.927398 a.u.

6	35.030665112	35.279114847	30.414406119
7	35.751180731	34.916209026	31.526179102
1	36.477430986	34.184150110	31.555956684
6	35.313452052	35.639958966	32.567102449
1	35.709757144	35.571998579	33.575974762
7	34.334259804	36.453954931	32.179561761
6	34.144833013	36.244146217	30.833998078
1	33.377920122	36.770468433	30.273593085
6	29.160648778	38.206605448	31.441647021
1	28.765265318	37.443173379	32.128733005
1	28.604325726	39.140403967	31.596120025
6	30.609839664	38.443572110	31.775745316
8	30.929372228	39.709498712	31.752122822
8	31.368925886	37.524821921	32.099276507
6	32.353126326	33.364049836	34.440752031
7	31.330483233	33.646143380	33.565754159
1	30.638478562	32.994774050	33.171325768
6	31.362549586	34.954391562	33.273100100
1	30.679127191	35.444021824	32.587975369
7	32.354787006	35.554605332	33.922535091
6	32.984919542	34.569610967	34.657730410
1	33.851214740	34.803064385	35.269097363
6	29.660892975	44.550354157	33.991534100
1	30.201834142	45.496782306	34.147123504
1	29.250288525	44.585462188	32.970106977
7	30.622264243	43.472881675	34.144106939
1	31.387419773	43.626613715	34.803641050
6	30.557071183	42.210725302	33.608044009
7	29.457923179	41.932515650	32.835138420
1	29.072895548	42.717309773	32.317756346
1	29.628945486	41.154577515	32.201261970
7	31.464056884	41.284854006	33.831529013
1	32.235122731	41.648117360	34.396105278
1	31.523057327	39.363522436	34.448895540
26	33.068660540	37.511571523	33.455060280
6	36.523115403	41.169378085	33.345389782
8	35.559896269	41.306379540	33.984843500

8	37.536875488	41.052367253	32.785155448
6	34.279808333	37.989000434	36.132409742
8	34.368938821	37.386668431	34.993680422
6	35.551461956	38.143225349	36.944825722
6	35.791516489	36.858741146	37.756071844
6	36.583062924	37.054662175	39.055393801
8	36.111576357	36.481280025	40.071978730
8	37.629959915	37.751307989	39.018239727
1	36.329007171	36.117706547	37.137635707
1	34.823699339	36.420330543	38.034776626
1	35.395913833	38.989043388	37.628903836
1	36.406612623	38.368298641	36.291683051
8	31.616334416	38.404514977	34.678333164
8	33.207057801	38.388880392	36.623605569
8	35.800343668	38.930482279	29.005094073
6	35.238823905	38.464087719	28.021284038
7	33.902492487	38.777067804	27.718825802
6	33.179213436	39.692958394	28.618778334
6	33.217438745	38.247251071	26.642763562
7	31.959117531	38.560350019	26.432754173
6	33.933638277	37.375721860	25.771229800
6	35.226121360	37.086250823	26.033160547
7	35.868187658	37.582437051	27.148036980
1	32.710181298	40.489406079	28.030718342
1	33.874124057	40.136691393	29.332717920
1	31.454338253	38.187404701	25.622221392
1	35.786233109	36.445002469	25.358308940
1	33.441724727	36.923024609	24.918380276
1	32.387016541	39.144682497	29.147308109
1	31.369564846	39.141189864	27.058860554
8	33.576027728	38.953082502	32.929886204
1	31.609272758	40.065951094	32.409731686
1	34.549787077	40.014972820	31.789132871
8	35.152894018	40.552390449	31.242785032
1	32.127121274	38.393356676	35.91720322
1	35.411168632	39.951099057	30.522380032
1	35.104697909	34.744778612	29.467267666
1	28.976123100	37.855571544	30.426367361
1	32.536729924	32.347354193	34.788152397
1	28.833560066	44.539515823	34.701090373
1	36.755005202	37.196776694	27.402582106

IM8

QM/MM (BS1) = -3580.809733 a.u.

QM/MM (BS2+ZPE) = -3582.969357 a.u.

6	34.989439548	35.268346148	30.413311463
7	35.753019447	34.922049656	31.501966613
1	36.497616706	34.209145342	31.509926852
6	35.323076194	35.628946756	32.558551415
1	35.741636400	35.565055159	33.558661395
7	34.309398379	36.414087220	32.205317362
6	34.085472830	36.202024803	30.866127742
1	33.281357027	36.705248104	30.336525791
6	29.034929403	38.122967364	31.747740848
1	28.530309233	37.332057968	32.3320740038
1	28.467894110	39.046804349	31.923063558
6	30.417381037	38.304420962	32.358646401
8	30.575392554	39.359614976	33.030101389
8	31.274256690	37.367322250	32.297842486
6	32.336408193	33.136721191	34.445418285
7	31.295645542	33.423071642	33.592819554

1	30.575605770	32.784860448	33.230988826
6	31.348682041	34.725218088	33.274234138
1	30.655147752	35.230675041	32.610040134
7	32.372188841	35.307697033	33.884566068
6	33.003338308	34.328257817	34.618471517
1	33.894516701	34.556517281	35.193926539
6	29.589739369	44.714697491	33.756461934
1	30.011874855	45.729370471	33.714979645
1	29.084939590	44.542116539	32.796581692
7	30.699635498	43.791074733	33.937450724
1	31.432149888	44.061519804	34.595275339
6	30.720493384	42.489037133	33.568992840
7	29.723036329	41.950770884	32.854895866
1	29.331168871	42.502341088	32.092564026
1	29.845589149	40.938659365	32.673035929
7	31.733873203	41.721626382	33.967063399
1	32.459097086	42.097262704	34.575396700
1	31.166565595	38.621891947	34.599390205
26	32.958879497	37.292780708	33.560459846
6	36.243663036	41.314233541	33.335292138
8	35.323709762	41.548551782	34.012520851
8	37.233456033	41.128500624	32.752334108
6	34.428261834	37.863986585	36.077858273
8	34.362271299	37.090529348	35.049401226
6	35.755101046	37.965395281	36.810883583
6	35.893048426	36.755630726	37.754254856
6	36.629248303	37.023757017	39.071721496
8	36.128211345	36.484891655	40.093861278
8	37.668735600	37.732598197	39.047057725
1	36.419908249	35.931492238	37.241140359
1	34.895342218	36.383394140	38.024135972
1	35.731798874	38.892675554	37.399779639
1	36.594339676	38.024512604	36.103030975
8	31.559430812	37.840807430	35.043511768
8	33.452728550	38.472496753	36.559461672
8	35.709621981	38.917617583	29.136172415
6	35.170440366	38.476644990	28.128179155
7	33.832970900	38.777307706	27.815834157
6	33.079398716	39.658635809	28.724951309
6	33.171439573	38.274444024	26.712634856
7	31.908146496	38.567319532	26.501377910
6	33.918627540	37.459473388	25.812970206
6	35.212138015	37.181841587	26.083110058
7	35.828000207	37.640161949	27.229019626
1	32.635905979	40.479012488	28.148423957
1	33.745124386	40.069044347	29.484585859
1	31.417988464	38.211697996	25.673603381
1	35.794811909	36.580590587	25.389866880
1	33.449571902	37.038100763	24.931886948
1	32.268583794	39.090646542	29.202202332
1	31.294887019	39.096100031	27.150459813
8	33.386910241	38.826392468	33.251973175
1	31.815384592	40.763458129	33.606100246
1	34.274010191	39.790304888	31.985322473
8	34.835236896	40.389143273	31.452731829
1	32.224891518	38.174009510	35.751847632
1	35.202621259	39.819961521	30.753948843
1	35.055539174	34.740407391	29.462007712
1	28.931411856	37.848800796	30.697891271
1	32.541700808	32.120384959	34.781547620
1	28.851073817	44.687459002	34.557522850
1	36.715979089	37.253274827	27.477584207

IM9

QM/MM (BS1) = -3580.809487 a.u.

QM/MM (BS2+ZPE) = -3582.964970 a.u.

6	35.056123634	35.265828735	30.419145070
7	35.809354446	34.865776794	31.495686655
1	36.544826344	34.144713451	31.481522453
6	35.392960490	35.536502427	32.578478410
1	35.814377544	35.428049741	33.573172933
7	34.394999906	36.352794535	32.254469689
6	34.170604829	36.199682585	30.907055802
1	33.386707402	36.745921943	30.390758050
6	29.276528658	38.226136306	31.827512382
1	28.814154681	37.455004603	32.460267933
1	28.779640005	39.187022160	32.030585469
6	30.760666256	38.388088627	32.155888170
8	31.318948153	39.466595814	31.915791831
8	31.334662976	37.374985689	32.716262645
6	32.366377930	33.063706557	34.483507712
7	31.287828848	33.403788068	33.701131590
1	30.534350159	32.797603020	33.351496080
6	31.363059469	34.713206685	33.417047562
1	30.640293799	35.259084927	32.819845546
7	32.439474511	35.249212226	33.980498712
6	33.082970033	34.225838392	34.643415551
1	34.020536114	34.393334638	35.164217041
6	29.369034969	44.333961541	33.717888226
1	29.690952561	45.300972685	33.295641146
1	28.715049932	43.847340594	32.983277770
7	30.524305200	43.492940985	34.001594733
1	31.179859877	43.804688865	34.719017380
6	30.809996784	42.299420119	33.428590463
7	30.035128952	41.777925814	32.470574676
1	29.649280736	42.414291752	31.771702799
1	30.415210966	40.904842939	32.046572432
7	31.859624376	41.606919228	33.873192572
1	32.440299859	41.973604147	34.626319946
1	32.153437290	40.754874683	33.383736283
26	33.088860072	37.222360276	33.635875404
6	36.211455271	41.262510470	33.415914223
8	35.297106651	41.486594429	34.10341888
8	37.198610515	41.085556429	32.825466171
6	33.890773529	37.351819008	36.035948726
8	34.617537873	36.819824112	35.151987030
6	34.406666127	37.557504019	37.443194081
6	35.905756829	37.839478285	37.506313999
6	36.590630731	37.640363105	38.868563873
8	36.050068413	36.902557678	39.734083880
8	37.701662543	38.220038623	38.993478274
1	36.134877349	38.858956126	37.160368405
1	36.421965442	37.166512142	36.801478013
1	34.196333342	36.629574027	37.996827722
1	33.810373782	38.342121666	37.932254858
8	30.395125376	38.382750959	37.132872038
8	32.707989509	37.696113082	35.712108559
8	35.713226387	38.982051634	29.193396436
6	35.183726298	38.552501532	28.174775058
7	33.849372500	38.855566862	27.852916517
6	33.095662053	39.750647398	28.750120609
6	33.195597335	38.346771626	26.747984399
7	31.927122802	38.616136636	26.537754464
6	33.956245550	37.558473799	25.837449495

6	35.250854109	37.291968786	26.109812649
7	35.852976765	37.730501015	27.270703992
1	32.622711188	40.539351590	28.153309110
1	33.769333134	40.201718862	29.478218788
1	31.445267059	38.258880296	25.706195307
1	35.847026812	36.723154494	25.402488752
1	33.498462953	37.152847648	24.943134669
1	32.309944256	39.192386567	29.276472242
1	31.308125457	39.139497068	27.185163759
8	33.585642132	38.740668701	33.372848022
1	31.258714114	38.196778176	36.713534750
1	34.239794346	39.800932349	32.000554750
8	34.786220228	40.440513695	31.502602859
1	29.769682584	38.084649539	36.458189667
1	35.175668325	39.908546597	30.786428515
1	35.104611674	34.758426051	29.455683214
1	29.082846244	37.962271654	30.787834602
1	32.566963608	32.038476989	34.794533502
1	28.775037756	44.520515825	34.612556950
1	36.738036826	37.338553873	27.521739080

Cartesian coordinates for direct hydrogen transfer from IM6

TS5

QM/MM (BS1) = -3580.768659 a.u.

QM/MM (BS2+ZPE) = -3582.923454 a.u.

6	34.986517860	35.264723205	30.439962813
7	35.771527088	34.921154791	31.516033557
1	36.521556303	34.213705606	31.509512268
6	35.353642128	35.616567654	32.582122923
1	35.793225959	35.554467111	33.572821559
7	34.322314908	36.393413090	32.250423653
6	34.079069351	36.184054949	30.910820311
1	33.257638557	36.679095890	30.401358449
6	29.250841203	38.158504310	31.655163771
1	28.835058961	37.368766534	32.299748095
1	28.729630448	39.099861878	31.880073764
6	30.739650998	38.349422603	31.936184555
8	31.190666354	39.508952166	31.939532972
8	31.433681909	37.297828598	32.183241701
6	32.326418475	33.105603960	34.467852812
7	31.271554467	33.415491003	33.639365524
1	30.545867099	32.789033132	33.266837150
6	31.325886932	34.722844241	33.345010007
1	30.636029853	35.249573024	32.692868015
7	32.364069330	35.286733322	33.951027217
6	33.003212491	34.288484527	34.653155730
1	33.913096622	34.494392766	35.206788938
6	29.376579454	44.426978270	33.689963722
1	29.706920416	45.415265292	33.328824110
1	28.723704425	43.997308950	32.920312403
7	30.532309186	43.572992761	33.913695757
1	31.234952436	43.885305405	34.584804779
6	30.756959523	42.358353425	33.357599213
7	29.891806421	41.796982424	32.505296911
1	29.443715986	42.404036048	31.820208561
1	30.240199206	40.899739606	32.093899156
7	31.850123877	41.682043575	33.713230699
1	32.502171395	42.059894705	34.397605924
1	32.091900374	40.827807315	33.196232586

26	32.968821912	37.256054330	33.567423903
6	36.192155621	41.328927221	33.366318223
8	35.274480990	41.612000012	34.028347585
8	37.189002450	41.097471564	32.811551635
6	34.726850102	37.648332970	36.146821742
8	34.684493422	36.926483654	35.137030353
6	35.975757788	37.826615574	36.965767567
6	36.056419154	36.640083974	37.944548735
6	36.697470845	36.983301972	39.287642695
8	36.139809852	36.497201619	40.304639371
8	37.721937795	37.713296187	39.274651467
1	36.627187941	35.811046088	37.490879211
1	35.047302022	36.264448838	38.159478504
1	35.890235759	38.767457003	37.526114547
1	36.859116222	37.886398098	36.316224947
8	32.014831550	38.048534451	34.851704384
8	33.685006771	38.241934109	36.649514622
8	35.697708979	38.924215995	29.168957639
6	35.165306664	38.490983433	28.154055726
7	33.831801074	38.797055448	27.831278417
6	33.072012253	39.677675379	28.738114138
6	33.180196869	38.299617689	26.720436055
7	31.920650314	38.596331352	26.495838467
6	33.931894691	37.486613497	25.822642756
6	35.222546815	37.206740467	26.100639531
7	35.829323531	37.658066254	27.254102532
1	32.633646101	40.499666260	28.160059004
1	33.731586360	40.085476772	29.503520858
1	31.436421957	38.237563015	25.666476163
1	35.810179174	36.611095909	25.406913373
1	33.469501230	37.075022026	24.933479904
1	32.259271999	39.114555468	29.216308673
1	31.306579169	39.134870546	27.135788114
8	33.547319031	38.929233881	33.444303270
1	32.712473874	38.966321840	34.265278956
1	34.271306058	39.810872573	32.050149591
8	34.790384144	40.432095977	31.495371932
1	32.872616234	38.104600866	35.993565840
1	35.160419914	39.877138953	30.787606987
1	35.050723518	34.743839867	29.484648466
1	29.036876035	37.882897051	30.622532727
1	32.536508309	32.085419969	34.789029096
1	28.779608641	44.566130285	34.591257169
1	36.716366526	37.269315777	27.503101087

IM7

QM/MM (BS1) = -3580.806871 a.u.

QM/MM (BS2+ZPE) = -3582.968370 a.u.

6	35.015169416	35.276934208	30.486930898
7	35.768757041	34.908157457	31.575098978
1	36.501953689	34.184075221	31.578808764
6	35.348866552	35.615869225	32.635532576
1	35.763611883	35.532966449	33.635859090
7	34.351998444	36.423760136	32.287308424
6	34.128046426	36.223466764	30.945838907
1	33.335377425	36.744804961	30.417332839
6	29.279800074	38.213702598	31.679717759
1	28.843298869	37.445826764	32.335016129
1	28.784618055	39.174132402	31.885337353
6	30.772278453	38.374801859	31.956938739
8	31.286466634	39.497436698	31.818104738

8	31.404587596	37.333139607	32.368559119	1	32.539693538	32.104049093	34.795944485
6	32.333054442	33.124359081	34.472934988	1	28.780323755	44.529225194	34.630975398
7	31.291994489	33.426115517	33.624717480	1	36.733096708	37.253382911	27.495651917
1	30.574352302	32.796704260	33.242886159	2OG rearrangement reaction states coordinates for			
6	31.342520729	34.734294086	33.332839507	AlkBH2-dsDNA			
1	30.648591378	35.252658953	32.679707324	ES1			
7	32.363741669	35.307941957	33.956553309	QM/MM (BS1) = -3275.477127 a.u.			
6	32.996420220	34.313902043	34.669913774	QM/MM (BS2+ZPE) = -3277.299466 a.u.			
1	33.888441196	34.531438343	35.247078107	6	40.282292761	37.751724933	43.589363266
6	29.302166645	44.272483363	33.709112636	7	39.163005387	36.975104270	43.775674071
1	29.575680357	45.201456024	33.179905494	1	39.034422972	36.278106088	44.520428839
1	28.598277627	43.715208062	33.076868921	6	38.288583132	37.250948135	42.797769544
7	30.479432250	43.457549849	33.979508854	1	37.317404389	36.772601631	42.700839951
1	31.147644455	43.785005541	34.679059930	7	38.779626021	38.173898505	41.975769360
6	30.774282098	42.274865956	33.392282093	6	40.028939760	38.494947045	42.459444409
7	30.003191252	41.754926982	32.435247036	1	40.669199452	39.209155104	41.951024720
1	29.597268756	42.391766279	31.748812506	6	41.400547203	39.782137053	37.309684846
1	30.384836186	40.879255986	32.003277806	1	41.255565919	38.871285437	36.712854810
7	31.830270549	41.580040739	33.836801492	1	41.336485989	40.665567937	36.656453231
1	32.437463066	41.980034021	34.551100474	6	40.358406632	39.891123473	38.410097035
1	32.178571987	40.782659886	33.290851769	8	40.106312067	41.007737343	38.911264455
26	32.964360096	37.294316909	33.645538355	8	39.780339824	38.808911892	38.744434771
6	36.203138340	41.349636843	33.313412892	6	38.782531252	34.187572378	39.668170403
8	35.293037204	41.570230216	34.009195322	7	39.930430542	34.700397421	34.700397421
8	37.187587875	41.191124983	32.713799558	1	40.781853960	34.193792693	38.879589937
6	34.359183407	37.757403751	36.216531822	6	39.780893195	36.031989019	38.976931727
8	34.314441624	37.042943614	35.146143500	1	40.534430554	36.699475294	38.569109734
6	35.697206843	37.906057213	36.915155373	7	38.591292727	36.408872739	39.431971381
6	35.914373343	36.680037211	37.823804537	6	37.960114495	35.267451468	39.871612205
6	36.636840520	36.977066994	39.140275832	1	36.968879627	35.300457449	40.317404650
8	36.116030077	36.481490447	40.174506341	6	38.994893188	44.666414464	34.930489515
8	37.682298302	37.676298977	39.103937050	1	39.292663714	45.703960115	35.161711995
1	36.487419608	35.903236178	37.287694267	1	39.910149120	44.074640574	34.784711565
1	34.941922950	36.246890255	38.091080366	7	38.193658745	44.065668876	35.988429154
1	35.644225574	38.816736359	37.528151509	1	37.184597960	44.183793637	35.954201292
1	36.511294985	38.021638970	36.185817697	6	38.662635124	43.196089911	36.916402194
8	31.487443089	37.924513730	35.127680813	7	39.963407624	43.000256170	37.096504289
8	33.358711967	38.266929278	36.759820360	1	40.687284053	43.718336753	36.930531761
8	35.728120965	38.918691003	29.155654594	1	40.213146286	42.304187678	38.829445444
6	35.191290035	38.485399470	28.142494225	7	37.774928313	42.475606170	37.614283991
7	33.860965651	38.803032208	27.819759403	1	36.772676060	42.591927881	37.462036500
6	33.115992116	39.704161912	28.718277733	1	38.069485928	41.851688789	38.370770508
6	33.200454774	38.298358798	26.717421264	26	38.224643878	38.465417155	39.969836429
7	31.941360380	38.601045951	26.497181122	6	35.913334785	40.253157098	39.832081770
6	33.942180479	37.471807441	25.824242676	8	35.246710180	41.281702713	39.783504357
6	35.232605580	37.186813249	26.098904719	8	37.137441473	40.107446920	39.495385406
7	35.846494814	37.643094486	27.246584738	6	35.254082741	38.916423606	40.298987917
1	32.683826509	40.523168302	28.131311820	8	36.002081530	37.975395969	40.545460052
1	33.785745513	40.112427753	29.474730192	6	33.757074341	38.822944079	40.383049575
1	31.450917360	38.240069760	25.672404091	6	33.211458010	37.414357027	40.166354010
1	35.813628155	36.582192470	25.407710197	6	31.688009331	37.253944649	40.322705916
1	33.472940496	37.054490647	24.941141210	8	31.062467699	38.169820787	40.936005044
1	32.299294643	39.158415139	29.209184566	8	31.189347866	36.216972997	39.839800767
1	31.336931311	39.153617052	27.134169313	1	33.689532205	36.715716548	40.875041787
8	33.387593213	38.852507344	33.453953315	1	33.470906170	37.050372288	39.159312089
1	31.356513086	38.835642693	34.822377645	1	33.325186726	39.549253263	39.677648042
1	34.228846098	39.697269156	32.030614600	1	33.458348069	39.200822250	41.379623275
8	34.807216532	40.300613967	31.523565940	8	39.281637951	41.845072898	43.986596878
1	32.154807701	38.044660339	35.906232205	6	40.467664377	41.739037891	43.765971257
1	35.173045300	39.752397884	30.807584630				
1	35.080215857	34.762064356	29.528418865				
1	29.058820751	37.933451407	30.649817413				

7	41.021162078	42.184824478	42.537327240
6	40.081116520	42.800364872	41.587148542
6	42.343179516	42.049414471	42.200793867
7	42.800942644	42.428226195	41.026782792
6	43.227719783	41.484053669	43.163765992
6	42.720293915	41.042832595	44.333258465
7	41.385954510	41.180291349	44.662790563
1	39.177590432	43.075622065	42.138397160
1	39.838707461	42.092988561	40.780341804
1	43.811672782	42.355653769	40.846885441
1	43.385671206	40.519314717	45.010180229
1	44.279080261	41.339672467	42.924470405
1	40.534978406	43.706692287	41.162822981
1	42.235097195	42.694369759	40.225410070
1	41.199885566	37.603295827	44.158625565
1	42.402551833	39.743273037	37.736936101
1	38.685261182	33.143525251	39.965779958
1	38.424407458	44.649306005	34.001877292
1	41.028694678	40.793622772	45.512981908

TS for 2OG rearrangement

QM/MM (BS1) = -3275.469836 a.u.

QM/MM (BS2+ZPE) = -3277.294776 a.u.

6	40.326673354	37.695317544	43.660963213
7	39.208358777	36.919617205	43.852890917
1	39.073882688	36.233695347	44.606106673
6	38.339884739	37.169373250	42.864611922
1	37.365561873	36.697761839	42.773577841
7	38.840569423	38.070149172	42.024907749
6	40.083685909	38.409762669	42.511813578
1	40.724577725	39.114835255	41.993606999
6	41.351067934	39.821771746	37.416453728
1	41.182739583	38.900115416	36.841814761
1	41.283818443	40.689559044	36.743709712
6	40.322340948	39.960390616	38.529506907
8	39.998531129	41.101815877	38.931475021
8	39.821858595	38.884637812	38.974648089
6	38.729312494	34.257486927	39.702731043
7	39.869867698	34.794800832	39.146197728
1	40.727359138	34.302802952	38.914063322
6	39.701234795	36.126098071	39.038959186
1	40.450658165	36.809309355	38.649926413
7	38.506446442	36.483444752	39.495963061
6	37.891244690	35.325459878	39.916150143
1	36.897506354	35.333588300	40.358899905
6	38.965147633	44.706294008	34.910747457
1	39.251451516	45.748189755	35.136838638
1	39.886535427	44.122515166	34.771307024
7	38.165666486	44.102443033	35.966676534
1	37.154148683	44.191460516	35.918039854
6	38.644417271	43.228402823	36.884208240
7	39.948504570	43.045663123	37.063803125
1	40.667281333	43.770793549	36.910584673
1	40.190626344	42.361908019	37.809668508
7	37.771587458	42.491341853	37.579516310
1	36.765752897	42.553523757	37.419354588
1	38.106143227	41.837668566	38.290246468
26	38.177305962	38.561608731	40.111255678
6	35.854844321	40.130863548	39.565378003
8	35.302009404	41.225499348	39.503362192
8	36.954537495	39.765962004	39.013981337

6	35.224537453	39.000084269	40.415120219
8	36.003792106	38.215574658	40.949230898
6	33.729748458	38.889283544	40.533091677
6	33.218325265	37.481086659	40.204620733
6	31.695525220	37.286327529	40.350997166
8	31.052845251	38.187272433	40.967346815
8	31.218243532	36.246987423	39.853446248
1	33.712965851	36.744093286	40.861002308
1	33.480242740	37.200639868	39.171311945
1	33.259898922	39.642935580	39.887651170
1	33.449368327	39.147050592	41.568918936
8	39.328670886	41.841674845	43.959125769
6	40.519362740	41.733753828	40.967346115
7	41.100246559	42.196312297	42.553482873
6	40.181548917	42.836291002	41.598681044
6	42.425552717	42.046067568	42.235017882
7	42.913117394	42.435526280	41.077168938
6	43.283258660	41.448227607	43.202502650
6	42.751340379	41.001407965	44.357697373
7	41.414975167	41.157625783	44.671134059
1	39.286226114	43.144786341	42.146024234
1	39.918810646	42.136185215	40.791977994
1	43.925396995	42.342278232	40.914829730
1	43.398294496	40.455979344	45.034441990
1	44.335347985	41.288917548	42.978935814
1	40.663427653	43.724388043	41.168375437
1	42.378496340	42.745570367	40.268597627
1	41.246178145	37.556610445	44.229591922
1	42.363374179	39.772413072	37.817536141
1	38.651302195	33.205119054	39.975684484
1	38.397693665	44.677002454	33.980583322
1	41.044377518	40.772773188	45.516425937

ES2

QM/MM (BS1) = -3275.479068 a.u.

QM/MM (BS2+ZPE) = -3277.302619 a.u.

6	40.319343381	37.637908109	43.663323312
7	39.195953788	36.869798728	43.852338043
1	39.057527550	36.183861863	44.604791414
6	38.330866632	37.128818196	42.863153330
1	37.351834333	36.668045134	42.770634562
7	38.840497127	38.027801932	42.027683188
6	40.083353803	38.358035915	42.516239161
1	40.725501710	39.065315811	42.002703767
6	41.356727876	39.813460393	37.454826878
1	41.213009463	38.901491383	36.858006971
1	41.292671949	40.691985528	36.795954467
6	40.294832246	39.913982723	38.541785412
8	39.912133556	41.041365266	38.928859784
8	39.829170337	38.819647803	38.981023230
6	38.710393799	34.203224399	39.725214499
7	39.849147191	34.739284244	39.163621719
1	40.710443998	34.248555251	38.943927037
6	39.674291068	36.068372421	39.041194144
1	40.421135165	36.752725940	36.649164091
7	38.477438496	36.425154724	39.493391704
6	37.866688987	35.269055462	39.925483285
1	36.870316332	35.275554526	40.362721448
6	38.973776915	44.686320118	34.922736470
1	39.266055020	45.726817466	35.148837430
1	39.891339827	44.096575056	34.781111176

7	38.174028905	44.086367872	35.981381026	1	24.286630960	32.946873121	42.130072392
1	37.162484966	44.174589895	35.931247551	6	24.760952510	36.673214524	43.929300794
6	38.649637948	43.218871791	36.907538766	1	25.606130192	36.730086462	44.628103175
7	39.953940977	43.041440342	37.102732843	1	24.542277838	37.685845202	43.560509909
1	40.673410788	43.771470864	36.985558728	6	25.104440547	35.799184373	42.730590159
1	40.179867509	42.349162769	37.844619512	8	24.441684111	35.817233953	41.700004739
7	37.777454843	42.477221309	37.597689691	8	26.187657422	35.075084240	42.874987718
1	36.773020533	42.520771416	37.424352508	6	29.291152868	31.708420762	44.707088266
1	38.122357932	41.830601589	38.311832090	7	28.358287786	32.418506392	45.423075863
26	38.169527712	38.504501155	40.107002760	1	28.145636934	32.346693997	46.427104882
6	35.836865148	40.050765263	39.562928907	6	27.770435003	33.290559018	44.591581594
8	35.286531943	41.144734930	39.469453815	1	26.986504080	33.983932733	44.885135936
8	36.913578895	39.653467171	38.990893593	7	28.279504025	33.181029911	43.369481854
6	35.236654262	38.971074180	40.498513061	6	29.226513348	32.187307825	43.421994335
8	36.031263692	38.200081581	41.028832370	1	29.759782402	31.866918841	42.533342382
6	33.751715410	38.874253317	40.696378377	6	24.315341461	42.184938532	41.133067381
6	33.217920502	37.519407183	40.204155438	1	24.000384534	42.695840470	40.206135259
6	31.697223847	37.313483725	40.355533554	1	23.488129066	42.255472022	41.849684562
8	31.051112497	38.201673653	40.984879426	7	24.645254715	40.791041138	40.899989986
8	31.226373996	36.279755279	39.840234926	1	25.560083087	40.582167739	40.51543784
1	33.720311170	36.703575259	40.751306626	6	23.867963786	39.720770770	41.186855814
1	33.456153803	37.367091947	39.137810797	7	22.616602115	39.846908951	41.588123614
1	33.256515384	39.702939132	40.176627145	1	22.055723820	40.692515828	41.505811236
1	33.538500795	38.982738659	41.772152390	1	22.075030630	39.010286732	41.883248576
8	39.609560165	41.900749690	43.785672748	7	24.412223629	38.502343281	41.034391689
6	40.802739406	41.712762795	43.699825244	1	25.431784735	38.385245633	41.107700751
7	41.525610228	42.127610564	42.545090556	1	23.891820578	37.654739640	41.292383410
6	40.731044170	42.796112314	41.502112970	26	27.387107058	34.172622306	41.681483033
6	42.844868494	41.823873761	42.313363489	8	26.920203753	34.877353679	39.782708628
7	43.484515081	42.141601841	41.211922009	8	27.843479673	35.229795374	38.981560965
6	43.541766233	41.106362599	43.331287830	6	29.733449426	35.532693330	40.696963160
6	42.888301362	40.753987084	44.450687522	8	30.614459498	36.342005283	40.408407214
7	41.566805994	41.077574637	44.686763690	8	28.813113197	35.660652442	41.587082738
1	39.879705891	43.288799394	41.981405341	6	29.668253418	34.175637754	39.956092410
1	40.371423080	42.067625667	40.760457037	8	28.986123211	33.282813794	38.487717946
1	44.446108286	41.769953516	41.129430203	6	30.543227171	33.938822426	38.760538085
1	43.421546307	40.134478019	45.157532100	6	32.002366637	33.630007813	39.155933510
1	44.578968559	40.813645526	43.192844319	6	32.969821454	33.608486343	37.957814907
1	41.347946598	43.547350382	40.994344645	8	34.094504933	34.164197852	38.125373941
1	43.123357102	42.603565229	40.367845535	8	32.583439643	33.049529311	36.904259137
1	41.235687476	37.496418157	44.236351601	1	32.046790548	32.628020471	39.616494006
1	42.361715986	39.765213483	37.874036582	1	32.373626563	34.356364300	39.891532379
1	38.637879069	33.153074715	40.008047620	1	30.517407221	34.853211142	38.151872068
1	38.405136178	44.663881473	33.993106682	1	30.127859004	33.116162395	38.161753300
1	41.114086386	40.724686222	45.505596531	8	24.871652072	33.225768863	38.048252749

Dioxygen Activation step reaction states cartesian coordinates for AlkBH2-dsDNA via "In-line" Fe(III)-superoxo Complex

RC1

QM/MM (BS1) = -3419.786229 a.u.

QM/MM (BS2+ZPE) = -3421.791578 a.u.

6	24.763326076	30.785773224	41.867313615	1	24.107103091	36.444624319	37.169878472
7	25.935481433	30.226951132	41.405918013	1	22.775217450	37.368156419	38.684703450
1	26.137727347	29.221911565	41.310700166	1	20.860225153	32.429764786	39.728343767
6	26.795100616	31.218067882	41.131308343	1	20.319822827	34.838354395	39.783008481
1	27.806566988	31.074998410	40.767272036	1	25.381660484	35.345661807	37.797197558
7	26.244946701	32.399107966	41.393799409	1	21.241541950	37.141146486	39.459448952
6	24.967788735	32.146680438	41.855162922	1	23.944326158	30.185820878	42.264004466
				1	23.887798936	36.328254300	44.483081075

1	29.842684596	30.874625307	45.141444355
1	25.182478824	42.699468266	41.547071324
1	23.015268866	31.747654137	38.871146359

TS1

QM/MM (BS1) = -3419.772852 a.u.

QM/MM (BS2+ZPE) = -3421.775893 a.u.

6	24.787971565	30.781619553	41.862134128
7	25.955283579	30.220051762	41.388026461
1	26.157264105	29.214152498	41.296970678
6	26.814534073	31.207903297	41.105745737
1	27.824836748	31.069153060	40.735298263
7	26.267681394	32.390981073	41.376845412
6	24.994789539	32.141618360	41.852252892
1	24.321226378	32.943608839	42.138150785
6	24.834532940	36.644675677	43.893292277
1	25.674990757	36.667910808	44.599896694
1	24.650246973	37.669904637	43.539793551
6	25.172138684	35.780463903	42.681288916
8	24.488274152	35.803072339	41.663688818
8	26.263879509	35.069577807	42.800020664
6	29.321222333	31.717790025	44.699920116
7	28.370620230	32.417397988	45.405524043
1	28.139091583	32.334567492	46.404818773
6	27.798537231	33.297658296	44.575269250
1	27.005286607	33.986035599	44.855465661
7	28.336772312	33.203642993	43.363876279
6	29.285210842	32.211115981	43.419749771
1	29.837553117	31.917659647	42.532875383
6	24.290330179	42.191898207	41.137915613
1	23.978731739	42.702954517	40.209723928
1	23.463532199	42.270551208	41.854330050
7	24.609341836	40.794968850	40.908095172
1	25.526495895	40.577044383	40.533597899
6	23.823209826	39.730551558	41.194297676
7	22.574906054	39.862411633	41.596459278
1	22.015338309	40.710023440	41.517771499
1	22.031948638	39.023341069	41.881858290
7	24.358804757	38.508904090	41.040295730
1	25.378684105	38.393033317	41.103274025
1	23.839197012	37.663445129	41.302405270
26	27.495954082	34.099859053	41.659150838
8	27.036495592	34.818197843	39.673133784
8	28.173023799	34.922156069	38.967827206
6	29.701025291	35.708486827	40.567998045
8	30.648596172	36.406902914	40.252949883
8	28.835740636	35.798877260	41.483235296
6	29.318002258	34.260823432	39.605270204
8	28.949443533	33.374096330	40.495528147
6	30.397648922	33.939660198	38.572659089
6	31.790021640	33.586376297	39.107693743
6	32.843847359	33.545450840	37.983087936
8	33.965660783	34.094175372	38.203039058
8	32.514665391	32.990863272	36.906597788
1	31.761643753	32.582233595	39.563164809
1	32.125460912	34.300103656	39.872498063
1	30.476342056	34.814250409	37.910120130
1	30.036447174	33.112143971	37.938311741
8	24.845994786	33.248117701	38.084765916
6	23.750393068	33.598781222	38.496072235
7	23.407023863	34.957738386	38.526894063

6	24.424661686	35.916725314	38.083289892
6	22.188728722	35.416001237	38.952073023
7	21.949190846	36.717171219	38.902003631
6	21.226732311	34.475679127	39.401746481
6	21.543046085	33.151910297	39.377209108
7	22.770263403	32.721049636	38.938064754
1	24.646008591	36.617767215	38.899853119
1	24.069838138	36.445700084	37.184892140
1	22.690818012	37.361920801	38.664246754
1	20.828157044	32.406941895	39.724752945
1	20.255193738	34.809070028	39.761260878
1	25.339212303	35.365782592	37.857191197
1	21.158771421	37.12992229	39.434581241
1	23.965852163	30.185790551	42.258586913
1	23.946982644	36.315549103	44.433660196
1	29.863399165	30.880089697	45.138519889
1	25.160899325	42.702056868	41.550122877
1	22.995687175	31.748490412	38.880748365

IMI

QM/MM (BS1) = -3419.850338 a.u.

QM/MM (BS2+ZPE) = -3421.846925 a.u.

6	24.597938474	30.621611704	41.853563754
7	25.783604223	30.071150370	41.423292172
1	26.012618738	29.071203631	41.358047041
6	26.624350781	31.070636571	41.120387553
1	27.646293180	30.930654282	40.785696019
7	26.047432283	32.248279374	41.326847618
6	24.775443177	31.985289791	41.792225559
1	24.080806855	32.779576793	42.050515001
6	24.766397125	36.705348854	43.918862111
1	25.587561881	36.764425430	44.646952765
1	24.548149393	37.719703735	43.551974047
6	25.163759237	35.819028377	42.737545574
8	24.602647358	35.970781304	41.638944194
8	26.105490631	34.979364130	42.963143186
6	29.295675084	31.674657973	44.669859170
7	28.376467702	32.407953180	45.380488525
1	28.156100007	32.344809035	46.382978135
6	27.794964512	33.273547244	44.534243038
1	27.006567004	33.970148655	44.808786174
7	28.291037755	33.138758872	43.309489971
6	29.223854545	32.132270365	43.375907812
1	29.743193383	31.790242402	42.486502633
6	24.104877980	42.226288500	41.217362115
1	23.769573807	42.738708992	40.297948348
1	23.300124699	42.316725850	41.960871909
7	24.436791010	40.835891741	40.975273028
1	25.426954961	40.598542965	40.876579767
6	23.648421358	39.758176225	41.176348534
7	22.385794785	39.836396247	41.536724787
1	21.847449529	40.696874258	41.619599453
1	21.853066428	38.973509347	41.761308876
7	24.219851691	38.556860048	40.944501995
1	25.239487401	38.569970721	40.897304936
1	23.861450598	37.667603505	41.332168972
26	27.231848179	33.955424849	41.620323579
8	27.999873161	35.402078954	40.428073309
8	28.913965750	35.014117126	39.391636496
6	29.187786321	36.779198101	41.763783669
8	30.273753198	36.482855724	41.432100412

8	28.262690392	37.259678332	42.292457379	1	23.226039915	42.335439510	41.936534555
6	29.379125162	33.774663007	39.504446502	7	24.342778756	40.895401009	40.870293120
8	29.000350956	33.011788480	40.384082418	1	25.330283030	40.690335723	40.696320051
6	30.427465245	33.476315261	38.462345657	6	23.627029924	39.795023254	41.189355267
6	31.848064314	33.789494036	38.961005132	7	22.403022637	39.839411912	41.671304092
6	32.923382531	33.678331618	37.864313426	1	21.812050027	40.669966288	41.684387528
8	34.066774146	34.145584302	38.132411225	1	21.909620982	38.961313696	41.922924947
8	32.589081365	33.140979750	36.781927851	7	24.231589710	38.609920963	40.961438662
1	32.138627260	33.104311539	39.774374509	1	25.244353815	38.653555024	40.850356219
1	31.900961041	34.797194147	39.402323332	1	23.910238200	37.710598246	41.359224413
1	30.214943709	34.067417149	37.560961679	26	27.219691818	33.941937999	41.602756662
1	30.348742393	32.417898124	38.179197183	8	27.775100288	35.303642016	40.549031734
8	24.980292050	33.172601175	38.184364842	8	29.058262019	34.880728835	39.452812265
6	23.883728489	33.552614762	38.570953975	6	28.979571547	36.934036470	41.918758036
7	23.608277126	34.922642340	38.675135544	8	30.065717370	36.571186737	41.693879957
6	24.712530574	35.845949693	38.388491950	8	27.987165113	37.424903641	42.284121673
6	22.389574767	35.418769501	39.057788857	6	29.418917195	33.660471441	39.643555924
7	22.224214867	36.729928645	39.125856165	8	28.889409682	32.910191809	40.490379199
6	21.340575149	34.503201006	39.334604122	6	30.563535697	33.189358817	38.761528059
6	21.599938524	33.170020531	39.265690824	6	31.861441841	33.976965199	39.452824806
7	22.841560221	32.703974970	38.910293653	6	32.934647878	33.749157447	37.893917273
1	25.042263432	36.312026291	39.327456895	8	34.095770873	34.185289868	38.144332880
1	24.384553003	36.592596926	37.650464358	8	32.582821860	33.191541736	36.826690076
1	23.026031574	37.349895094	39.126335329	1	32.315803518	33.768924604	39.959391455
1	20.830258867	32.442047858	39.517436449	1	31.629300254	35.054990131	38.987523898
1	20.361188449	34.866694991	39.641896885	1	30.254933401	33.303001525	37.711021863
1	25.543435404	35.268366505	37.976676621	1	30.713477954	32.115485778	38.945222664
1	21.368007713	37.114787659	39.570582096	8	24.992534397	33.139608651	38.165870754
1	23.797191340	30.020831138	42.284764470	6	23.906312134	33.531265862	38.568400112
1	23.884822579	36.350430446	44.452647240	7	23.651360144	34.903828956	38.694271996
1	29.842881154	30.844957127	45.117329108	6	24.766680367	35.817056732	38.415863241
1	24.998923159	42.721745379	41.595876341	6	22.438556953	35.411045477	39.080941537
1	23.029440730	31.723783148	38.847864449	7	22.285531905	36.723179540	39.155465495
				6	21.379463538	34.506117503	39.356714063
				6	21.621908550	33.170626355	39.276413971
				7	22.855987070	32.693026843	38.910115723
				1	25.062983076	36.313035120	39.350131580
				1	24.467570753	36.538761031	37.641031927
				1	23.091600467	37.337106229	39.148670970
				1	20.844632358	32.449672228	39.525557817
				1	20.405846241	34.880340170	39.669535887
				1	25.613728674	35.225476832	38.060708486
				1	21.433198196	37.111460468	39.605034900
				1	23.771439585	30.032241993	42.291838549
				1	23.895929898	36.335329495	44.475139839
				1	29.828959521	30.889430549	45.111762348
				1	24.921516249	42.753105603	41.560436267
				1	23.032429946	31.711303698	38.838981590

TS2

QM/MM (BS1) = -3419.840647 a.u.

QM/MM (BS2+ZPE) = -3421.852688 a.u.

6	24.564900806	30.637996376	41.854176313
7	25.744958292	30.089242511	41.403834473
1	25.973763988	29.089053102	41.337804328
6	26.578543838	31.087324964	41.084767865
1	27.595065885	30.955236502	40.732448077
7	26.002435240	32.265371720	41.303335135
6	24.737996944	32.001382817	41.791220673
1	24.047837451	32.794688285	42.061863239
6	24.788451603	36.669273010	43.946032992
1	25.611561979	36.689143288	44.674023874
1	24.606179505	37.695569728	43.593707722
6	25.148220285	35.794516601	42.744446744
8	24.600858019	36.004832151	41.651834851
8	26.043714595	34.895119943	42.949000787
6	29.268519634	31.718721102	44.680193541
7	28.331087498	32.421148743	45.399598692
1	28.113063640	32.342610796	46.401665046
6	27.729992013	33.283952208	44.566715174
1	26.925296941	33.957484057	44.849654708
7	28.233640434	33.178073821	43.341467591
6	29.191214839	32.191777981	43.393501108
1	29.717708466	31.877857930	42.497807542
6	24.018882168	42.276393341	41.178252472
1	23.667484038	42.823661858	40.286096180

IM2

QM/MM (BS1) = -3419.849387a.u.

QM/MM (BS2+ZPE) = -3421.854806 a.u.

6	24.599400903	30.651292426	41.839371569
7	25.774969596	30.107069217	41.368999047
1	26.007463493	29.107207342	41.302185656
6	26.599368662	31.107425619	41.035350807
1	27.611183513	30.989497532	40.665013142
7	26.019918452	32.282253675	41.267781743
6	24.764568987	32.014518976	41.777143817
1	24.075170027	32.805526603	42.055589303
6	24.780396112	36.619820814	43.933332489

1	25.616883454	36.617751419	44.645839037
1	24.618524750	37.650443773	43.584628495
6	25.084008648	35.740379551	42.720474808
8	24.498338436	35.943130777	41.653102559
8	25.984817416	34.827252706	42.896657002
6	29.246436644	31.759082392	44.633640914
7	28.289175125	32.439612553	45.348375382
1	28.065967119	32.347903357	46.348364101
6	27.682672803	33.299763294	44.520024479
1	26.863100808	33.954403436	44.802115567
7	28.203709465	33.215732704	43.298894916
6	29.180012601	32.245972622	43.351003524
1	29.724608721	31.959667007	42.456863707
6	24.009092050	42.264730957	41.177959800
1	23.660491182	42.806288435	40.281205185
1	23.216391517	42.332981868	41.935598584
7	24.326358471	40.879625553	40.881679782
1	25.312180421	40.665886178	40.705447512
6	23.600117022	39.788421832	41.204891598
7	22.374102640	39.846179528	41.680431923
1	21.786903042	40.679337012	41.680469717
1	21.875729905	38.971643331	41.933174444
7	24.192113691	38.594421377	40.992578267
1	25.205857123	38.615766477	40.885462187
1	23.832471799	37.704453143	41.370488072
26	27.202810762	33.976116812	41.542940011
8	27.481617406	35.430095916	40.562338283
8	29.038125570	34.868939639	39.218112387
6	28.893662415	36.936694199	41.907481893
8	29.944012265	36.521446457	41.622465307
8	27.940443672	37.459915325	42.331509205
6	29.382413602	33.723915983	39.581033352
8	28.807947713	33.053772546	40.507484002
6	30.585680982	33.107398278	38.867793661
6	31.849156319	33.970335275	38.984470249
6	32.974581149	33.590733928	38.004881239
8	34.160997208	33.732416295	38.411060931
8	32.633934397	33.216937519	36.851893471
1	32.255784557	33.971948461	40.007844374
1	31.572294508	35.014542542	38.758839987
1	30.331873063	33.020295290	37.799650056
1	30.753697362	32.090237890	39.254051105
8	24.986484155	33.184917072	38.201778499
6	23.890245328	33.567851389	38.583372373
7	23.617945358	34.938193187	38.694024749
6	24.723593385	35.863248169	38.416751703
6	22.394621525	35.433761675	39.060095858
7	22.223520174	36.745385865	39.111921563
6	21.344965256	34.519392380	39.339709555
6	21.603211776	33.186080934	39.271400673
7	22.845088151	32.719927235	38.918374010
1	24.957361371	36.427123978	39.328552716
1	24.450161372	36.525701534	37.581320450
1	23.023364256	37.366462115	39.088945988
1	20.832544558	32.457812329	39.519065257
1	20.364131775	34.884903472	39.639778922
1	25.607470746	35.276588232	38.155785683
1	21.373664851	37.129885462	39.569636837
1	23.804215718	30.046835453	42.275696695
1	23.887677649	36.303850862	44.473039868
1	29.811157618	30.937340918	45.073979982
1	24.912967512	42.742180273	41.556270023

1	23.030836821	31.739836221	38.848434579
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IM3

QM/MM (BS1) = -3419.876731 a.u.

QM/MM (BS2+ZPE) = -3421.892680 a.u.

6	24.623812045	30.602038782	41.857291781
7	25.806238410	30.051937531	41.420096090
1	26.025383361	29.051496631	41.329635382
6	26.668420144	31.048154460	41.169227417
1	27.689827708	30.909484366	40.831164289
7	26.101392661	32.218710034	41.422140153
6	24.819545566	31.964449320	41.852142405
1	24.134639961	32.758184358	42.133759879
6	25.032758154	36.780239701	44.100208815
1	25.777987779	36.676958447	44.904288745
1	24.891586761	37.851425816	43.904214003
6	25.585883055	36.161595021	42.814203895
8	25.538009040	36.822558503	41.771732482
8	26.167607854	35.013325223	42.921934127
6	29.197852601	31.747192314	44.617764898
7	28.233390630	32.406951743	45.340977950
1	28.036925417	32.322593910	46.346825370
6	27.591719384	33.243980852	44.514299998
1	26.770685441	33.890737206	44.808026493
7	28.095000535	33.162983236	43.287666939
6	29.099348722	32.223886382	43.332424444
1	29.657666703	31.961497675	42.438909384
6	24.352215886	42.151597216	41.107164673
1	24.409865985	42.423509051	40.036581302
1	23.410447862	42.561984428	41.501111682
7	24.407234096	40.720194936	41.326972827
1	25.322019996	40.281527999	41.491587973
6	23.353111703	39.894118568	41.202391807
7	22.149446916	40.351543161	40.858775868
1	21.865674669	41.309923900	41.024942261
1	21.365092550	39.675688588	40.878144819
7	23.490317601	38.572950391	41.357406260
1	24.393359280	38.122193289	41.573745450
1	22.643804350	38.092823433	41.719354598
26	27.171634713	33.994148733	41.558242483
8	26.506168128	34.673643743	40.263684867
8	29.354987742	35.440406130	39.569728343
6	29.641592971	36.531278417	41.994913188
8	30.787215751	36.304736123	41.991197755
8	28.517638767	36.792879074	42.103090829
6	29.505964853	34.234996312	39.768997058
8	28.875096019	33.567609094	40.697598527
6	30.543463369	33.453984171	38.959315454
6	31.921575448	34.120998753	39.053890837
6	32.990470786	33.654107614	38.049921573
8	34.191768585	33.784868333	38.420827066
8	32.614265630	33.241176382	36.921880829
1	32.344837182	34.039499906	40.067732866
1	31.777896141	35.201148046	38.877999643
1	30.224761466	33.460667061	37.903458503
1	30.572793754	32.403248270	39.285080709
8	24.829274378	33.299620241	38.176328005
6	23.731894826	33.637156220	38.582963880
7	23.404395752	34.996614181	38.719371138

6	24.463258493	35.973627569	38.426996331
6	22.157093300	35.436791130	39.077197962
7	21.946002812	36.744599746	39.139730023
6	21.148490634	34.477161723	39.345724179
6	21.470879649	33.154984669	39.288785813
7	22.728503666	32.742798932	38.937839779
1	24.680723392	36.564824053	39.328435111
1	24.151413605	36.612381704	37.586340580
1	22.732504564	37.384082241	39.144434541
1	20.736533004	32.394479771	39.547594499
1	20.148909927	34.790993947	39.641268767
1	25.371056317	35.423553920	38.170652950
1	21.101528122	37.137176170	39.590218340
1	23.815072117	30.006177024	42.280323482
1	24.098740095	36.395645456	44.509799896
1	29.782771719	30.940212630	45.059036630
1	25.171998003	42.642639132	41.631476074
1	22.962992038	31.772429153	38.879786405

Substrate hydroxylation step reaction states cartesian coordinates for AlkBH2-dsDNA

Snapshot 1

RC2

QM/MM (BS1) = -3309.777979 a.u.

QM/MM (BS2+ZPE) = -3311.663829 a.u.

6	24.526979716	36.782905040	44.666764018
7	25.711314055	36.185705437	45.033308847
1	25.888946115	35.670164403	45.907803361
6	26.621915804	36.448315960	44.077811118
1	27.649418977	36.095040176	44.113177785
7	26.089352609	37.187368679	43.112339235
6	24.777153409	37.410224036	43.465585829
1	24.126735503	38.040545060	42.862806232
6	25.126171798	41.663270377	40.230351723
1	25.728389165	42.539451050	40.521688214
1	25.086340198	41.683323014	39.131028523
6	25.908338392	40.417255677	40.637403885
8	25.503237809	39.618236105	41.540792625
8	27.014103356	40.204566561	40.080211516
6	28.855036481	39.935627750	45.058633519
7	27.844882146	40.830825578	44.805324529
1	27.551675441	41.629162109	45.382825388
6	27.272108439	40.497737530	43.640311092
1	26.415329789	41.015156646	43.223026578
7	27.865310785	39.434805930	43.113279191
6	28.862568531	39.067435139	43.991108379
1	29.494880002	38.207173091	43.789164011
6	24.424833235	43.058298664	34.911541255
1	23.489165386	43.231533330	34.353179520
1	24.436385915	43.765564066	35.758545804
7	24.542434903	41.690551163	35.385608344
1	25.275806354	41.084205244	35.002789769
6	23.765899533	41.183423560	36.356058759
7	22.716251144	41.869790963	36.808736129
1	22.349185858	42.717846158	36.362323239
1	22.219017457	41.499769699	37.627534478
7	24.052968068	39.985013709	36.885472238
1	24.988427108	39.586455186	36.791415724
1	23.321594028	39.473471324	37.399209699
26	27.092567525	38.257238191	41.512603829

8	26.463283795	37.363101363	40.329923889
8	29.538342314	38.359424244	39.558478855
6	29.711168105	37.576131709	40.488837013
8	28.874811406	37.431122145	41.478940425
6	31.014801508	36.771658209	40.566734401
6	30.989247830	35.369723020	41.176512606
6	32.365986021	34.665110225	41.207090658
8	32.361168317	33.407287687	41.192437713
8	33.404630561	35.378815624	41.267620222
1	30.287853671	34.710613833	40.643342021
1	30.617075391	35.416441455	42.216251796
1	31.723699760	37.393192657	41.141702278
1	31.413770959	36.739019567	39.54573697
8	23.451389915	33.311773734	42.187055389
6	22.608664800	34.162492271	42.365850633
7	22.441531119	35.233260342	41.452873276
6	23.366750686	35.270305628	40.307788510
6	21.488273446	36.200182123	41.602191961
7	21.405773331	37.194171644	40.726002709
6	20.579644120	36.110094507	42.697988591
6	20.727478209	35.101960962	43.598765159
7	21.742735099	34.187784203	43.465454217
1	23.896998503	34.313506917	40.278025428
1	24.097885733	36.086449232	40.428454105
1	20.736098882	37.953170647	40.888844048
1	20.046421364	34.999985003	44.449793800
1	19.771483594	36.832597234	42.800226397
1	22.800907904	35.392571878	39.373729043
1	21.999731665	37.286353363	39.906646972
8	27.112043037	39.689189551	37.270211256
1	28.036895672	39.376753783	37.195006967
1	27.053739187	39.939291821	38.216799312
1	23.667809963	36.855312866	45.333586154
1	24.121789146	41.803954440	40.629714712
1	29.396231933	39.959311554	46.004473826
1	25.265334090	43.308305688	34.264144840
1	21.887207241	33.495073176	44.172031694

TS7

QM/MM (BS1) = -3309.739955 a.u.

QM/MM (BS2+ZPE) = -3311.629373 a.u.

6	24.375061929	36.710689454	44.851814148
7	25.567182460	36.131664550	45.220133245
1	25.770178885	35.645108035	46.104034170
6	26.462038863	36.361045355	44.243758982
1	27.489875661	36.009090779	44.278165531
7	25.910805908	37.059051679	43.261143189
6	24.604742429	37.292998078	43.626257266
1	23.947541301	37.909231165	43.016937626
6	25.004673850	41.450203661	40.253148388
1	25.694561621	42.248741909	40.573578103
1	24.974925151	41.493266132	39.155169055
6	25.613602397	40.112452185	40.662620906
8	25.212595931	39.456240852	41.662995834
8	26.607027259	39.666364522	40.013368423
6	28.766898814	39.806310901	44.959635176
7	27.752192343	40.695875431	44.709819128
1	27.468767157	41.501304519	45.282314736
6	27.154939594	40.333236750	43.563255275
1	26.283830084	40.839138619	43.161995661
7	27.731129173	39.259068478	43.042181439

6	28.747115941	38.914953414	43.907153223	7	26.096321968	37.146544782	43.102986783
1	29.377864852	38.048754679	43.719254585	6	24.782452188	37.359211604	43.460809851
6	24.417850979	43.091246415	34.894524422	1	24.120426155	37.968140346	42.849141272
1	23.480415377	43.265744555	34.339522424	6	25.069308168	41.583851381	40.228555536
1	24.430858494	43.793177598	35.745712039	1	25.705020333	42.434394237	40.526718573
7	24.540036360	41.720787890	35.357960399	1	25.045166842	41.596783351	39.129124575
1	25.267311673	41.113144509	34.965565822	6	25.765021122	40.305053341	40.675626088
6	23.763134381	41.205047108	36.322809532	8	25.379086920	39.608440050	41.650132218
7	22.716665723	41.888306875	36.786625775	8	26.826129172	39.948614115	40.067637683
1	22.350709291	42.742684097	36.351683400	6	28.874690341	39.933009053	45.055919707
1	22.221261587	41.511598610	37.603320476	7	27.872517602	40.836049118	44.800154780
7	24.047734240	39.998763898	36.834436400	1	27.573625248	41.628399654	45.382176076
1	24.978191222	39.594300752	36.721954982	6	27.313249821	40.514120429	39.629124575
1	23.313638573	39.481346058	37.338004196	1	26.460984483	41.041388312	43.207196273
26	26.733713986	37.924275034	41.450277778	7	27.903496067	39.453804822	43.090090385
8	25.696499187	36.884526170	40.508925264	6	28.887119741	39.075711747	43.977690058
8	29.394156399	38.331334631	39.561424430	1	29.516447118	38.212004733	43.778138439
6	29.484870376	37.442333686	40.407515154	6	24.411537079	42.999332920	34.906026958
8	28.530210071	37.119794422	41.232606654	1	23.486199866	43.213400627	34.344850419
6	30.823673290	36.693497586	40.542852315	1	24.436519754	43.686456385	36.769065737
6	30.855259023	35.294570606	41.159709101	7	24.484164249	41.618966943	35.352439361
6	32.252726982	34.626223402	41.179722341	1	25.209175657	41.001849971	34.970912338
8	32.278001419	33.368240571	41.154404041	6	23.707489674	41.129179907	36.331468935
8	33.276935381	35.360146410	41.244087440	7	22.679776681	41.839982843	36.795186530
1	30.167653842	34.610579658	40.640796652	1	22.328082582	42.696278623	36.352098450
1	30.492771089	35.333053662	42.203551632	1	22.181416757	41.482352428	37.618712104
1	31.485555985	37.359425539	41.125740160	7	23.972364805	39.922795006	36.854867357
1	31.259543752	36.676659505	39.532316030	1	24.897289165	39.506213071	36.747317013
8	23.672748822	33.354607203	42.218060725	1	23.249617170	39.433661076	37.400213098
6	22.840395381	34.218417401	42.359382711	26	27.038423533	38.187985785	41.400858962
7	22.745050542	35.297885018	41.424088018	8	26.200480752	37.074713839	40.188185255
6	23.715756163	35.307113366	40.361721398	8	29.523501723	38.360119080	39.617579492
6	21.765913465	36.260797964	41.510986627	6	29.699708328	37.516773230	40.500756884
7	21.716323799	37.244768213	40.625411078	8	28.844830044	37.290339105	41.452721772
6	20.800956672	36.171013958	42.555317150	6	31.013751043	36.730999975	40.539572347
6	20.897555481	35.172352601	43.474268257	6	31.005812189	35.329441228	41.147683865
7	21.916429075	34.255510958	43.407596295	6	32.385176068	34.635611324	41.180030190
1	24.240318960	34.347990890	40.328881388	8	32.387731433	33.377499220	41.154069331
1	24.694872856	36.165523099	40.531343884	8	33.419048556	35.354831729	41.253512811
1	21.002121874	37.972570994	40.735132625	1	30.308736825	34.663914359	40.616531584
1	20.170957245	35.082417483	44.288612643	1	30.632704810	35.376404534	42.186926899
1	19.993232939	36.900538296	42.614032604	1	31.727901734	37.357160317	41.103043933
1	23.271211523	35.582115696	39.395898723	1	31.396418475	36.707348954	39.508689853
1	22.377557728	37.369627362	39.864899322	8	23.414892221	33.305354845	42.135888600
8	27.048507169	39.637045753	37.239292302	6	22.587978706	34.162607442	42.340318895
1	27.995705652	39.397655126	37.183968525	7	22.458983914	35.270303654	41.425729689
1	26.889187785	39.693083597	38.207439775	6	23.372518268	35.292024480	40.383305681
1	23.529220283	36.822653104	45.530108603	6	21.488836469	36.244157123	41.578876147
1	24.021304260	41.682056254	40.662166666	7	21.384652502	37.223448661	40.687476880
1	29.335049539	39.870787487	45.887597913	6	20.608545035	36.157763127	42.691364218
1	25.255587862	43.346065528	34.245423924	6	20.740828817	35.142379864	43.588421146
1	22.014304175	33.567170375	44.126331433	7	21.732123942	34.201311667	43.436182741

IM10

QM/MM (BS1) = -3309.767645 a.u.

QM/MM (BS2+ZPE) = -3311.653160 a.u.

6	24.548571841	36.763564511	44.680134977	1	26.223383035	36.133522068	40.415079949
7	25.744888113	36.194936887	45.056242225	1	20.718722887	37.982978000	40.863184767
1	25.934376384	35.702075580	45.941019298	1	20.063659054	35.048044156	44.443060030
6	26.645473383	36.445378270	44.088321589	1	19.806702695	36.886141679	42.801854369
1	27.679623086	36.112236939	44.128350366	1	23.583157013	36.227026211	39.870658474
				1	21.877152248	37.261508952	39.797333002
				8	27.065763327	39.652539163	37.243142924
				1	28.010883541	39.403080029	37.185704967
				1	26.938033237	39.788575949	38.205888407

1	23.688750973	36.838227278	45.345868305
1	24.069525251	41.763880794	40.623638874
1	29.410947431	39.952274735	46.004668616
1	25.266241883	43.237947900	34.273089433
1	21.876499667	33.508524941	44.142705707

TS8

QM/MM (BS1) = -3309.753653 a.u.

QM/MM (BS2+ZPE) = -3311.643711 a.u.

6	24.353001672	36.700556752	44.869996779
7	25.551282515	36.130900788	45.234322106
1	25.765771723	35.656392931	46.122035706
6	26.434192371	36.348846285	44.245674328
1	27.465310317	36.006243636	44.276500797
7	25.870398066	37.029227149	43.256850059
6	24.567707430	37.266060898	43.634710222
1	23.901058674	37.870943874	43.024142808
6	24.976190869	41.424645940	40.233062772
1	25.674707404	42.216751578	40.550745882
1	24.932662463	41.479453600	39.135928609
6	25.587292736	40.080255348	40.615442738
8	25.183067645	39.402139210	41.607186907
8	26.576893509	39.653815459	39.957421339
6	28.761138027	39.812602972	44.953538917
7	27.744044151	40.697328208	44.696892349
1	27.449730973	41.497221054	45.271604781
6	27.165427634	40.337610575	43.538047514
1	26.297148264	40.841860437	43.126922312
7	27.754178594	39.271194860	43.016902075
6	28.758824871	38.927955240	43.894786372
1	29.397224040	38.065862334	43.712899351
6	24.421679486	43.062384823	34.895618872
1	23.489572985	43.263649743	34.340742865
1	24.444939441	43.750036725	35.758121600
7	24.517649299	41.682841262	35.337447383
1	25.240812328	41.072055610	34.942539516
6	23.742639987	41.171362949	36.306139951
7	22.707671763	41.864639116	36.780541481
1	22.345531604	42.721873318	36.347933370
1	22.213728490	41.491202510	37.599805569
7	24.018228169	39.959488511	36.808578852
1	24.946462437	39.550873503	36.695096770
1	23.287467154	39.451153284	37.325965297
26	26.671858050	37.884039693	41.463025933
8	25.503003060	36.739572171	40.353628251
8	29.331248797	38.251929622	39.564106432
6	29.418610902	37.355040782	40.402708060
8	28.445111897	36.999484630	41.194756637
6	30.772674775	36.639021169	40.557770768
6	30.828102594	35.235691414	41.161164968
6	32.236061015	34.590577118	41.175245401
8	32.278033757	33.333127665	41.134935424
8	33.249652669	35.337408219	41.248327742
1	30.154622175	34.543859303	40.633685341
1	30.463099094	35.257221403	42.204573463
1	31.407766951	37.315794367	41.158213895
1	31.230360823	36.642881232	39.556547236
8	23.699415815	33.401134372	42.213997004
6	22.860028576	34.255853833	42.372468000
7	22.764955412	35.353555734	41.434319575
6	23.707167653	35.366961588	40.414702556

6	21.759755376	36.303900081	41.527382522
7	21.695060013	37.292125904	40.643994174
6	20.799066615	36.185493354	42.567046522
6	20.902097748	35.183123882	43.482086369
7	21.935265118	34.277484440	43.411117001
1	24.329388968	34.476528986	40.384510713
1	26.050273583	36.020414246	40.000891001
1	20.971571915	38.008243626	40.762317170
1	20.174529959	35.077713383	44.292723271
1	19.980896690	36.902863257	42.629422132
1	23.437631269	35.869977647	39.492205733
1	22.361684829	37.445914152	39.894268161
8	27.024291865	39.588546568	37.205807543
1	27.977042687	39.370775028	37.161936971
1	26.858288041	39.672779129	38.171830978
1	23.512112983	36.815359724	45.553951314
1	23.999275241	41.659747199	40.655473214
1	29.326859542	39.878067929	45.882915499
1	25.267483481	43.309876953	34.254190333
1	22.033734294	33.584139920	44.124944491

PD

QM/MM (BS1) = -3309.851902 a.u.

QM/MM (BS2+ZPE) = -3311.714112 a.u.

6	24.435134797	36.690708076	44.876468447
7	25.612850134	36.107028290	45.279963459
1	25.785563306	35.609704971	46.164062910
6	26.539700239	36.343346694	44.338826288
1	27.566387325	35.993595823	44.413903866
7	26.027347937	37.049391088	43.337303411
6	24.708741591	37.277847744	43.661427476
1	24.050233232	37.857707912	43.020016104
6	24.795746703	41.269155958	40.113610501
1	25.594276849	41.948404948	40.439169161
1	24.647579232	41.370024470	39.029898719
6	25.144585388	39.810908605	40.416853894
8	26.050992894	39.617676659	41.297809419
8	24.555253741	38.901245850	39.795527365
6	29.004003433	39.916463395	45.317919602
7	28.092889827	40.859459624	44.912219736
1	27.792037797	41.708196006	45.409733252
6	27.597146166	40.470841658	43.723510196
1	26.840135796	41.017228661	43.166033786
7	28.137041762	39.321155474	43.342194210
6	29.020622980	38.958624428	44.330892688
1	29.596681798	38.037148631	44.275680573
6	24.484649303	42.864162931	34.943529940
1	23.576546123	43.171626396	34.398950034
1	24.569559090	43.520334740	35.828091728
7	24.438909027	41.466138924	35.340462535
1	25.226624965	40.846107434	35.117851112
6	23.610916281	41.030063733	36.308545257
7	22.611899756	41.797203604	36.743074387
1	22.319051966	42.674240217	36.298580151
1	22.068612895	41.457746384	37.545326327
7	23.801756647	39.817253530	36.838451564
1	24.697189604	39.350647612	36.716056274
1	23.141004524	39.427828543	37.521911049
26	27.166719498	38.071258529	41.889620240
8	24.506035229	36.288675048	40.532608935
8	29.165699331	38.170198704	39.458182340

6	29.479530936	37.335633233	40.324198747
8	28.721090654	37.031320812	41.323780814
6	30.844393718	36.641429815	40.276792789
6	30.933031547	35.278612086	40.967913839
6	32.332627121	34.630091635	41.017400289
8	32.366264379	33.371892561	41.002419752
8	33.348053877	35.373564148	41.106367838
1	30.244760127	34.554626128	40.508068616
1	30.587730549	35.385846389	42.011736405
1	31.564084481	37.330421234	40.754894511
1	31.152328129	36.582405676	39.222722187
8	23.493505274	33.467766873	42.083359853
6	22.642406263	34.304406571	42.279003169
7	22.445587438	35.382507821	41.375416242
6	23.431037620	35.474555055	40.243169682
6	21.465436521	36.320991956	41.538648616
7	21.313113988	37.318309594	40.677100095
6	20.581166817	36.204670256	42.653656814
6	20.760829674	35.195387819	43.546091861
7	21.787734094	34.298024185	43.392586103
1	23.778177271	34.445760213	40.096614508
1	24.379765642	37.227224468	40.255020225
1	20.606493330	38.028239996	40.883564124
1	20.093236141	35.081390011	44.406419167
1	19.758961143	36.907772868	42.773732387
1	22.860499851	35.785221269	39.352487688
1	21.823679141	37.466770245	39.804213804
8	26.662025672	38.557812080	37.840678645
1	27.482330366	38.509846586	38.367889979
1	25.949800805	38.382537780	38.479739666
1	23.576602237	36.797254803	45.539519698
1	23.876236927	41.570003437	40.615666162
1	29.483068343	39.950949284	46.296374945
1	25.353767789	43.057002651	34.314631519
1	21.943990785	33.598142854	44.089524023

Snapshot 2

RC2

QM/MM (BS1) = -3461.229779 a.u.

QM/MM (BS2+ZPE) = -3463.249318 a.u.

6	23.741634603	37.364676179	43.845800212
7	24.922306855	36.902004778	44.375894064
1	25.042991384	36.504612831	45.318949730
6	25.893464347	37.100639952	43.468525626
1	26.931665706	36.821629549	43.629020725
7	25.402713579	37.677782388	42.377508001
6	24.054697340	37.853046491	42.597069245
1	23.421450384	38.362634810	41.875400200
6	24.366742305	41.597055147	38.852054998
1	24.851759220	42.569579969	39.027759901
1	24.499936938	41.376119037	37.783605719
6	25.163661847	40.549334545	39.617859834
8	24.625623668	39.698575520	40.390132041
8	26.419238049	40.505224859	39.467629853
6	27.791454702	40.845904325	44.250957068
7	26.796081610	41.671052516	43.779885809
1	26.417333741	42.526537152	44.206567510
6	26.339624803	41.157718156	42.628077788
1	25.551471839	41.622341760	42.046537699
7	26.991690588	40.045798527	42.320991918
6	27.908944920	39.835326542	43.327907387
1	28.575987607	38.978418975	43.304550763

6	25.120607388	42.422664140	33.295314691
1	24.252132270	42.398281060	32.614386367
1	24.993895525	43.311159493	33.939302559
7	25.237956872	41.216491460	34.084267507
1	26.089264130	40.645458714	34.040954482
6	24.299371886	40.794523416	34.959357658
7	23.136327962	41.431562736	35.096931566
1	22.877804307	42.264897489	34.560990120
1	22.410373888	40.985373127	35.679944705
7	24.556518797	39.711134177	35.687325283
1	25.511231888	39.352157180	35.776537762
1	23.939576766	39.394266248	36.447663617
26	26.494307128	38.648460301	40.805871849
8	26.145687877	37.583227192	39.649995996
8	28.987625540	38.353787633	38.884726259
6	29.193165868	37.909901024	40.016707505
8	28.356370867	38.043344514	41.006708760
6	30.533450129	37.235773279	40.348954505
6	30.491205306	35.930454103	41.152210384
6	31.873554454	35.314606881	41.487184472
8	31.905823667	34.070856849	41.655734924
8	32.872337188	36.077846731	41.602456957
1	29.908652054	35.158620594	40.626841327
1	29.968349900	36.099689406	42.111544029
1	31.135454699	37.970743819	40.913251115
1	31.048684298	37.079866776	39.390419796
8	22.827921688	34.038616645	41.831908413
6	21.860267245	34.758884466	41.903814002
7	21.544942693	35.676385856	40.864373680
6	22.442838648	35.672159518	39.697575888
6	20.486358580	36.538170654	40.920139633
7	20.263069599	37.418651766	39.955611981
6	19.609742467	36.461221678	42.043040208
6	19.864978725	35.577996813	43.036902001
7	20.973066386	34.770890530	42.989773354
1	21.852055303	35.688232563	38.774094066
1	23.033515368	34.752512289	39.730572365
1	20.796339066	37.510435501	39.080657580
1	19.196928284	35.507732156	43.899939690
1	18.742609947	37.105491571	42.107321655
1	23.117697340	36.539353460	39.710248948
1	19.494722273	38.072885310	40.083207824
8	27.517154743	42.905874799	40.330885981
1	28.215744723	42.689733357	40.963606220
1	27.286767236	42.048913028	39.915970493
8	23.655390120	38.343719930	37.944770482
1	22.678545932	38.205380122	37.743364621
1	23.687820129	38.690887145	38.851533224
8	26.729836180	38.347158291	36.909265910
1	25.993499167	37.918548230	37.378734413
1	27.364902733	38.538348337	37.625991429
1	22.832404926	37.476485828	44.436450119
1	23.304025126	41.703872432	39.069516679
1	28.257776706	41.005122901	45.223202177
1	26.019628251	42.586727926	32.701250818
1	21.162317607	34.151649869	43.751808442

TS7

QM/MM (BS1) = -3461.191003 a.u.

QM/MM (BS2+ZPE) = -3463.210017 a.u.

6	23.494496111	37.292507208	44.081041010
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6	31.504271175	33.832607720	40.872043840
8	31.154222255	32.646482963	40.660019153
8	32.681944273	34.224000771	41.068124622
1	29.535104807	34.499979078	40.314310832
1	30.028205450	34.988087363	41.938491051
1	31.715717841	36.570719950	40.980762554
1	31.211993732	36.137490648	39.338988096
8	22.274330175	34.637095370	41.720542743
6	21.774314413	35.675190931	42.081856449
7	21.951932545	36.865147847	41.330519457
6	22.788572343	36.766089973	40.123487674
6	21.371113777	38.052558590	41.665551649
7	21.537464683	39.120869325	40.897380026
6	20.589698134	38.118060293	42.853020030
6	20.419273769	37.000110965	43.604731897
7	21.000411218	35.814189496	43.243583850
1	22.194057759	37.014723242	39.234782777
1	23.140582351	35.734718979	40.036010526
1	21.047416261	39.983914597	41.130762100
1	19.822912098	37.032304865	44.519393705
1	20.158989377	39.061913572	43.160568677
1	23.652342541	37.443679987	40.210769725
1	22.106526905	39.135665550	40.053684194
8	27.579071418	39.865052952	38.450603066
1	26.806809932	39.526168932	38.930085502
1	28.278591088	39.268759809	38.793763447
8	23.543729688	40.973276178	39.326332288
1	22.790947503	41.496931383	39.730205693
1	24.147804426	40.791734815	40.092456598
1	23.845628325	37.268998604	45.272208223
1	25.636787949	43.053020317	42.096137366
1	30.202636734	38.340294512	46.704388860
1	28.380067737	45.488980709	36.756547034
1	20.905571209	35.003981344	43.821978705

TS7

QM/MM (BS1) = -3386.878586 a.u.

QM/MM (BS2+ZPE) = -3388.828717 a.u.

6	24.546414623	36.916959486	44.875006563
7	25.576636482	36.051224438	45.137907435
1	25.606308487	35.344441852	45.889400428
6	26.559234632	36.294787511	44.259481192
1	27.493631153	35.741734923	44.238989269
7	26.207674874	37.277310841	43.437895677
6	24.950293871	37.682002941	43.811962872
1	24.442311620	38.508988091	43.321486715
6	26.765476861	42.769009147	41.739921622
1	27.596051896	42.924481465	42.444446647
1	26.918357962	43.404849277	40.856878731
6	26.700213250	41.321827652	41.252905305
8	27.063898374	40.411252696	42.071349021
8	26.330196563	41.122855615	40.082403834
6	29.604250134	38.594380768	45.711558624
7	28.943798144	39.795423852	45.696346318
1	28.912290205	40.492634590	46.452773566
6	28.319295699	39.912027059	44.514728986
1	27.718341059	40.768379445	44.229479975
7	28.538274589	38.848880570	43.751282895
6	29.346693973	38.011469268	44.489174625
1	29.687297190	37.054152990	44.100861354
6	27.459813499	45.395774741	37.312269994

1	26.843360618	46.288813711	37.125958220
1	27.733160483	45.407797775	38.382044719
7	26.787388461	44.161555889	36.945172656
1	27.315843060	43.466457231	36.407126195
6	25.709020257	43.656630368	37.577279706
7	25.005964307	44.390375312	38.440234790
1	25.111144794	45.407245632	38.531872070
1	24.199795535	43.976058393	38.928392330
7	25.352211220	42.398558793	37.290733729
1	26.065365459	41.786821686	36.894971997
1	24.656184490	41.919031864	37.880581557
26	27.157940003	38.407674202	41.955535284
8	25.745996083	38.132442754	40.958409879
8	28.863369218	37.702240209	38.929370673
6	29.184052700	37.207652556	40.015009254
8	28.608601235	37.482997026	41.147152201
6	30.350302952	36.235124692	40.110451123
6	30.053757986	34.923903100	40.837140261
6	31.254184071	33.955880476	40.813163605
8	30.979332133	32.733469627	40.958409879
8	32.408125046	34.442644211	40.897030769
1	29.188521221	34.407244740	40.394085588
1	29.790322036	35.128284186	41.890805137
1	31.185018318	36.739912971	40.626541019
1	30.692444244	36.018727366	39.090294210
8	22.634546293	34.848017622	41.722477553
6	22.104717156	35.897353870	41.987822917
7	22.463201859	37.089908486	41.274565964
6	23.550160144	36.977194822	40.342382700
6	21.768611840	38.271617572	41.428014253
7	22.119374741	39.343283650	40.743790960
6	20.682446231	38.304059010	42.346663391
6	20.411934224	37.219574052	43.121004380
7	21.133855655	36.061882401	42.986245065
1	23.335436215	37.468871449	39.385955445
1	23.848915368	35.931275746	40.227776381
1	21.605599445	40.231199433	40.829131729
1	19.612204189	37.249437228	43.865600183
1	20.092882762	39.2111289080	42.427185277
1	24.664693967	37.568384966	40.735216611
1	22.917922097	39.409932699	40.112043205
8	27.435687646	40.023727788	37.799236880
1	27.052206441	40.349151682	38.637055442
1	27.833756792	39.172978213	38.066232552
8	23.834516481	41.028322910	39.221744934
1	23.413556742	41.847774084	39.611426748
1	24.730273480	40.966546805	39.633374131
1	23.713016665	37.096628910	45.554148718
1	25.853981014	43.093847681	42.241641229
1	30.117157770	38.266463740	46.615695504
1	28.375127719	45.482932848	36.726889215
1	20.991233644	35.288584601	43.604016835

Snapshot 4

RC2

QM/MM (BS1) = -3387.759704 a.u.

QM/MM (BS2+ZPE) = -3389.705321 a.u.

6	25.791583624	38.862391534	45.691503203
7	27.157436618	38.756990131	45.775370177
1	27.720823816	38.859531924	46.634749626
6	27.628247595	38.527310975	44.538094406

1	28.683756316	38.399391826	44.313103289
7	26.631867580	38.480121155	43.660169511
6	25.471177505	38.693744115	44.364790359
1	24.503356788	38.763803489	43.871644297
6	23.623288598	40.661675446	39.596286299
1	23.995247848	41.611577914	39.183451642
1	23.275245742	40.077820635	38.729665339
6	24.811382239	39.931117387	40.191620573
8	24.778530556	39.451604032	41.375072853
8	25.848628624	39.805548484	39.492405730
6	28.631810197	42.253580314	42.849030356
7	27.374260656	42.725753606	42.575539447
1	27.040743112	43.687405301	42.721894078
6	26.647101143	41.717958639	42.075049642
1	25.607619810	41.823973035	41.787904848
7	27.374540633	40.611335921	41.994773057
6	28.623614395	40.928128574	42.481521583
1	29.409304246	40.180105359	42.534102190
6	22.079003904	39.003877967	34.855261503
1	21.012854588	38.818619796	34.671497607
1	22.168269036	40.031602834	35.248753339
7	22.652907352	38.037051972	35.774146230
1	23.498720708	37.525337175	35.500034442
6	22.284867676	37.905446902	37.061736470
7	21.197631086	38.522949766	37.532527186
1	20.561278775	39.073170786	36.945643174
1	20.903815336	38.360110158	38.505226461
7	23.026674964	37.136849037	37.869029892
1	24.014922774	36.974724697	37.643178096
1	22.850750104	37.145789614	38.884556647
26	26.682960919	38.641440305	41.540920972
8	26.073106169	37.172518447	41.273124030
8	28.193365251	36.759134509	39.322613230
6	28.904323500	37.405415704	40.086352084
8	28.471688671	38.277458455	40.966413558
6	30.421521256	37.270804120	40.027939192
6	31.067532375	36.521585493	41.200094506
6	32.582841191	36.339220562	40.984225733
8	33.101736251	35.256022827	41.362314728
8	33.204699692	37.283406037	40.436661755
1	30.613631727	35.530565048	41.349638420
1	30.915568968	37.085801822	42.138294981
1	30.874901670	38.272314255	39.964832958
1	30.654023430	36.741062424	39.096555806
8	25.574112618	34.584525071	46.271218747
6	24.527801888	35.171777772	46.136458945
7	23.910758646	35.276695126	44.865655948
6	24.610183276	34.632915002	43.740431713
6	22.738295165	35.943262135	44.650874026
7	22.244107068	36.011094027	43.425774221
6	22.080749163	36.544555760	45.765589515
6	22.642859117	36.448543681	47.001936104
7	23.838076786	35.804416513	47.187555767
1	23.948571795	33.898408863	43.262353888
1	25.485778547	34.113526463	44.136965419
1	21.371970050	36.506121457	43.190668437
1	22.149865146	36.886762150	47.873676732
1	21.130649010	37.049739059	45.614931620
1	24.931407127	35.391425394	43.008980879
1	22.693633775	35.556848901	42.632795737
8	22.736527496	37.219015230	40.667835440
1	21.813617852	37.600829728	40.679110149

1	23.322499609	37.853126925	41.118258737
8	25.915461377	37.354982308	37.884765840
1	25.877243011	38.276988673	38.199134460
1	26.603680843	36.973827228	38.478097232
1	25.169051284	39.201486050	46.519474046
1	22.769232005	40.886278718	40.235197891
1	29.364835625	42.904442014	43.325601534
1	22.597495657	38.971119334	33.897054587
1	24.300685024	35.801107276	48.074096890

TS7

QM/MM (BS1) = -3387.728665 a.u.

QM/MM (BS2+ZPE) = -3389.668228 a.u.

6	25.790958543	38.887644745	45.921499728
7	27.159027886	38.854086923	46.001658566
1	27.727997957	39.006075058	46.848871622
6	27.637237311	38.601210874	44.773955516
1	28.696054453	38.512113232	44.548474635
7	26.639725306	38.466745591	43.910218255
6	25.473070393	38.649483635	44.608231368
1	24.499421456	38.640197336	44.121157138
6	23.632613448	40.599152525	39.565714343
1	23.988113819	41.566246130	39.180533801
1	23.222338045	40.072471553	38.688002860
6	24.871714960	39.816679897	39.988254613
8	24.848525878	39.118996265	41.078621387
8	25.848548591	39.852001774	39.226296023
6	28.569439202	42.075444827	42.841962591
7	27.295642713	42.513361305	42.590410248
1	26.944636793	43.468252321	42.742821228
6	26.586605637	41.478402209	42.112498479
1	25.540797185	41.555665416	41.838509423
7	27.333287176	40.387166690	42.029476596
6	28.583192726	40.744225139	42.485117083
1	29.392489507	40.019700320	42.531896807
6	22.075455533	39.036642691	34.828648919
1	21.005879106	38.877277565	34.642442082
1	22.188867393	40.055976585	35.236958238
7	22.627571229	38.041539046	35.729169857
1	23.465015567	37.520673483	35.446848249
6	22.241617274	37.879700043	37.006944506
7	21.158180181	38.498796259	37.482290103
1	20.535970492	39.076391814	36.906934821
1	20.865908073	38.325508501	38.453259303
7	22.963590580	37.074586270	37.797665610
1	23.962074790	36.946100896	37.588984778
1	22.780393549	37.067119780	38.810652975
26	26.533375846	38.254646471	41.820052244
8	25.726410455	36.729962449	42.068908477
8	27.930659995	36.520373873	39.326218118
6	28.677802087	37.030243434	40.160974908
8	28.273275625	37.779480359	41.149078507
6	30.187186372	36.855939232	40.035348208
6	30.957756730	36.391146598	41.274930784
6	32.465541931	36.250489586	40.977703057
8	33.040910887	35.198281128	41.364846577
8	33.024229426	37.190741994	40.359510310
1	30.581187690	35.427813331	41.649529866
1	30.830434524	37.129328116	42.087012334
1	30.613847468	37.822099512	39.713754345
1	30.346327815	36.149332492	39.212296147

8	25.690354762	34.745553819	46.158062109	1	23.418840296	38.045876997	32.353111959
6	24.629348737	35.302386072	46.029512414	1	22.587014852	38.222657886	33.890226418
7	24.042531925	35.452790254	44.732874407	7	23.875623552	36.533413536	35.209018917
6	24.798124735	34.938113229	43.623723137	1	24.657888044	36.199305213	35.789227448
6	22.810585948	36.037198791	44.536556738	1	23.068364061	36.934008577	35.706648598
7	22.335007681	36.154889107	43.313129213	26	26.587135190	39.617034841	38.877778966
6	22.091215124	36.503014472	45.676149199	8	25.684050467	38.283552265	39.001118287
6	22.645379599	36.396573697	46.915314578	8	28.544341955	36.916391377	38.532650204
7	23.886443867	35.843589351	47.091579244	6	28.975382897	37.876556656	39.176627663
1	24.184901867	34.332868592	42.946689923	8	28.308590607	38.969503391	39.417821219
1	25.688098266	34.410029239	43.975080219	6	30.398946227	37.879006402	39.722934184
1	21.411691623	36.564181653	43.103476452	6	30.503609956	37.881582559	41.250905132
1	22.109862765	36.756110219	47.797990310	6	31.944253074	37.647723093	41.747582135
1	21.105449367	36.941501637	45.540668335	8	32.897791117	38.101533278	41.066619404
1	25.279108981	35.881631078	42.857985046	8	32.067008035	37.009811546	42.822492086
1	22.865504455	35.911577160	42.477821999	1	29.867215655	37.100901080	41.694297663
8	22.754699697	37.165982256	40.615041961	1	30.144180571	38.843747958	41.658849836
1	21.840658656	37.568758915	40.608879258	1	30.930170979	38.757371557	39.321325213
1	23.391672765	37.836834145	40.937483158	1	30.907923103	36.987856558	39.340137787
8	25.824992293	37.323765480	37.800725879	8	22.751702808	38.269821137	43.064554217
1	25.879377452	38.259695462	38.073774301	6	21.871381941	38.780926988	42.414616735
1	26.483558739	36.896767495	38.397418847	7	21.735840010	38.503247719	41.025045942
1	25.147250023	39.239954913	46.727467598	6	22.719337422	37.561297272	40.448677005
1	22.809132615	40.803244257	40.250033867	6	20.763717850	39.067972058	40.248493866
1	29.301033031	42.759152453	43.272522315	7	20.708013832	38.841306339	38.944352464
1	22.592862811	39.002629416	33.869899672	6	19.785589983	39.906720057	40.870296147
1	24.331681322	35.836112759	47.986945202	6	19.890034527	40.184908039	42.196173409

Snapshot 5

RC2

QM/MM (BS1) = -3307.735939 a.u.

QM/MM (BS2+ZPE) = -3309.615721 a.u.

6	24.041723945	41.695961846	41.500221569
7	25.181630939	41.650996126	42.262388432
1	25.338855231	42.107413356	43.176498134
6	26.101890622	40.944694970	41.594926685
1	27.102950570	40.755052645	41.972180908
7	25.605594283	40.522756692	40.435914541
6	24.314940667	40.987522687	40.355252736
1	23.690569866	40.812043294	39.481602773
6	24.974164088	40.560362112	34.962892107
1	25.570974074	41.426409105	34.630149141
1	24.816004682	39.926756411	34.080420516
6	25.806534860	39.755498831	35.963017946
8	25.812746644	40.187090075	37.176923525
8	26.470150187	38.805785258	35.535059567
6	28.547063218	43.487502530	39.294856756
7	27.648716764	43.706981271	38.282185680
1	27.417429835	44.606970772	37.841908130
6	27.086767806	42.531757708	37.965436695
1	26.325247211	42.402553981	37.206633943
7	27.577417194	41.555207382	38.717044366
6	28.497552701	42.137030136	39.560201480
1	29.046171721	41.552182779	40.294426520
6	25.813986760	36.977140846	32.165911670
1	25.108974781	37.259099047	31.368702001
1	26.319905156	37.897997886	32.508817438
7	25.149391233	36.324447785	33.278413214
1	25.667677369	35.596432957	33.780153083
6	24.123799940	36.896986675	33.946994124
7	23.353755574	37.804343530	33.342845286

1	23.418840296	38.045876997	32.353111959
1	22.587014852	38.222657886	33.890226418
7	23.875623552	36.533413536	35.209018917
1	24.657888044	36.199305213	35.789227448
1	23.068364061	36.934008577	35.706648598
26	26.587135190	39.617034841	38.877778966
8	25.684050467	38.283552265	39.001118287
8	28.544341955	36.916391377	38.532650204
6	28.975382897	37.876556656	39.176627663
8	28.308590607	38.969503391	39.417821219
6	30.398946227	37.879006402	39.722934184
6	30.503609956	37.881582559	41.250905132
6	31.944253074	37.647723093	41.747582135
8	32.897791117	38.101533278	41.066619404
8	32.067008035	37.009811546	42.822492086
1	29.867215655	37.100901080	41.694297663
1	30.144180571	38.843747958	41.658849836
1	30.930170979	38.757371557	39.321325213
1	30.907923103	36.987856558	39.340137787
8	22.751702808	38.269821137	43.064554217
6	21.871381941	38.780926988	42.414616735
7	21.735840010	38.503247719	41.025045942
6	22.719337422	37.561297272	40.448677005
6	20.763717850	39.067972058	40.248493866
7	20.708013832	38.841306339	38.944352464
6	19.785589983	39.906720057	40.870296147
6	19.890034527	40.184908039	42.196173409
7	20.923693974	39.678223876	42.940155658
1	23.554821492	38.079987779	39.905134700
1	22.201596614	36.863580731	39.778370147
1	21.308398854	38.205354272	38.405624958
1	19.143563315	40.812196052	42.691931369
1	18.956250957	40.306373940	40.288071885
1	23.153216141	36.989231625	41.274705588
1	20.019279985	39.379113030	38.405379970
8	26.510792820	36.250833382	36.490252379
1	26.608572097	37.170826524	36.155314444
1	26.863619433	36.334104254	37.396118859
1	23.208836993	42.362226674	41.724849749
1	24.012870757	40.941925611	35.306973124
1	29.068758308	44.327594083	39.753275493
1	26.576543734	36.343428764	31.713160978
1	21.059730263	39.985203769	43.882084509

TS7

QM/MM (BS1) = -3307.696418 a.u.

QM/MM (BS2+ZPE) = - 3309.580645 a.u.

6	23.999011690	41.794394752	41.633831373
7	25.160901653	41.772031441	42.362207904
1	25.350617269	42.259354643	43.252664351
6	26.055135876	41.032981103	41.695125635
1	27.065156229	40.849850209	42.049992586
7	25.520392179	40.566178427	40.573799457
6	24.232590538	41.037565625	40.513913812
1	23.581355281	40.828530139	39.667872127
6	24.960759631	40.528485655	35.052084609
1	25.598216891	41.386521270	34.778302186
1	24.804588836	39.950781931	34.131009405
6	25.739073280	39.628516665	36.017401169
8	25.675136424	39.920221490	37.266785447
8	26.417825442	38.717644109	35.526278871

6	28.484729842	43.357153971	39.307702952
7	27.578215284	43.549770992	38.298001037
1	27.338099329	44.444500053	37.852995965
6	27.031249747	42.355639883	38.006391971
1	26.267108020	42.208794848	37.252503234
7	27.534214105	41.395969586	38.766573997
6	28.450591538	42.007699539	39.591281536
1	29.015121706	41.447895728	40.334210674
6	25.845833076	36.982669140	32.152977891
1	25.146191356	37.280310201	31.356554637
1	26.350697631	37.895402626	32.518094746
7	25.173985460	36.307100296	33.246879399
1	25.687515446	35.565393674	33.732737373
6	24.149835889	36.868489395	33.925753732
7	23.387242339	37.794435485	33.341620653
1	23.455825140	38.056161541	32.357153719
1	22.623619254	38.209597151	33.895467606
7	23.894178295	36.470871871	35.176264623
1	24.675256218	36.122472444	35.749977726
1	23.094089648	36.873282191	35.683164738
26	26.275563558	39.374736792	39.051150980
8	24.991148788	38.240366501	39.349976033
8	28.422832265	36.680589762	38.527019176
6	28.752166096	37.637924599	39.240751388
8	27.955105078	38.601817634	39.580040160
6	30.186229488	37.756628972	39.750775554
6	30.350497409	37.797829707	41.273509282
6	31.811306429	37.585099395	41.726192631
8	32.741865701	38.038795658	41.015219380
8	31.969481219	36.959434776	42.804755191
1	29.737995487	37.024750230	41.761065777
1	29.998295077	38.766724691	41.671352792
1	30.634867663	38.664018382	39.312008989
1	30.751061652	36.902078281	39.362876433
8	22.873566020	38.251269399	43.058894052
6	22.007681601	38.764689142	42.398072083
7	21.884811655	38.453019771	40.997160868
6	22.823404584	37.489949224	40.477338346
6	20.913880012	39.025204625	40.204566434
7	20.861633453	38.799179782	38.903635349
6	19.937452312	39.867605687	40.817955643
6	20.031782427	40.166785681	42.139700920
7	21.062741969	39.676637943	42.897044900
1	23.890922580	37.975761313	39.904966400
1	22.376514164	36.856186098	39.703378984
1	21.455731770	38.164115864	38.355215850
1	19.279164757	40.800743963	42.618476423
1	19.109380867	40.260535903	40.230029316
1	23.264463248	36.912129675	41.295436001
1	20.166085671	39.335527552	38.370000417
8	26.518143955	36.153842082	36.432388963
1	26.600425450	37.083977801	36.117156160
1	26.936772203	36.198689960	37.315470971
1	23.177288646	42.477651948	41.848303213
1	24.004182026	40.925020377	35.392359228
1	29.027293704	44.205748254	39.724331709
1	26.608245330	36.353552184	31.693623198
1	21.178139149	39.991699906	43.839059732

Dioxygen activation step reaction states cartesian coordinates for AlkB-ssDNA

RC1			
QM/MM (BS1) = -3425.036952 a.u.			
QM/MM (BS2+ZPE) = -3427.041479 a.u.			
6	28.069778968	29.955598654	39.667639263
7	28.221667068	29.211622708	38.518265786
1	27.465895238	28.738993149	38.008269947
6	29.529971338	29.214927208	38.193582999
1	29.947750500	28.697137647	37.333843217
7	30.230842093	29.920593674	39.070005845
6	29.333325273	30.386520351	40.001698297
1	29.669866742	30.970153971	40.854425111
6	33.352042106	31.589649717	43.259226271
1	33.797124830	30.671727711	43.682790065
1	34.040604283	32.412361739	43.502273905
6	33.332116328	31.437585708	41.736042170
8	32.319768442	30.850048326	41.181242270
8	34.316098875	31.830456094	41.102167018
6	31.677318972	25.932796409	40.764529988
7	31.616207805	26.657885960	41.934066970
1	31.385569140	26.305922150	42.871044781
6	31.901091769	27.938299144	41.632724848
1	31.928870400	28.755935770	42.344560113
7	32.141701801	28.076123200	40.337850953
6	32.008867923	26.830503822	39.777347798
1	32.152297575	26.672398996	38.710366012
6	36.661289752	34.960907454	41.774312925
1	36.736723969	36.005629901	41.456260206
1	36.349563738	34.939446200	42.829188109
7	35.698898532	34.264448947	40.933777541
1	35.503741725	33.272111237	41.114994343
6	34.864483924	34.846724291	40.068226742
7	34.849799467	36.185498481	39.907269210
1	35.088245974	36.755123769	40.722276693
1	34.119186168	36.588561542	39.328371753
7	34.046919923	34.086721487	39.327468204
1	34.071549589	33.067642382	39.384822419
1	33.491031781	34.492035916	38.584735470
6	33.411105055	31.235069072	36.985201650
8	33.935105374	32.023000205	36.216542374
8	32.880790223	31.511685048	38.134527553
6	33.318763493	29.716475198	36.636369626
8	32.616258702	29.027696598	37.390472099
6	34.001407378	29.187470884	35.424763397
6	34.261603582	27.683811450	35.435456979
6	34.826631082	27.161419063	34.095959631
8	34.239233784	27.559529347	33.057248325
8	35.791802753	26.362759946	34.149930757
1	33.313420247	27.146869991	35.623218264
1	34.956070377	27.422523579	36.248691061
1	34.929543902	29.755614766	35.267788549
1	33.378083178	29.457113828	34.550011888
26	32.390235352	30.016586411	39.357625073
8	34.397042827	29.458623994	39.372077174
8	35.182903491	29.633932379	38.420253364
8	28.862979400	33.338453776	37.895392508
6	28.114155958	33.602889580	38.80265685
7	28.603141258	34.004091915	40.071873927
6	30.069960049	34.016933137	40.251046993
6	27.798391305	34.338563613	41.125670637
7	28.302514604	34.787089725	42.250272559
6	26.384144480	34.165778695	40.970794580

6	25.886570104	33.795556528	39.768214690
7	26.703839834	33.545044659	38.694884127
1	30.435228413	35.044747207	40.375073292
1	30.524890311	33.565399499	39.364889941
1	29.274086499	35.120004943	42.428197265
1	24.809803788	33.709744823	39.648681122
1	25.709518715	34.396215342	41.793067782
1	30.323024780	33.430496433	41.145665387
1	27.675638704	34.997809915	43.017953302
1	27.130320972	30.009063628	40.217755150
1	32.405198891	31.755428693	43.773106196
1	31.338816367	24.899215296	40.692464751
1	37.675245120	34.572949208	41.677100599
1	26.323798831	33.212022621	37.831960227

TS1

QM/MM (BS1) = -3425.020416 a.u.

QM/MM (BS2+ZPE) = -3427.023464 a.u.

6	28.085685962	29.957627176	39.685034636
7	28.248312455	29.233723526	38.523235480
1	27.496189122	28.769313947	38.000060709
6	29.559494158	29.240015094	38.211097972
1	29.997612973	28.748019426	37.346108185
7	30.250846649	29.925180789	39.112427334
6	29.346192726	30.377642720	40.042320795
1	29.673329270	30.948609451	40.906616614
6	33.401343000	31.491073356	43.237318296
1	33.801547476	30.547878565	43.649376803
1	34.113258239	32.284427990	43.506654566
6	33.392766905	31.383790342	41.709095422
8	32.429738026	30.722066088	41.143510482
8	34.329150396	31.883054344	41.084320869
6	31.677782447	25.856983708	40.772374469
7	31.634263672	26.577107535	41.945990646
1	31.410428167	26.224706994	42.884557671
6	31.919621297	27.856785263	41.647282868
1	31.965706666	28.669808320	42.362607819
7	32.141934581	27.997552735	40.349543183
6	31.998428055	26.756483377	39.784074117
1	32.125915258	26.606658994	38.714080889
6	36.696724292	35.007264688	41.779421153
1	36.771266575	36.050678173	41.456343932
1	36.390017281	34.989507944	42.835803915
7	35.731740653	34.304928626	40.948552847
1	35.541108767	33.314634037	41.138197728
6	34.893529982	34.875170802	40.079932523
7	34.872686627	36.211709128	39.905140156
1	35.104698925	36.787721299	40.717644640
1	34.142462674	36.606520092	39.320121456
7	34.086286414	34.098755290	39.345538395
1	34.089931810	33.084061910	39.466817211
1	33.466841549	34.495809437	38.651027441
6	33.396570482	31.315584496	37.051709646
8	33.842184442	32.005811126	36.168867494
8	32.808327601	31.564875744	38.142388984
6	33.614495453	29.578637309	36.954100495
8	32.546163566	29.060863237	37.508446695
6	34.075744536	29.123473759	35.581480160
6	34.329980665	27.614668156	35.524546800
6	34.853349537	27.131649631	34.152607214
8	34.239775555	27.542522834	33.136010855

8	35.830788061	26.343235591	34.168849548
1	33.384690040	27.077952317	35.728510704
1	35.055068190	27.320244624	36.298602414
1	34.991493396	29.672023436	35.324561383
1	33.315790491	29.412564089	34.842252527
26	32.414498589	29.883983504	39.333449246
8	34.374697878	29.519585954	39.140561720
8	34.757110056	29.572929688	37.849635753
8	28.855903046	33.332660286	37.913313842
6	28.101679069	33.599635595	38.814746679
7	28.584568422	33.997992613	40.087892794
6	30.049994080	34.001480785	40.275191276
6	27.775294248	34.342410922	41.134964947
7	28.275292430	34.789889565	42.262252762
6	26.361250494	34.178931470	40.970472485
6	25.869553102	33.806874979	39.765828339
7	26.692000192	33.547610153	38.698700172
1	30.426025322	35.028723185	40.369317293
1	30.504911219	33.516514549	39.406631639
1	29.249838873	35.111487169	42.447004224
1	24.793012026	33.727269358	39.640584822
1	25.682033254	34.415856994	41.787189030
1	30.289866053	33.443140065	41.191096958
1	27.642753497	35.009869314	43.022576607
1	27.142243373	30.007182524	40.228659197
1	32.453034610	31.683229268	43.739169498
1	31.324734717	24.828526095	40.696879032
1	37.708083394	34.613833860	41.677282694
1	26.317123970	33.215144645	37.833306041

IMI

QM/MM (BS1) = -3425.120278 a.u.

QM/MM (BS2+ZPE) = -3427.118763 a.u.

6	28.017477767	29.968887739	39.673237153
7	28.174057965	29.196111994	38.543741140
1	27.423593041	28.704850771	38.045007342
6	29.482275730	29.205932761	38.217188982
1	29.906010666	28.661892945	37.376693884
7	30.176721390	29.947468708	39.066204469
6	29.277337881	30.424743390	39.989417427
1	29.612008327	31.028344022	40.829505487
6	33.381126497	31.562096807	43.261874480
1	33.857799012	30.680996340	43.726917929
1	34.057973610	32.407626042	43.461111858
6	33.359619877	31.322764003	41.745476819
8	32.274298839	30.915579472	41.191084443
8	34.428800532	31.490044038	41.134958481
6	31.735064683	25.989375003	40.732212286
7	31.663169265	26.717057756	41.899884739
1	31.406893914	26.369393511	42.831376173
6	31.993667154	27.989051794	41.604133136
1	32.005724685	28.808663113	42.314312061
7	32.280362809	28.122039577	40.317126446
6	32.121064295	26.877847125	39.755377004
1	32.281485278	26.718379646	38.691352927
6	36.635798835	34.781198897	41.874251652

1	36.643789554	35.834747534	41.579253699	6	33.357212676	31.567515571	43.259222979
1	36.349071683	34.720954639	42.934779434	1	33.841239887	30.696830266	43.736518421
7	35.697741211	34.051696600	41.033910746	1	34.024549728	32.422526112	43.448975257
1	35.559353148	33.042432732	41.180433952	6	33.353817824	31.304806838	41.745721293
6	34.820280394	34.616460368	40.195869718	8	32.294497154	30.818865667	41.197033644
7	34.689128745	35.953842737	40.116198866	8	34.417303759	31.510275072	41.144371581
1	34.913195780	36.524736114	40.933657804	6	31.772013828	25.996919991	40.703267455
1	33.984841368	36.345560761	39.499578664	7	31.693563375	26.720732881	41.873909042
7	34.089152453	33.840645658	39.391108600	1	31.431753476	26.370480917	42.802943685
1	34.191700585	32.822514065	39.372221412	6	32.030200313	27.992044185	41.586875798
1	33.338817760	34.228421375	38.831083318	1	32.038471326	28.809881374	42.298648123
6	31.769979671	33.339938087	36.584507012	7	32.327707085	28.130096459	40.302151534
8	31.833002839	32.746581522	35.589454057	6	32.169716630	26.888090505	39.733498774
8	31.698985388	33.983783675	37.553925632	1	32.342947813	26.734755549	38.670426592
6	33.489443011	29.561239157	36.674551553	6	36.634746333	34.780160112	41.869343068
8	32.704356147	28.952744954	37.406940693	1	36.641039991	35.840761475	41.602511070
6	34.103185641	29.039585523	35.408840988	1	36.344745035	34.693350986	42.927256502
6	34.409649808	27.544043573	35.428771158	7	35.699879458	34.069558607	41.009370834
6	34.960291539	27.057774672	34.069793097	1	35.541851520	33.063121483	41.153421634
8	34.324147142	27.437968363	33.052998529	6	34.849757371	34.651058850	40.153491431
8	35.970695667	26.315659419	34.090409318	7	34.748017176	35.993130126	40.075482413
1	33.478891767	26.984135614	35.632663173	1	34.949402701	36.552820143	40.906442229
1	35.131406130	27.296771850	36.221775270	1	34.057966895	36.394196670	39.448831371
1	35.006306184	29.621001732	35.179949417	7	34.119222850	33.896350570	39.331471499
1	33.398505345	29.251389029	34.587179186	1	34.169686918	32.871762708	39.305405889
26	32.315151667	30.069795512	39.313255159	1	33.379254776	34.306526185	38.772835857
8	33.246185225	31.362430812	38.103860906	6	31.166333191	33.793831278	36.744236164
8	33.876757968	30.798019751	36.949456785	8	30.728549129	33.304246076	35.788495189
8	28.810135871	33.272240865	38.025732733	8	31.609586586	34.305338696	37.692968446
6	28.042755024	33.569855748	38.907848219	6	33.504336053	29.670799814	36.673550641
7	28.503050006	33.992313864	40.179841230	8	32.793648473	28.999425150	37.471348284
6	29.963431282	33.995641277	40.404105490	6	34.049578642	29.084894356	35.387369060
6	27.677116162	34.370373124	41.201650927	6	34.370291758	27.593807782	35.437190548
7	28.161861715	34.847259713	42.324436417	6	34.915717707	27.082620004	34.084390266
6	26.265502179	34.210360439	41.013176190	8	34.294552269	27.462592690	33.058070899
6	25.794981878	33.819785099	39.805610334	8	35.912379297	26.321419174	34.116624151
7	26.636119884	33.532978867	38.759811567	1	33.449394389	27.028565802	35.669383555
1	30.329508620	35.023934174	40.519567023	1	35.103673713	27.372554552	36.227235580
1	30.442377761	33.536614040	39.537469459	1	34.934273190	29.662130837	35.088270893
1	29.138817957	35.155889410	42.519806044	1	33.300318845	29.274916742	34.601665085
1	24.720542678	33.747085908	39.661168600	26	32.314535477	30.085293118	39.260689041
1	25.570930803	34.463899901	41.811830693	8	33.120153392	31.425990471	38.413717443
1	30.184978491	33.422119128	41.315115584	8	33.818759659	30.895303532	36.863257002
1	27.516140570	35.101000971	43.062758687	8	28.806169127	33.289533022	38.142042791
1	27.082432262	30.013674561	40.231584150	6	28.018283047	33.587830418	39.007169471
1	32.436649705	31.734176326	43.778032932	7	28.453918465	34.007634789	40.285966484
1	31.390772587	24.957585187	40.661926864	6	29.910700605	34.002830219	40.542278676
1	37.667512872	34.454640860	41.743893224	6	27.606907454	34.410984748	41.281292892
1	26.279507564	33.200773408	37.886633646	7	28.068836430	34.909607424	42.404174555

TS2

QM/MM (BS1) = -3425.105649 a.u.

QM/MM (BS2+ZPE) = -3427.116983 a.u.

6	28.028933925	29.971653924	39.671382445	1	29.047154213	35.208734606	42.613438550
7	28.190129475	29.216515751	38.530236712	1	24.682926605	33.774675152	39.684108089
1	27.441238155	28.726152679	38.026688919	1	25.487478185	34.510336146	41.843734900
6	29.495659205	29.237984361	38.201276003	1	30.091694248	33.538581558	41.520794890
1	29.924697163	28.711214884	37.352657706	1	27.404885636	35.186634328	43.117412097
7	30.184640538	29.970224790	39.065841464	1	27.090566082	30.010466768	40.224579224
6	29.284527659	30.428161409	39.999058264	1	32.411673735	31.734895171	43.774982130
1	29.617078761	31.021265985	40.847208175	1	31.426092883	24.965827107	40.630786465

1	37.668072594	34.460198962	41.735443761
1	26.280953937	33.221363314	37.941572711

IM2

QM/MM (BS1) = -3425.110527 a.u.
QM/MM (BS2+ZPE) = -3427.123113 a.u.

6	28.042722675	29.955511864	39.676054530
7	28.199973241	29.204414827	38.532449239
1	27.447327403	28.726927622	38.022070620
6	29.506868931	29.208919888	38.210028680
1	29.930569576	28.686669833	37.356060760
7	30.198730829	29.925211735	39.084787830
6	29.301511587	30.393204881	40.013996668
1	29.634371977	30.983184083	40.863980919
6	33.404204864	31.523283598	43.238113305
1	33.871644978	30.642950936	43.714174245
1	34.079255437	32.369090699	43.438477433
6	33.411205668	31.274548076	41.724354603
8	32.367826066	30.740154198	41.180733757
8	34.449849165	31.529499139	41.104881485
6	31.767323143	25.967597428	40.672308665
7	31.689537516	26.689115007	41.843575972
1	31.438880006	26.336809670	42.774752413
6	32.006740335	27.964342333	41.553593010
1	32.017729547	28.777407317	42.269660804
7	32.290460188	28.108771912	40.266637327
6	32.146104989	26.865224973	39.699502051
1	32.321512579	26.711366682	38.636710593
6	36.635259968	34.827604747	41.835924535
1	36.658586652	35.885322570	41.557549774
1	36.341360105	34.755882301	42.894125466
7	35.691589245	34.123154679	40.980817260
1	35.545809687	33.115231382	41.115072973
6	34.823582471	34.710847983	40.146755402
7	34.742425609	36.053859767	40.059952415
1	34.970055283	36.610791616	40.885893366
1	34.026162200	36.457686747	39.464320786
7	34.054259617	33.963405535	39.355179110
1	34.070450536	32.940381196	39.350905565
1	33.312199658	34.380456152	38.802930781
6	31.163793961	33.884937206	36.805513440
8	30.768126899	33.329860007	35.867368380
8	31.557210770	34.475493015	37.730512154
6	33.629340425	29.781322615	36.730178417
8	33.006050040	29.106284156	37.631238566
6	34.108940010	29.096225729	35.461114148
6	34.368688817	27.595746391	35.528501347
6	34.879150125	27.055422278	34.170527897
8	34.250020575	27.435567470	33.149381216
8	35.863716898	26.277102448	34.192994260
1	33.431776094	27.063940894	35.778113657
1	35.105176407	27.352948958	36.309634558
1	35.009018217	29.623026581	35.116665602
1	33.349669937	29.303961926	34.688523085
26	32.307273662	30.140061286	39.241793185
8	32.715033377	31.656511326	38.457953311
8	33.856032455	31.010487157	36.810027306
8	28.804724610	33.258911218	38.165530731
6	28.016350011	33.576760892	39.022391413
7	28.450716524	34.005181851	40.299162434
6	29.907575533	33.996147308	40.556975166

6	27.602516886	34.422815902	41.287173501
7	28.062324115	34.926824904	42.408732268
6	26.195136739	34.269516206	41.065380811
6	25.750497508	33.863042349	39.853186163
7	26.615083369	33.551796077	38.833540489
1	30.311642855	35.016058868	40.524206966
1	30.394047061	33.392500125	39.787741262
1	29.042501094	35.219208865	42.619160612
1	24.679214226	33.796007128	39.685206577
1	25.482489414	34.539004768	41.842663449
1	30.082000329	33.564329465	41.551286771
1	27.395631527	35.219082466	43.113216822
1	27.106115595	30.000154929	40.231789619
1	32.455958875	31.698107885	43.746378327
1	31.420671705	24.936327348	40.606111041
1	37.664211701	34.491097590	41.709083728
1	26.281385323	33.227477322	37.948421593

IM3

QM/MM (BS1) = -3425.123364 a.u.
QM/MM (BS2+ZPE) = -3427.140790 a.u.

6	28.275017068	29.882160145	39.668316371
7	28.435021492	29.170442881	38.498961352
1	27.679077753	28.723743277	37.967429052
6	29.751003262	29.159773064	38.200186660
1	30.184585318	28.683564664	37.324483008
7	30.447545124	29.817617036	39.118501638
6	29.540252040	30.272363774	40.045369761
1	29.873994659	30.831184586	40.915043640
6	33.388825296	31.416719079	43.112141941
1	33.763347483	30.443214301	43.474527803
1	34.131754746	32.173439757	43.400452291
6	33.350225118	31.386690874	41.577866360
8	32.378204422	30.742021124	40.997015969
8	34.264797056	31.936271314	40.970133632
6	31.722825538	25.771306536	40.741430676
7	31.667513005	26.518992543	41.895148926
1	31.417010106	26.193431492	42.836615869
6	31.992269951	27.784875129	41.573355642
1	32.031318665	28.615927561	42.268858206
7	32.252418635	27.886177588	40.280227922
6	32.093374519	26.637702394	39.740440812
1	32.245360951	26.447174904	38.679745858
6	36.721373691	35.014519872	41.722714656
1	36.781176012	36.061104288	41.405883257
1	36.392743491	34.983783903	42.772473733
7	35.793302372	34.298809125	40.862245636
1	35.610686082	33.307387076	41.042298380
6	34.975989175	34.856459486	39.963600472
7	34.871841822	36.194780742	39.860944716
1	35.022814255	36.751500482	40.705169366
1	34.205134189	36.585684421	39.203518662
7	34.294305615	34.069847475	39.124236946
1	34.337739763	33.056597505	39.241907683
1	33.525366536	34.432955991	38.572170204
6	31.093919338	33.787135265	36.700336011
8	30.529729569	33.471387049	35.738771826
8	31.665165517	34.111007977	37.663928744
6	33.500725683	30.151705874	36.660875856
8	32.612426438	29.521699123	37.417658495
6	33.913143036	29.438050477	35.385222093

6	34.330026418	27.973721656	35.543337376	1	36.676690964	35.853773182	41.367375917
6	34.772734183	27.315453987	34.212523668	1	36.347304199	34.801336092	42.767958047
8	34.142503236	27.647380089	33.176302241	7	35.768084023	34.037773015	40.873160621
8	35.705450800	26.475541080	34.271662078	1	35.683480895	33.028528156	41.023893310
1	33.478874198	27.385849236	35.936607360	6	34.855268107	34.556945475	40.038432438
1	35.149576738	27.872227105	36.272266098	7	34.628836586	35.881270994	39.999946403
1	34.731020929	30.017860395	34.941026953	1	34.840547655	36.458204537	40.816156647
1	33.079092994	29.492792059	34.668957222	1	33.935343398	36.254887351	39.360523631
26	32.597728106	29.746739326	39.302842851	7	34.193099825	33.750645663	39.204405521
8	34.200610666	29.648999547	39.430065174	1	34.341098409	32.741992746	39.215941649
8	33.939679201	31.257915691	36.955965771	1	33.363703601	34.072210675	38.714460140
8	28.774403368	33.277302519	38.200800035	6	31.101084303	33.952784164	36.806595020
6	27.980939020	33.598203784	39.053133336	8	30.618892273	33.464108533	35.872295714
7	28.410824752	34.012808867	40.335290561	8	31.597053997	34.463284393	37.730436207
6	29.865729620	33.987098144	40.598169244	6	33.784766715	29.916332803	36.920628304
6	27.561216189	34.438311471	41.318761022	8	32.945854820	29.310421439	37.756007046
7	28.020092013	34.928086690	42.447276026	6	34.015628508	29.229244157	35.581916604
6	26.154159073	34.307816007	41.083944773	6	34.372099644	27.741466100	35.636562844
6	25.713684589	33.913134008	39.866302927	6	34.805534404	27.170607707	34.261869235
7	26.581945501	33.593886460	38.852309252	8	34.156753487	27.549588070	32.254398754
1	30.284302357	35.001051210	40.557189107	8	35.759766791	26.352898749	34.268611313
1	30.341992398	33.366675175	39.836006429	1	33.497811779	27.158043600	35.983137154
1	29.004467955	35.202379690	42.663995117	1	35.187207903	27.555630628	36.353950872
1	24.642794808	33.863042566	39.690795032	1	34.817017884	29.787341689	35.080150292
1	25.438583763	34.582725228	41.856681724	1	33.114903313	29.359891760	34.960439804
1	30.031557227	33.562853278	41.596879847	26	32.186629537	30.119323386	39.289955866
1	27.350079156	35.236839289	43.141492588	8	32.101634696	31.626173668	38.712417071
1	27.318244842	29.963976191	40.184029827	8	34.349871364	30.962254223	37.200100927
1	32.456874478	31.620067592	43.639573810	8	28.760492986	33.298961844	38.161006742
1	31.347468600	24.750322863	40.672388428	6	27.971108118	33.591715954	39.025536531
1	37.739325972	34.634857750	41.634981275	7	28.407436498	34.005208410	40.305862734
1	26.254820694	33.277070284	37.962034371	6	29.866363944	33.985966044	40.555185875

IM4

QM/MM (BS1) = -3425.131228 a.u.

QM/MM (BS2+ZPE) = -3427.147412 a.u.

6	27.926273337	29.928082622	39.667485124	1	29.005912858	35.227638151	42.612964592
7	28.088178911	29.147615471	38.545616243	1	24.635283105	33.788256142	39.698115782
1	27.335142371	28.677172896	38.030146066	1	25.441301919	34.538767808	41.852336634
6	29.401366704	29.116080994	38.247737861	1	30.037472048	33.624347003	41.576998065
1	29.826835584	28.576328048	37.405738280	1	27.358804108	35.232307320	43.116463721
7	30.089098533	29.834539489	39.120272752	1	26.991869170	29.974703038	40.226754926
6	29.188199085	30.349618065	40.016128829	1	32.461305137	31.679260746	43.707413265
1	29.515457250	30.962357381	40.851670187	1	31.392332930	24.975171932	40.543019307
6	33.401950971	31.490220148	43.190193400	1	37.705161262	34.488895535	41.634045367
1	33.869869863	30.612688792	43.670655073	1	26.236014163	33.225170808	37.957493575
1	34.085821029	32.333655455	43.370504055				
6	33.389206780	31.224438896	41.679801466				
8	32.319077009	30.702793569	41.169807692				
8	34.416419350	31.444548818	41.035091785				
6	31.713376411	26.014727980	40.608758420				
7	31.644623063	26.714642596	41.793709367				
1	31.423942037	26.340962410	42.724615176				
6	31.920426720	28.000864813	41.521756172				
1	31.931200092	28.800779742	42.250636300				
7	32.169095248	28.173110484	40.229841093				
6	32.045583760	26.936495972	39.641307392				
1	32.205489472	26.805232032	38.573092634				
6	36.668288974	34.815111047	41.714956574				

2OG rearrangement reaction state coordinates for AlkB-ssDNA

ES1

QM/MM (BS1) = -3274.903190 a.u.

QM/MM (BS2+ZPE) = -3276.725383 a.u.

6	27.983339902	29.969201568	39.678452190
7	28.130917065	29.212825708	38.536962528
1	27.375018650	28.736202417	38.031870792
6	29.438112714	29.212719608	38.209079748

1	29.849197149	28.678474190	37.356149403
7	30.141654454	29.931236159	39.070470908
6	29.247704918	30.406418225	40.000799257
1	29.590367751	30.991441957	40.850637265
6	33.323595061	31.624227259	43.269676188
1	33.830113279	30.760131427	43.734927227
1	33.983647919	32.488780961	43.442463704
6	33.267152630	31.357447560	41.760802078
8	32.179316275	30.911652379	41.245577666
8	34.312589048	31.535702499	41.108905148
6	31.727974734	25.988192493	40.762277973
7	31.647299260	26.710046586	41.933057803
1	31.388743452	26.357253035	42.862378424
6	31.970135832	27.984842792	41.646596843
1	31.972415998	28.800553138	42.361577347
7	32.260989360	28.125578201	40.360474059
6	32.113280172	26.882625787	39.791317828
1	32.284524205	26.728147480	38.728244085
6	36.621504196	34.732669618	41.899836552
1	36.630772937	35.802219422	41.679010177
1	36.334876101	34.605489291	42.953914028
7	35.675302222	34.058638897	41.021455358
1	35.484888510	33.056574026	41.160426512
6	34.867018900	34.664076277	40.144174319
7	34.853555128	36.004684124	40.007689595
1	35.098246953	36.576772536	40.819006537
1	34.144302301	36.419052469	39.411191533
7	34.071576752	33.919979080	39.365275034
1	34.091584552	32.898658311	39.386825222
1	33.531833601	34.342730588	38.620352761
6	33.522005081	31.157007908	36.987349300
8	34.024224495	31.928388779	36.184258884
8	33.022119793	31.449463271	38.136912841
6	33.458551468	29.625827288	36.672518767
8	32.854687931	28.922125816	37.484336310
6	34.117952253	29.098415978	35.447525385
6	34.321146638	27.587496470	35.412351788
6	34.906316010	27.108581355	34.066305157
8	34.301192428	27.504207665	33.036848145
8	35.908135555	26.354628915	34.104323928
1	33.348875245	27.080608209	35.552569397
1	34.984605265	27.267821330	36.230713656
1	35.069054398	29.634368241	35.304350161
1	33.514795088	29.428468887	34.578699735
26	32.261095571	30.067525230	39.371812686
8	28.875921784	33.315765619	37.872583466
6	28.131724695	33.578583606	38.784061739
7	28.626845054	33.980329586	40.050917211
6	30.094445509	33.988412266	40.225137004
6	27.827742322	34.313614102	41.109513284
7	28.339118536	34.759046791	42.232043874
6	26.412005942	34.144667571	40.960218755
6	25.908826664	33.772743221	39.760260331
7	26.721111233	33.519462013	38.683507811
1	30.455417017	35.011085866	40.394961540
1	30.545011827	33.581561096	39.315860214
1	29.311533468	35.090273474	42.405940144
1	24.831469210	33.686786960	39.644504946
1	25.741414488	34.378363124	41.784976963
1	30.357011062	33.358085892	41.086916463
1	27.720211897	34.965486763	43.007557572
1	27.051524321	30.011506696	40.242364697

1	32.385050981	31.778723631	43.801966709
1	31.384587421	24.956632181	40.684587578
1	37.655313966	34.421217273	41.750497647
1	26.336326732	33.184835838	37.823310910

TS for 2OG rearrangement

QM/MM (BS1) = -3274.893943 a.u.

QM/MM (BS2+ZPE) = -3276.718908 a.u.

6	27.926032218	29.906776549	39.703487306
7	28.092383081	29.149112873	38.566114172
1	27.343258918	28.680929837	38.043448529
6	29.407627511	29.130839568	38.269259727
1	29.837712928	28.616943735	37.413196351
7	30.097669770	29.829596788	39.158225371
6	29.186712356	30.322930783	40.061140640
1	29.513411276	30.915052877	40.911876493
6	33.236120543	31.655748183	43.288164683
1	33.736029798	30.776771861	43.731992945
1	33.893732836	32.511720869	43.508816456
6	33.250813689	31.462093975	41.767530762
8	32.160281971	31.132360006	41.152219105
8	34.346708000	31.592991328	41.213161406
6	31.719705112	26.124113045	40.714216767
7	31.656901710	26.841179730	41.888513604
1	31.419114114	26.478884480	42.819463625
6	31.964139164	28.122517710	41.595225549
1	31.981158044	28.929535092	42.319770540
7	32.224619880	28.273973758	40.305786294
6	32.074795328	27.029930577	39.739350220
1	32.218310056	26.873512010	38.671804770
6	36.666037705	34.707826858	41.902660771
1	36.663897025	35.782566022	41.709261801
1	36.369144006	34.551705969	42.950003789
7	35.739604481	34.040908168	40.998728847
1	35.526778949	33.044454110	41.147655787
6	34.966848934	34.650040808	40.094285393
7	34.942866262	35.993819956	39.983592165
1	35.139072506	36.555276605	40.815479327
1	34.273373664	36.414197342	39.347603880
7	34.214347916	33.912832356	39.266083558
1	34.284585988	32.888487636	39.208980253
1	33.713521497	34.367912492	38.512569769
6	33.855055112	31.079989292	37.116146184
8	34.270916430	31.939253947	36.352147441
8	33.729399212	31.158193043	38.397290157
6	33.367017304	29.719715398	36.577385773
8	32.431708057	29.202257186	37.194040393
6	34.040355125	29.138933519	35.379236966
6	34.228203274	27.620651018	35.402151753
6	34.826112229	27.107475184	34.070649284
8	34.254963223	27.516601097	33.027390345
8	35.801816490	26.324166647	34.134923100
1	33.250178555	27.127027924	35.547998856
1	34.888451717	27.321868716	36.231567139
1	35.002042762	29.648633351	35.228589829
1	33.436627676	29.413640483	34.493631333
26	32.167143299	30.301109810	39.298965103
8	28.875590800	33.263407325	37.916438173
6	28.125125580	33.553877342	38.815828609
7	28.613131839	33.986298663	40.074886205
6	30.080016285	34.023167797	40.248275094

6	27.808959149	34.315313454	41.131614186
7	28.312217434	34.767774136	42.254753018
6	26.394842602	34.137600499	40.976832640
6	25.897968116	33.761837507	39.775697664
7	26.716096178	33.502482843	38.704217618
1	30.405057425	35.035136316	40.518099573
1	30.535988338	33.735308196	39.298311432
1	29.282437250	35.101631126	42.436426135
1	24.821323157	33.674789527	39.654845175
1	25.719620423	34.369424426	41.798295027
1	30.376647576	33.314065706	41.035029162
1	27.685622347	34.975526335	43.023666109
1	26.987155915	29.962481155	40.254373507
1	32.288659197	31.794616740	43.808837170
1	31.408293821	25.081622461	40.648614103
1	37.703364245	34.407390560	41.755151438
1	26.334680589	33.169716408	37.841801744

ES2

QM/MM (BS1) = -3274.906024 a.u.

QM/MM (BS2+ZPE) = -3276.727311 a.u.

6	27.923549387	29.907144941	39.708879321
7	28.097440809	29.156442941	38.568408595
1	27.352671568	28.684236655	38.043188242
6	29.414087479	29.149371159	38.273933749
1	29.849424039	28.646878959	37.413741615
7	30.097871773	29.846649303	39.169251716
6	29.180913833	30.329188277	40.071879975
1	29.500217056	30.920352174	40.926112885
6	33.213997103	31.676072209	43.301050954
1	33.717823539	30.800483383	43.747090059
1	33.864389016	32.536525153	43.527174319
6	33.242788039	31.484807485	41.781293927
8	32.153656476	31.171322634	41.151106626
8	34.345900761	31.602620925	41.240952340
6	31.718438108	26.144532392	40.711673875
7	31.658956114	26.859849437	41.886938979
1	31.422368269	26.496103040	42.817618718
6	31.966138951	28.141788128	41.593913305
1	31.985665321	28.946901387	42.320663960
7	32.222382736	28.295138397	40.304004792
6	32.070323712	27.051989822	39.737034726
1	32.210284347	26.895475967	38.668993649
6	36.693352210	34.712742089	41.910224132
1	36.689369723	35.784998232	41.702868932
1	36.395453127	34.568887286	42.958879605
7	35.771045722	34.031491983	41.013347162
1	35.559088649	33.037736612	41.175504539
6	35.011768627	34.622289202	40.085759061
7	34.979891846	35.964358897	39.957658040
1	35.156343735	36.537649870	40.785945495
1	34.323752836	36.371685258	39.300025987
7	34.282650279	33.866260922	39.254194067
1	34.359024632	32.841345939	39.223577179
1	33.794575286	34.301634513	38.481122035
6	33.902369003	31.056066041	37.153125392
8	34.330278168	31.931971145	36.413373021
8	33.807904922	31.082123856	38.438378336
6	33.343770335	29.746208926	36.567686393
8	32.381218642	29.261121985	37.168125450
6	33.987056858	29.170593379	35.350097651

6	34.223583218	27.658002692	35.404563997
6	34.808445345	27.126377718	34.073977396
8	34.233275661	27.525717799	33.029434721
8	35.777593571	26.335780230	34.143192807
1	33.263864698	27.139787562	35.584772267
1	34.909453814	27.397616391	36.225939440
1	34.926590627	29.704531736	35.155740463
1	33.338974550	29.398710515	34.484915651
26	32.169267940	30.337988511	39.309138509
8	28.862577654	33.270275537	37.918139806
6	28.112659423	33.560246768	38.818387906
7	28.601767366	33.995955386	40.075822012
6	30.068942494	34.039703528	40.243898904
6	27.798774900	34.320203830	41.134957115
7	28.302366197	34.772899112	42.257906730
6	26.384900907	34.138070265	40.982498049
6	25.886811530	33.762650662	39.781744980
7	26.703790462	33.506039877	38.708762102
1	30.387067129	35.047354199	40.535907821
1	30.522073157	33.779739733	39.284536017
1	29.271615808	35.109839311	42.438713948
1	24.810174678	33.673902282	39.662208618
1	25.710452919	34.366981426	41.805412990
1	30.376135951	33.313943514	41.011357021
1	27.675934832	34.977302461	43.027836031
1	26.982134002	29.959600964	40.255736482
1	32.262538145	31.808404151	43.816105737
1	31.410983253	25.100891164	40.645705523
1	37.730552081	34.410367944	41.765816286
1	26.322259799	33.172821721	37.846571573

Substrate hydroxylation step reaction states cartesian coordinates for AlkB-ssDNA

Snapshot 1

RC2

QM/MM (BS1) = -3371.376168 a.u.

QM/MM (BS2+ZPE) = -3373.322789 a.u.

6	24.428634865	27.784285884	25.352006656
7	25.464882364	26.935186433	25.669233319
1	25.770322112	26.126901375	25.114739416
6	25.986888664	27.335373828	26.843976580
1	26.824167068	26.847491227	27.335946810
7	25.332726321	28.394620090	27.299268218
6	24.367710466	28.700352838	26.374735539
1	23.685920774	29.534780946	26.517340087
6	21.983414961	31.225851746	31.109367927
1	21.685973611	30.391751729	31.763637021
1	22.003428762	32.161623530	31.680702986
6	23.391224478	31.013519856	30.570833115
8	23.611468234	29.844084783	30.022857575
8	24.235475649	31.880423074	30.709885333
6	24.293225011	25.212480623	30.263139088
7	23.100310497	25.871276479	30.463884477
1	22.270311047	25.471407845	30.906568515
6	23.306237669	27.179963439	30.245556300
1	22.558400116	27.956289562	30.363085657
7	24.565429735	27.398130905	29.887250364

6	25.199093344	26.175387458	29.896010004	1	25.708489185	26.068969384	24.978094160
1	26.257540908	26.074824196	29.674748608	6	26.027996888	27.372287132	26.611247035
6	26.168050532	36.182217498	32.207509913	1	26.904630363	26.916850124	27.064783624
1	26.090388484	36.915545948	31.390194482	7	25.391810744	28.442527115	27.059789186
1	25.252914305	35.579613085	32.224095519	6	24.344219272	28.677286436	26.206285535
7	27.323672915	35.318430563	32.070327495	1	23.647624989	29.495863975	26.371009120
1	28.240201374	35.688565071	32.347902304	6	22.139818017	31.309110939	30.820524633
6	27.320386549	34.109252749	31.488918743	1	21.917608299	30.495679717	31.530245147
7	26.245060326	33.644328328	30.857194563	1	22.207401948	32.254706237	31.369888348
1	25.415994695	34.202323342	30.646865503	6	23.504419386	31.059008906	30.204230457
1	26.167466405	32.655404674	30.626662156	8	23.633580736	30.049721141	29.400390245
7	28.423790891	33.353246064	31.538299399	8	24.458753517	31.761281838	30.5262853625
1	29.123720297	33.480872128	32.267899562	6	24.355693417	25.399517258	26.371588319
1	28.406081477	32.433668871	31.090907266	7	23.170352524	26.083075852	30.326561055
26	25.243618407	29.283930572	29.200582187	1	22.325145611	25.703388488	30.754769099
8	25.579203785	30.722488583	28.527218981	6	23.402529931	27.382484436	30.057897237
8	27.919262480	30.867269441	30.271358253	1	22.654467621	28.166077321	30.116979220
6	27.998521934	29.675394554	29.969719971	7	24.668040950	27.571569188	29.711055100
8	26.967940420	28.880495622	29.902968939	6	25.278418114	26.341104071	29.783299865
6	29.324256969	29.063228305	29.550372497	1	26.338143483	26.211590717	29.580453551
6	29.507147871	27.559642453	29.807298471	6	26.175961123	36.408122260	32.228553710
6	30.233750060	27.263985346	31.130147559	1	26.160215512	37.185212102	31.449707148
8	29.636940767	26.616386759	32.020827176	1	25.241594548	35.842025484	32.175415456
8	31.420558445	27.701658069	31.208066247	7	27.303029784	35.511401524	32.081161595
1	30.150370627	27.145694000	29.015323291	1	28.237717745	35.851976239	32.334685996
1	28.540126281	27.039132572	29.786897603	6	27.224843999	34.251569969	31.628789455
1	30.137006648	29.637672683	30.016969107	7	26.096899475	33.787591008	31.907042846
1	29.378155847	29.293460843	28.470193232	1	25.350934305	34.389747531	30.740496295
8	26.659341018	30.116740059	23.287640349	1	25.962269957	32.794070259	30.906650579
6	25.706039571	30.869396353	23.301329889	7	28.276261311	33.437171908	31.728656738
7	25.557565278	31.860688234	24.296200660	1	29.042755051	33.604003313	32.376963025
6	26.608281425	31.940996089	25.333755332	1	28.241313245	32.521546913	31.272530487
6	24.524930403	32.767061867	24.314849268	26	25.441009094	29.566010569	28.856010316
7	24.440662233	33.672052935	25.270825204	8	25.873009249	30.993011079	27.888009970
6	23.548862739	32.70388505	23.274072615	8	28.151101160	31.031160435	30.266474227
6	23.636563444	31.722107709	22.347057682	6	28.149595074	29.854466791	29.909505151
7	24.679666000	30.827688433	22.349364757	8	27.059543658	29.155429741	29.752961964
1	26.234190999	31.585074180	26.304985125	6	29.436826332	29.154530383	29.516245994
1	26.937766744	32.983169146	25.436204836	6	29.536485166	27.647221817	29.801065372
1	24.795489671	33.550472541	26.245470026	6	30.264611566	27.326478538	31.119263737
1	22.872173347	31.612372270	21.580512813	8	29.664920543	26.670328727	32.001727126
1	22.709129376	33.396941917	23.273287120	8	31.457711795	27.745702301	31.199228759
1	27.449831083	31.316325799	25.026619127	1	30.151596265	27.186649837	29.011814158
1	23.659572674	34.333718567	25.195525572	1	28.542669914	27.178175540	29.793237247
8	28.912719310	32.124673528	27.712237529	1	30.275795367	29.691598295	29.978614367
1	29.851208562	31.808534668	27.713598647	1	29.503138464	29.356423437	28.431276801
1	28.562248948	31.789740922	28.554635061	8	26.542104884	29.970368155	23.582715319
8	24.335775349	33.199059657	27.926272216	6	25.630579297	30.767159261	23.523131025
1	24.709127811	32.402165356	28.350215001	7	25.477586645	31.787326556	24.509001908
1	24.185025425	33.856088595	28.672729849	6	26.462009457	31.827011378	25.566009137
1	23.670310045	27.565675365	24.600195357	6	24.502289792	32.767980657	24.424418868
1	21.227724132	31.311752909	30.328586476	7	24.433120081	33.728308895	25.320839455
1	24.347242504	24.124188674	30.290889201	6	23.577875025	32.709547629	23.338410805
1	26.217132468	36.751731785	33.135578744	6	23.667967356	31.708436954	22.433442068
1	24.684213220	30.106503347	21.656657107	7	24.673142155	30.772485964	22.503205865

TS7

QM/MM (BS1) = -3371.336675 a.u.

QM/MM (BS2+ZPE) = -3373.285174 a.u.

6	24.350133050	27.715431373	25.226912557	1	26.093009324	31.324011194	26.699009542
7	25.423423507	26.901576465	25.505308093	1	26.726493172	32.853063521	25.843698047
				1	24.734828929	33.643368655	26.328992309
				1	22.936263073	31.615635812	21.631949006
				1	22.770632727	33.438051136	23.278612193
				1	27.331037728	31.213609379	25.320187111
				1	23.692086282	34.423662644	25.170248336

8	28.989604054	32.233884874	27.649258372
1	29.918406929	31.891470956	27.643967012
1	28.646995695	31.929218614	28.506472793
8	24.444209917	33.363496343	27.932408200
1	24.952856528	32.601221734	28.280960289
1	24.253333159	33.990279172	28.694094534
1	23.567795003	27.475247128	24.506963930
1	21.306780027	31.360437565	30.119467856
1	24.393145709	24.313582465	30.258671271
1	26.198197299	36.918226199	33.191552590
1	24.691571874	30.058373575	21.803437090

**Snapshot 2
RC2**

QM/MM (B1) = -3369.665144 a.u.
QM/MM (B2+ZPE) = -3371.606048 a.u.

6	43.336524795	30.520830215	31.354033780
7	42.488813868	29.446448970	31.496181404
1	42.752933345	28.485431219	31.735625489
6	41.242414197	29.860319809	31.202048390
1	40.369234085	29.214547090	31.220731686
7	41.247352373	31.140714181	30.867911032
6	42.547170154	31.574498351	30.954269626
1	42.828588520	32.590139815	30.681007173
6	40.781551461	35.173614218	27.353355980
1	40.572674278	34.823956641	26.329780006
1	40.183519478	36.087719655	27.494766259
6	40.262557969	34.114044671	28.303560528
8	41.039759298	33.435263521	29.047566960
8	39.028638250	33.858825929	28.311152301
6	40.606763956	29.085236464	26.973786987
7	41.313360700	30.153236895	26.458405807
1	41.917708418	30.159997356	25.640565221
6	41.048351480	31.232381407	27.215006298
1	41.501048038	32.200046508	27.036391503
7	40.200070608	30.926712261	28.187541639
6	39.911210507	29.586398583	28.047768793
1	39.217514009	29.091547151	28.721957563
6	35.737281256	38.390099183	29.756346952
1	36.005856024	38.893451159	30.696059736
1	36.502552898	38.631288611	29.017194398
7	35.653493415	36.952688306	29.957335715
1	34.912744757	36.620899151	30.587301116
6	36.455190412	36.033806468	29.409921505
7	37.400301148	36.340833706	28.514974878
1	37.693115865	37.294638961	28.274679452
1	37.983942727	35.570040824	28.191793933
7	36.281658158	34.736139873	29.728041832
1	35.850144936	34.472180440	30.628275522
1	36.996308408	34.098021104	29.390486555
26	39.658013878	32.180923730	29.856339983
8	39.272013614	33.229943288	31.031414572
8	37.830460512	31.309191696	32.370788257
6	37.582199350	30.751782275	31.309092989
8	38.306626563	30.894984931	30.212369817
6	36.451935649	29.743346623	31.203707430
6	35.743153774	29.590423664	29.867601452
6	34.843159706	28.339551244	29.805060808
8	34.290300992	28.135146419	28.693619502
8	34.743563510	27.628696576	30.832551154
1	36.466990382	29.511961103	29.040242163

1	35.121689267	30.470144057	29.626492660
1	35.743271230	29.950915076	32.017243122
1	36.878306766	28.759859069	31.462249675
8	41.815923540	31.355717611	35.117960366
6	42.257515498	32.407286469	34.706895183
7	41.398180150	33.431788763	34.254101272
6	39.951634738	33.153903851	34.369201753
6	41.841989642	34.603648029	33.697565623
7	40.998606570	35.502118056	33.230106237
6	43.259678209	34.826737997	33.637523389
6	44.101566128	33.878368085	34.112780043
7	43.626171227	32.703194825	34.645558640
1	39.811885392	32.432179491	35.179498008
1	39.553411781	32.734340277	33.432199378
1	41.394725512	36.407456116	32.933513169
1	45.184686953	34.009414136	34.064363595
1	43.639533693	35.745019012	33.192036358
1	39.424121942	34.084559867	34.609629753
1	39.970928281	35.387929025	33.139679783
8	38.285026320	35.427691790	32.430095649
1	37.384341157	35.220312756	32.742045045
1	38.472849286	34.705161302	31.795071218
8	35.457096365	34.086915087	32.343923378
1	35.623691147	33.292472925	32.919206026
1	34.503782143	34.246338486	32.492769984
1	44.422465245	30.448199664	31.413409441
1	41.843508862	35.409878789	27.420384740
1	40.726153318	28.070269352	26.594768159
1	34.805686024	38.825714968	29.395186967
1	44.275857646	32.006479657	34.949644181

TS7

QM/MM (BS1) = -3369.626225 a.u.
QM/MM (BS2+ZPE) = -3371.567654 a.u.

6	43.440532080	30.457823943	31.398793629
7	42.596520044	29.382737458	31.548569026
1	42.860172861	28.415371543	31.759342319
6	41.343035468	29.801479209	31.296547223
1	40.471786271	29.153551945	31.328760380
7	41.338430536	31.085768707	30.980393789
6	42.641214550	31.516481067	31.035009284
1	42.918247418	32.534598392	30.764579215
6	40.782574953	35.152604569	27.444010943
1	40.565916225	34.789938334	26.425689646
1	40.193296631	36.073681630	27.572777225
6	40.248725381	34.112907882	28.413395807
8	41.035292020	33.387766883	29.109932605
8	39.009988181	33.925311160	28.471394544
6	40.593458122	29.080625298	27.057557264
7	41.286667253	30.157060021	26.542961198
1	41.870852583	30.176559742	25.711157043
6	41.039220082	31.224374431	27.320868376
1	41.487114293	32.195413710	27.151387127
7	40.214773967	30.902005896	28.309266171
6	39.922438134	29.563417187	28.156102653
1	39.243699329	29.057781346	28.837747102
6	35.721953631	38.398747701	29.761175800
1	35.987475174	38.898369597	30.703606888

1	36.491042933	38.641956565	29.026516464	7	37.196252692	38.605411028	34.491996699
7	35.633571342	36.960870746	29.954458224	6	37.496275417	39.759452420	35.179349806
1	34.884773649	36.625632170	30.572874601	1	36.817911999	40.607758169	35.199093325
6	36.439801773	36.045346564	29.407498831	6	33.967330723	42.121818180	32.359880231
7	37.389890432	36.357782448	28.520546574	1	34.347072445	42.070511720	31.330734460
1	37.680644924	37.313218745	28.285822814	1	32.878908681	42.284222217	32.351758667
1	38.000622743	35.592593845	28.232887012	6	34.245499676	40.813103977	33.081175190
7	36.266866537	34.745784525	29.718051458	8	35.249725358	40.151810553	32.580473557
1	35.833634976	34.473768649	30.614747725	8	33.548735093	40.451787985	34.020135103
1	36.975332848	34.108371706	29.365479676	6	39.197837881	38.813010671	30.361061951
26	39.744433603	32.119207661	29.987458628	7	38.770348925	40.123749225	30.434410792
8	39.451216679	33.269213658	31.252420011	1	39.219885490	40.944570233	30.025034520
8	37.776817148	31.714157580	32.491802130	6	37.631891719	40.138653084	31.154058634
6	37.570978930	30.757013314	31.419677408	1	37.059299657	41.029391086	31.387501150
8	38.337575425	30.901165509	30.354512647	7	37.311814547	38.912887484	31.544516581
6	36.440292527	29.752340810	31.272418047	6	38.280774740	38.072043812	31.054416452
6	35.774639995	29.594188209	29.914141622	1	38.241468830	37.003102007	31.236642258
6	34.869858624	28.346502913	29.828335680	6	28.445085068	38.731952025	32.265216930
8	34.320356428	28.158895449	28.712119983	1	27.972223655	38.943657104	33.238917102
8	34.765105379	27.619188430	30.843904774	1	28.786648164	39.684890684	31.837388623
1	36.525613410	29.506440736	29.111739507	7	29.552598111	37.793623198	32.380644871
1	35.166902647	30.475454478	29.645703826	1	29.347508917	36.809424949	32.200495769
1	35.705287427	29.966293871	32.060644028	6	30.788635205	38.113635530	32.798864928
1	36.851795552	28.767320473	31.547507358	7	31.069384506	39.357023055	33.205259471
8	41.757619045	31.293440482	34.710647118	1	30.403224657	40.139896900	33.170554974
6	42.218562221	32.378412066	34.432544228	1	32.024022586	39.610658218	33.484543882
7	41.387522997	33.420705331	33.927847761	7	31.759152371	37.195864271	32.781027950
6	40.000664391	33.106590806	33.733940860	1	31.544044766	36.206964657	32.641391489
6	41.866101556	34.663707451	33.566704651	1	32.676580829	37.400848958	33.190558398
7	41.050138617	35.592460328	33.113371297	26	35.797773036	38.357119841	32.928428892
6	43.272832365	34.903329985	33.687609307	8	34.490579091	37.911059277	33.786107613
6	44.074774842	33.930854985	34.183347708	8	34.354839967	35.454753972	32.495014775
7	43.569867726	32.713027700	34.577246868	6	35.546610205	35.530445756	32.218232282
1	39.749478334	32.118075762	34.116482654	8	36.265333230	36.619732638	32.322435199
1	39.704768767	33.029747311	32.391708179	6	36.332184827	34.359123753	31.659133166
1	41.456401962	36.522596841	32.923470348	6	35.636373764	33.020814101	31.808762711
1	45.152327462	34.079686637	34.270361360	6	36.087802921	31.962639422	30.792306801
1	43.681060994	35.860189165	33.366937620	8	36.615867347	32.354503171	29.731737855
1	39.327536044	33.912838595	34.047344530	8	35.822492229	30.757708208	31.089553472
1	40.030675276	35.484815436	32.956077599	1	34.553065891	33.167436617	31.659598371
8	38.309285789	35.542389275	32.302556830	1	35.744959443	32.625688038	32.8278755076
1	37.423854737	35.315484469	32.642208750	1	37.338703980	34.36331294	32.107481421
1	38.511075696	34.805980855	31.683721085	1	36.506436916	34.543243526	30.585099294
8	35.430537562	34.093802302	32.325616015	8	36.751541901	36.523673245	39.170070459
1	35.583846905	33.312946290	32.920409560	6	36.201204134	37.585002026	38.961758686
1	34.475128238	34.256019111	32.458797969	7	34.977099643	37.647452879	38.263704668
1	44.527820826	30.387242228	31.428605205	6	34.427503216	36.367948563	37.785005568
1	41.846645259	35.383428949	27.494427342	6	34.313523882	38.818819698	37.978688616
1	40.708328120	28.075204422	26.652586817	7	33.193711479	38.789436729	37.296455780
1	34.792479067	38.835679730	29.396162426	6	34.890513428	40.045265958	38.450573030
1	44.205932662	32.010880707	34.897221073	6	36.065995743	40.009310904	39.124885659

Snapshot 3

RC2

QM/MM (BS1) = -3446.808270 a.u.

QM/MM (BS2+ZPE) = -3448.819020 a.u.

6	38.731158862	39.615048522	35.771533460	1	36.713495411	38.821004613	39.368575719
7	39.157576076	38.353465221	35.425596676	1	33.351752434	36.319324174	37.992728456
1	40.052357160	37.911441110	35.660772428	1	34.950918768	35.559411235	38.302028266
6	38.217381380	37.777040275	34.662437716	1	32.677879874	39.653273624	37.083311821
1	38.303622365	36.780397640	34.236708920	1	36.541390967	40.929080569	39.475926547
				1	34.395196607	40.994713889	38.253773344
				1	34.569736954	36.267398985	36.697834199
				1	32.762034847	37.941710938	36.856304592
				8	31.191282279	40.319638445	36.129406751
				1	30.248210352	40.649848779	36.121048910
				1	31.164643698	39.599827680	35.478311530

8	31.852308458	36.819341275	35.967747441
1	30.874181793	36.775839656	35.829930683
1	32.227728728	35.993448665	35.588052271
8	33.073533606	34.628354711	34.770702037
1	33.447923764	33.748216813	35.044519274
1	33.666840613	34.941132904	34.055082292
1	39.380008419	40.340446404	36.262307834
1	34.457446267	42.959690082	32.855687399
1	40.161084823	38.494874542	29.962298800
1	27.683422277	38.327107738	31.598855004
1	37.594642969	38.834924896	39.841183068

TS7

QM/MM (BS1) = -3446.767386 a.u.

QM/MM (BS2+ZPE) = -3448.776399 a.u.

6	38.891593482	39.688946865	35.933965977
7	39.314240778	38.420426828	35.614860740
1	40.224376735	37.990321805	35.802207510
6	38.339950283	37.799672139	34.936067773
1	38.413212915	36.785186498	34.552503201
7	37.298640579	38.607051462	34.790219078
6	37.623925987	39.794070889	35.407510329
1	36.939772116	40.637833476	35.425056302
6	33.957480517	41.972645346	32.503161644
1	34.341196730	41.868897268	31.478068445
1	32.871808281	42.153533434	32.475065465
6	34.199299433	40.688984940	33.293213990
8	35.215458687	40.001358952	32.870469335
8	33.450510218	40.376708481	34.213085432
6	39.122062170	38.721901695	30.548868904
7	38.636161730	40.012147193	30.593286429
1	39.031882181	40.831327376	30.133529133
6	37.534551352	40.007915993	31.369944801
1	36.930993378	40.880157741	31.593658372
7	37.294327498	38.786642996	31.828633963
6	38.279745941	37.970842854	31.324602327
1	38.305823674	36.911131244	31.557892652
6	28.439416241	38.733844913	32.244081633
1	27.967588756	38.935473045	33.220658127
1	28.762021070	39.693995137	31.816705805
7	29.564943213	37.815989838	32.354109056
1	29.385183146	36.832627122	32.145485413
6	30.762630557	38.149046225	32.864782098
7	30.973870500	39.373795857	33.354434929
1	30.296009361	40.143510254	33.281173101
1	31.905786810	39.648899435	33.692887665
7	31.764283331	37.261606426	32.857812633
1	31.586427763	36.278607901	32.644716765
1	32.619873327	37.450679177	33.386323103
26	35.870114651	38.243183603	33.285650306
8	34.573904013	37.773525004	34.326984130
8	34.390124580	35.572257764	32.401323266
6	35.618512275	35.524882303	32.357253734
8	36.402535741	36.475409147	32.792096354
6	36.354215921	34.352127839	31.738093275
6	35.559610396	33.059697473	31.776105897
6	36.049765094	31.992382322	30.788974868
8	36.608237569	32.380115376	29.743169682
8	35.783097231	30.787631568	31.087858200
1	34.512901195	33.287382965	31.510285846
1	35.531411435	32.646065495	32.793599773

1	37.343473994	34.249835061	32.208887525
1	36.558907528	34.602946239	30.682304922
8	37.211822002	36.880272892	38.109335277
6	36.482486697	37.837037582	38.265977516
7	35.229235779	37.911048270	37.597890641
6	34.909976562	36.849357320	36.691571868
6	34.359956836	38.982483336	37.724223475
7	33.181554034	38.926800226	37.155259924
6	34.816653805	40.120888371	38.461973333
6	35.998477563	40.056041753	39.125465452
7	36.779356081	38.924217455	39.091531575
1	33.899694780	36.445677498	36.819584617
1	35.704624114	36.103606672	36.666368923
1	32.540894697	39.729312373	37.161585253
1	36.370479268	40.915807655	39.686658200
1	34.211119935	41.024738459	38.501881632
1	34.801556568	37.349536450	35.383116512
1	32.799026692	38.103935325	36.636805271
8	30.882236955	40.182452932	36.315388948
1	29.981278721	40.603647832	36.192853225
1	30.842501306	39.435764280	35.695673123
8	31.845651816	36.860795084	35.909501325
1	30.862190398	36.823180313	35.811821327
1	32.197983511	36.040225541	35.497615747
8	33.079099577	34.695229492	34.680631534
1	33.445212132	33.812332421	34.956514457
1	33.666205410	35.014141405	33.962179564
1	39.556486867	40.438978366	36.362261267
1	34.454897606	42.829260220	32.957974260
1	40.069069578	38.440246808	30.088526841
1	27.680140717	38.318312849	31.581585516
1	37.629002660	38.898771173	39.618243715

Snapshot 4

RC2

QM/MM (BS1) = -3370.511712 a.u.

QM/MM (BS2+ZPE) = -3372.448429 a.u.

6	36.513129844	33.978991689	42.373119936
7	37.239677146	33.769299028	41.224526323
1	38.256358709	33.689311040	41.127223179
6	36.397099752	33.749850531	40.182499690
1	36.696984610	33.610757482	39.147278398
7	35.154462209	33.945158990	40.600066848
6	35.202465517	34.087953290	41.965959954
1	34.306739724	34.266235180	42.554515473
6	30.573235193	36.355770982	41.476410058
1	30.811665576	37.245542076	40.877557766
1	29.512529677	36.102092543	41.329856134
6	31.416469128	35.172234055	41.018672283
8	32.501387694	35.536571808	40.384233858
8	31.063578511	34.016204020	41.211948923
6	36.160160983	38.005167651	38.632506158
7	35.286401141	38.488297467	39.586732363
1	35.307615095	39.405222032	40.036535671
6	34.367578539	37.531144636	39.823309255
1	33.546199525	37.628576333	40.526391648
7	34.609531628	36.456805297	39.080029135
6	35.728927124	36.740541507	38.332212642
1	36.152110487	36.012329444	37.647716018
6	26.681996493	33.053241172	37.553514837

1	26.348737828	32.157218479	38.106895373	7	35.217310246	33.904050395	40.672350624
1	26.517331874	33.926845356	38.198473533	6	35.271318701	34.112225354	42.029484740
7	28.077724110	32.948319887	37.156510608	1	34.381060129	34.335011527	42.609990611
1	28.271917830	32.466524015	36.277546371	6	30.596970963	36.302632855	41.474206771
6	29.118880786	33.042538430	38.010928195	1	30.837053717	37.180748444	40.858774794
7	28.946402563	33.550022243	39.238139941	1	29.535530007	36.049096029	41.3322861188
1	28.083750290	34.013918197	39.543361583	6	31.437786499	35.108287022	41.039200005
1	29.730926584	33.580921770	39.892049919	8	32.522765470	35.436012790	40.408168735
7	30.324373156	32.621887053	37.636981673	8	31.059172830	33.957622390	41.261712889
1	30.521790418	32.145152264	36.733345384	6	36.149799713	37.949029300	38.639654242
1	31.140272815	32.860358049	38.206282126	7	35.255432942	38.429822296	39.573727293
26	33.650149606	34.548125170	39.245968505	1	35.253403855	39.354342370	40.006456617
8	32.778363157	33.175398073	39.196957325	6	34.356434013	37.456431227	39.822290340
8	32.992071997	34.374558853	36.424116949	1	33.526114840	37.551756460	40.514583015
6	34.190601659	34.121205286	36.565034834	7	34.632813675	36.372754651	39.104646381
8	34.769685249	34.099736782	37.727309102	6	35.754147712	36.667032569	38.363136792
6	35.109902648	33.882639984	35.380162936	1	36.205840616	35.934252305	37.702575781
6	34.685138097	32.694782446	34.483921978	6	26.705090693	33.054916383	37.549215505
6	34.895481402	33.106681952	33.020336386	1	26.366795637	32.162135530	38.104898755
8	33.955329110	33.747696367	32.480344267	1	26.537453749	33.931878938	38.88249268
8	36.015451627	32.870490180	32.502948534	7	28.105350845	32.943869374	37.165334067
1	33.627255102	32.461949188	34.657995771	1	28.303912781	32.447685898	36.295166889
1	35.293932222	31.811909316	34.724666495	6	29.131450857	33.019915669	38.040977276
1	36.147188266	33.771843471	35.723037799	7	28.938239391	33.534549487	39.261856411
1	35.059048910	34.814294314	34.792563063	1	28.074455191	34.008869015	39.546069595
8	35.796981620	29.351046350	41.914331934	1	29.706314767	33.560125840	39.932740956
6	35.008271633	29.869508300	42.670878639	7	30.338463405	32.579229641	37.694382159
7	33.690713376	30.182290668	42.257583339	1	30.545489091	32.106913614	36.790034820
6	33.357049192	29.908896201	40.848565716	1	31.144683486	32.767252662	38.296100121
6	32.741660724	30.718982446	43.085361403	26	33.726604627	34.477107662	39.278812404
7	31.540391517	30.987434360	42.606010605	8	32.879664838	32.969378368	39.282791494
6	33.098246951	30.983275673	44.443061834	8	33.070662740	34.347703652	36.563723401
6	34.373787106	30.743800139	44.846131070	6	34.271022186	34.069212399	36.651272909
7	35.311338788	30.219980317	43.992162558	8	34.879425360	34.000693311	37.796186559
1	33.218404260	30.857156494	40.301654346	6	35.146246044	33.858239150	35.429828089
1	32.444908791	29.297514192	40.794358423	6	34.707042601	32.679776916	34.529237019
1	31.343558859	30.944316982	41.612618356	6	34.904391186	33.102885894	33.065432633
1	34.693810714	30.985321922	45.860098223	8	33.957595518	33.743028013	32.535337727
1	32.368778960	31.423018490	45.121369111	8	36.020891167	32.873193058	32.537707277
1	34.185169691	29.347179033	40.408542943	1	33.650603799	32.447407529	34.712964438
1	30.753059243	31.286840318	43.198100197	1	35.317368530	31.794537765	34.758159245
8	30.986702730	31.359339316	35.254144274	1	36.196374328	33.750559052	35.732717716
1	31.715125665	30.686216182	35.196624496	1	35.064314319	34.798128992	34.859246694
1	31.244481712	32.095391462	34.649016458	8	35.944780159	30.534576171	41.591047710
8	31.628173043	33.716466692	33.986498174	6	35.096396721	30.636263056	42.447688509
1	32.010602011	34.083352496	34.810428833	7	33.743882629	30.927971395	42.100045631
1	32.385418410	33.747380544	33.344369147	6	33.423954257	30.936902426	40.702568814
1	36.982302261	34.162062580	43.339778928	6	32.755199655	31.145058747	43.039213479
1	30.745688974	36.610652861	42.522049692	7	31.564730829	31.541373829	42.630158381
1	37.071540860	38.509308339	38.311108879	6	33.074374808	30.934365656	44.412677545
1	26.028381050	33.172577918	36.689447179	6	34.350163041	30.622574183	44.761118634
1	36.267805356	30.168758426	44.279426407	7	35.333645996	30.455101992	43.816508965

TS7

QM/MM (BS1) = -3370.472795 a.u.

QM/MM (BS2+ZPE) = -3372.413181 a.u.

6	36.578788246	34.000734053	42.444048669	1	32.455084923	30.458752458	40.509482048
7	37.301280956	33.729012738	41.307971310	1	31.448981688	32.089116643	41.769953039
1	38.315684839	33.636280865	41.207635980	1	34.635909574	30.549937408	45.811773285
6	36.457569715	33.669620244	40.268456877	1	32.316059259	31.121279575	45.171061385
1	36.757095219	33.473944409	39.242627279	1	34.252766687	30.544712524	40.112151988
				1	30.753621944	31.555015632	43.265450263
				8	30.996628005	31.349879627	35.295559056
				1	31.722330831	30.674232254	35.226389504
				1	31.259602205	32.096075630	34.705717552

8	31.657380420	33.725443400	34.074716107
1	32.040320388	34.083186631	34.900968558
1	32.412946046	33.755346069	33.429060431
1	37.046630672	34.213950483	43.405157158
1	30.768682217	36.577532181	42.514885844
1	37.045692255	38.475384971	38.310422425
1	26.053008482	33.171557924	36.683622720
1	36.281398184	30.337877177	44.113151221

IM10

QM/MM (BS1) = -3370.497094 a.u.

QM/MM (BS+ZPE) = -3372.433476 a.u.

6	36.523982041	34.030838168	42.293123306
7	37.254117912	33.771476572	41.158490538
1	38.263221762	33.617273713	41.080391760
6	36.431157499	33.816444149	40.101364117
1	36.735981047	33.648550342	39.072161116
7	35.199219629	34.107033453	40.493392186
6	35.234934912	34.240812494	41.859934445
1	34.345195829	34.481176109	42.433699242
6	30.584517337	36.259747558	41.524416738
1	30.726876992	37.159521070	40.910478766
1	29.545379345	35.918468424	41.413669624
6	31.517266223	35.169190889	41.028183450
8	32.536227427	35.603132548	40.371140282
8	31.253047737	33.967481396	41.212941485
6	36.191204203	38.097061624	38.552211003
7	35.315064530	38.581002595	39.504277727
1	35.350524792	39.488672120	39.972372136
6	34.371348784	37.642685574	39.709304599
1	33.547790470	37.740350999	40.409941738
7	34.598149967	36.580647363	38.942187029
6	35.734010528	36.851977647	38.214162554
1	36.152682316	36.123404061	37.527352711
6	26.702596607	33.055917200	37.493118097
1	26.409148941	32.132143997	38.023100245
1	26.517460448	33.904713682	38.164355296
7	28.090838286	33.013107412	37.062457834
1	28.282280840	32.567054521	36.164737503
6	29.156403152	33.145462056	37.880719164
7	29.003354931	33.681171754	39.103311399
1	28.134420763	34.115009588	39.433213625
1	29.773380495	33.655503853	39.766275536
7	30.355326067	32.748340026	37.475703064
1	30.519027197	32.201244640	36.605337932
1	31.204271776	33.006194732	38.001306096
26	33.710163333	34.726921012	39.107014640
8	32.694073254	33.235216153	39.043052202
8	33.098984571	34.482284365	36.345887274
6	34.281932598	34.163563453	36.502594909
8	34.845235430	34.127431532	37.669004507
6	35.197281147	33.863969627	35.329367233
6	34.732172678	32.679246533	34.448623136
6	34.922115444	33.086742204	32.981841059
8	33.972871214	33.720021366	32.449130038
8	36.040221308	32.861637743	32.454001110
1	33.674624165	32.462529939	34.645271831
1	35.334372869	31.789533998	34.682007543
1	36.226592667	33.715317975	35.681981873
1	35.188153516	34.787331173	34.725928355
8	35.900884864	30.442978928	41.789318016

6	35.080794899	30.530964605	42.672641720
7	33.705255061	30.809141617	42.349176195
6	33.396839072	30.831709678	41.001724863
6	32.739762645	31.050472759	43.316877555
7	31.543234744	31.470367905	42.932785944
6	33.095684670	30.839675975	44.675143180
6	34.378225649	30.520478090	44.997064360
7	35.342821125	30.359580340	44.030259828
1	32.228192377	33.219519396	39.904092247
1	32.353272215	30.787412499	40.707580223
1	31.412382482	32.009956674	42.075638188
1	34.682188961	30.445122572	46.040126720
1	32.359224364	31.035360282	45.452693041
1	34.217355564	30.754785906	40.297622317
1	30.727681474	31.448050638	43.561406901
8	30.987281153	31.349744592	35.178783407
1	31.718499964	30.677638520	35.154095674
1	31.269294171	32.089156172	34.589162987
8	31.661727643	33.725590602	33.965934600
1	32.054758391	34.109464404	34.777364892
1	32.415460321	33.742857184	33.318930888
1	36.984057526	34.179338216	43.270029446
1	30.765624737	36.547285679	42.560075591
1	37.121961011	38.583131597	38.259815617
1	26.031958568	33.179335924	36.642777127
1	36.301071322	30.250650685	44.294576656

TS8

QM/MM (BS1) = -3370.487244 a.u.

QM/MM (BS2+ZPE) = -3372.420750 a.u.

6	36.653754237	34.040814525	42.473578267
7	37.381586154	33.802450644	41.332653243
1	38.392729030	33.682545853	41.235591610
6	36.548664101	33.823309658	40.282453895
1	36.850592324	33.657033218	39.251838218
7	35.315170259	34.080636208	40.686105067
6	35.356116000	34.212052864	42.050214248
1	34.465185082	34.431684696	42.630285939
6	30.588356306	36.316894827	41.515039426
1	30.789165631	37.210417693	40.907180817
1	29.532897768	36.033730505	41.392415336
6	31.460679797	35.175593600	41.025089594
8	32.562404223	35.527985695	40.475627796
8	31.071120451	33.994010665	41.128333420
6	36.191701307	38.014588525	38.593209000
7	35.308600481	38.499852576	39.537794422
1	35.326170410	39.417969182	39.984471160
6	34.390141752	37.542388891	39.771279997
1	33.567492157	37.635912709	40.473410496
7	34.640948024	36.466162812	39.032905366
6	35.766090210	36.747448593	38.293252539
1	36.196988862	36.012559832	37.620101401
6	26.716383473	33.034353143	37.498757591
1	26.397074180	32.123091367	38.035061424
1	26.531983612	33.893792247	38.156334540
7	28.117192260	32.958186693	37.109275738
1	28.325392175	32.479440829	36.231805364
6	29.143985532	33.060758955	37.980124433
7	28.944022732	33.592800329	39.191384755
1	28.073625245	34.061008558	39.466058117
1	29.700951365	33.632885923	39.874976968

7	30.354068006	32.624610977	37.633071704	8	31.004153477	33.871055416	41.028177936
1	30.555173755	32.123337260	36.740713987	6	36.255938106	38.023907982	38.672778234
1	31.168195488	32.838865394	38.209444309	7	35.386487641	38.516784947	39.624116815
26	33.793352362	34.548801035	39.306156664	1	35.391793659	39.448258642	40.041263880
8	32.962560507	32.872101778	39.576219543	6	34.498283145	37.537247039	39.907518792
8	33.041190065	34.246575240	36.568003704	1	33.690176425	37.639906214	40.626611294
6	34.251185839	34.003591705	36.659495196	7	34.756187086	36.447094116	39.200677007
8	34.877673344	33.995576924	37.793005087	6	35.852477597	36.735991170	38.425592265
6	35.124162636	33.795131308	35.432339151	1	36.283250638	35.994970922	37.756408147
6	34.682300501	32.634028384	34.512860877	6	26.657029228	32.968631906	37.473096088
6	34.887075760	33.078263324	33.056985070	1	26.349690485	32.039957325	37.984050087
8	33.943401852	33.726774514	32.530752692	1	26.487804064	33.804737357	38.161653851
8	36.006697437	32.858001163	32.531264634	7	28.045238082	32.903168781	37.046988062
1	33.624368043	32.405013267	34.690870166	1	28.237803514	32.387889054	36.186336894
1	35.288325828	31.742530416	34.730167430	6	29.116860181	33.202392304	37.802524515
1	36.173391335	33.680814237	35.735182999	7	28.993471149	33.914723228	38.928962609
1	35.049463436	34.743918069	34.874474087	1	28.097622111	34.277424104	39.273783606
8	35.925106270	30.611125835	41.555674486	1	29.734779957	33.863029924	39.630790555
6	35.084254739	30.657342276	42.421806005	7	30.325188893	32.780876754	37.419584335
7	33.695672613	30.868214420	42.071173107	1	30.480386542	32.151768377	36.602822403
6	33.399461727	30.891271461	40.715167482	1	31.161802820	33.284477755	37.711587268
6	32.702982551	31.017102090	43.031649843	26	34.028024295	34.401750165	39.548470425
7	31.466999639	31.291123103	42.636672923	8	33.005141061	32.448361070	40.316049607
6	33.059308803	30.868183727	44.397253113	8	32.950138859	33.967206261	36.688534226
6	34.350960183	30.614833542	44.740300060	6	34.183208111	33.820564535	36.759425536
7	35.330255171	30.479217229	43.782692782	8	34.826469238	33.761733990	37.873402013
1	32.247182024	33.125316971	40.204250526	6	35.028195617	33.758778239	35.496667266
1	32.394039183	30.604042538	40.421346503	6	34.682366018	32.586758314	34.551389505
1	31.286663039	31.741175918	41.743510475	6	34.908228446	33.046021612	33.103153334
1	34.653011789	30.564086132	45.787120351	8	33.970236091	33.700856444	32.572290709
1	32.300401999	31.025674222	45.161793596	8	36.029715404	32.824191224	32.582955721
1	34.240929553	30.760759878	40.046856580	1	33.630035626	32.307544569	34.689743358
1	30.669996185	31.290236911	43.290578271	1	35.321906537	31.722476027	34.783140390
8	30.973018450	31.333990297	35.272868359	1	36.094075904	33.741951074	35.762556364
1	31.696498695	30.654332078	35.216617167	1	34.834830821	34.707851665	34.970707272
1	31.244843489	32.076194378	34.680703872	8	35.782382191	30.611768780	41.584150615
8	31.644372333	33.705158396	34.068646793	6	34.973680554	30.721011676	42.476043471
1	32.035697395	34.035742430	34.903551848	7	33.615244064	31.040556549	42.204193059
1	32.399676906	33.739157325	33.422508100	6	33.228564437	31.156858468	40.754676729
1	37.113682848	34.241441823	43.441194764	6	32.654975501	31.149797799	43.179704499
1	30.775981995	36.590325348	42.553355214	7	31.410872152	31.460212396	42.858609110
1	37.102879774	38.525666784	38.282371205	6	33.037726489	30.925640227	44.535316241
1	26.060519302	33.158114075	36.637019382	6	34.336669836	30.648316232	44.820312983
1	36.279682215	30.367546595	44.076104527	7	35.280612657	30.524134228	43.833255763

PD

QM/MM (BS1) = -3370.577826 a.u.

QM/MM (BS2+ZPE) = -3372.485246 a.u.

6	36.890681544	33.969772802	42.641096544	1	34.068586234	30.730353496	40.198850674
7	37.632200494	33.736128521	41.509184762	1	30.634195031	31.372834606	43.530583543
1	38.647174813	33.697476721	41.401087704	8	30.932821368	31.256738372	35.206406581
6	36.799788774	33.668936393	40.457985434	1	31.662921483	30.582506559	35.192330164
1	37.122240586	33.494292248	39.434138394	1	31.227416978	31.995295612	34.621905126
7	35.553298915	33.856919959	40.852921009	8	31.661209430	33.656151714	34.089322928
6	35.586471016	34.041244725	42.211742677	1	32.044823613	33.917485756	34.952209087
1	34.683999223	34.236859450	42.783377780	1	32.427874316	33.706466744	33.451766352
6	30.623016755	36.180831837	41.574976518	1	37.329187071	34.244027399	43.600557138
1	30.823862275	37.052008002	40.932952744	1	30.820938142	36.502685843	42.597377830
1	29.565749218	35.902717627	41.469415340	1	37.153979246	38.540521795	38.334104948
6	31.499481771	35.034175986	41.107662412	1	25.990470887	33.121327266	36.624301988
8	32.676015271	35.319471433	40.750006649	1	36.240039045	30.409632496	44.090865651

Snapshot 5**RC2****QM/MM (BS1) = -3369.803340 a.u.****QM/MM (BS2+ZPE) = -3371.752763 a.u.**

6	27.876122977	22.152655995	36.130907149
7	29.183237979	22.358925482	36.508160822
1	29.799117650	21.655490652	36.934042270
6	29.504247164	23.634600630	36.227433540
1	30.479623384	24.072597628	36.423391029
7	28.470194332	24.267193385	35.684773977
6	27.439538141	23.352999042	35.615300068
1	26.474859653	23.633963030	35.196291141
6	24.099329271	26.985660418	35.126197645
1	24.133967435	27.667703363	35.987031771
1	23.849179448	27.584387406	34.236890163
6	25.459584390	26.336041305	34.884707708
8	26.437929696	26.899175525	35.567146209
8	25.620843002	25.389351631	34.129760695
6	28.744303739	26.173446499	39.707386787
7	27.401683060	26.480281169	39.614320067
1	26.757370405	26.635021021	40.386249780
6	27.103406615	26.668943315	38.314817438
1	26.117168578	26.946849944	37.955948653
7	28.182662032	26.483498466	37.566197104
6	29.217300939	26.181294949	38.422268651
1	30.222889490	26.002656860	38.054411928
6	26.289576574	31.862606052	30.619661464
1	26.341992448	31.468355883	29.593720258
1	25.368802048	31.498689016	31.096929880
7	27.477494988	31.516594146	31.407110258
1	28.219075306	32.215652549	31.455893881
6	27.748558922	30.395415344	32.094167396
7	26.917613859	29.351437820	32.135466114
1	26.044766155	29.298064754	31.600133168
1	27.211253854	28.515222289	32.633307269
7	28.899805173	30.352578896	32.776706662
1	29.499006108	31.174946779	32.757147763
1	29.201177305	29.568028877	33.361629681
26	28.317247709	26.407441334	35.449018347
8	28.370287906	26.541500113	33.834497698
8	30.500407169	28.848917758	34.587366695
6	30.891616506	27.886472657	35.249226868
8	30.106947062	26.991273173	35.783328836
6	32.363935708	27.618628000	35.539356201
6	33.399286389	28.604400128	34.981805658
6	34.651678686	27.886156151	34.413367569
8	34.420325647	26.844381787	33.730771654
8	35.784833023	28.363897673	34.638029511
1	33.703883058	29.351209474	35.729971307
1	32.950280219	29.167744029	34.145565823
1	32.551154507	26.636887181	35.085627552
1	32.465963913	27.476151550	36.627949723
8	29.543475883	21.201387705	31.443638014
6	28.373856466	21.347103894	31.706397722
7	27.728400348	22.595948507	31.520986487
6	28.579329208	23.726536049	31.105120179
6	26.391067722	22.795099306	31.731536452
7	25.870902695	23.995379539	31.556563084
6	25.591710307	21.681349888	32.135872972
6	26.202370126	20.495436499	32.392570039

7	27.555675688	20.336340127	32.230538791
1	28.619892290	24.484969884	31.904674865
1	28.186008719	24.172255727	30.179336716
1	26.458140478	24.815581832	31.453053040
1	25.631401728	19.636947179	32.749900866
1	24.517699772	21.802761119	32.269636989
1	29.587387689	23.343819234	30.922126474
1	24.884787781	24.188818562	31.785866826
8	26.647010712	29.483422008	36.635842306
1	27.462083981	29.944892329	36.303736708
1	26.565727573	28.659565041	36.125337167
8	31.852331874	26.697729716	32.614957265
1	31.564276202	27.611352749	32.751517677
1	32.775474510	26.690509161	32.964278518
1	27.354783589	21.214048615	36.318760156
1	23.321336800	26.242348568	35.300216414
1	29.235788905	25.871784087	40.632324323
1	26.252043122	32.951283761	30.581722011
1	27.992827119	19.489404957	32.533147357

TS7**QM/MM (BS1) = -3369.767004 a.u.****QM/MM (BS2+ZPE) = -3371.719255 a.u.**

6	27.809743914	21.829926174	36.205695775
7	29.118068324	22.042902639	36.569311804
1	29.741807738	21.360936519	37.015874313
6	29.443345044	23.305898731	36.248146739
1	30.421606025	23.740999505	36.432272724
7	28.409192663	23.923845866	35.692708180
6	27.372606125	23.014361845	35.661491770
1	26.395456691	23.298680272	35.277717877
6	24.128941035	26.907890598	35.172860167
1	24.198316484	27.590743179	36.033443114
1	23.892991890	27.538122381	34.300636024
6	25.474242891	26.236473806	34.916770150
8	26.528299607	26.993780537	35.130385654
8	25.582262234	25.080737592	34.518730046
6	28.678978120	26.058289761	39.515302468
7	27.343823497	26.392269092	39.424803506
1	26.717561448	26.606572177	40.196974079
6	27.033672156	26.512963823	36.115842485
1	26.045251876	26.804687947	37.772551699
7	28.090243253	26.255841990	37.360198143
6	29.127179794	25.980886592	38.221601130
1	30.124551927	25.757371542	37.853994337
6	26.272428760	31.885694267	30.563108561
1	26.275974453	31.503340368	29.531826295
1	25.370016976	31.523947525	31.074468328
7	27.485222653	31.510074773	31.292552771
1	28.270873403	32.157491952	31.244672824
6	27.699684016	30.455432882	32.093875258
7	26.813719527	29.464985054	32.225824007
1	25.976817791	29.368477073	31.641338962
1	26.984861275	28.733471026	32.906984402
7	28.840715521	30.429485829	32.790912748
1	29.445289469	31.247877871	32.743107733
1	29.167739600	29.631744231	33.347784526
26	28.270743120	25.988809201	35.117437751
8	28.282137581	25.613541827	33.408781761
8	30.393372212	28.770225836	34.448480782
6	30.776783953	27.761685857	35.045763195

8	29.996055493	26.782265093	35.400350206	6	42.572583505	27.244276610	26.735013640
6	32.227448809	27.564424776	35.481377187	1	41.971055433	26.835615235	25.928593186
6	33.287775889	28.527835890	34.919025440	7	42.444427983	28.460734765	27.243682529
6	34.556449059	27.800149862	34.395378982	6	43.404275295	28.588555868	28.220066111
8	34.348700850	26.736580417	33.737442325	1	43.508174088	29.506127585	28.793541978
8	35.682334559	28.293938504	34.623332719	6	33.383600999	32.044620588	25.929921161
1	33.583264930	29.290190337	35.654945821	1	33.357730084	33.141262711	25.872465302
1	32.865888439	29.079556746	34.061385057	1	32.723641535	31.681948204	25.128348764
1	32.485310649	26.544041455	35.177427490	7	34.700359659	31.505984275	25.669825855
1	32.224316122	27.564786353	36.585772079	1	34.744457909	30.621333257	25.147507822
8	29.669255389	21.439353025	31.686567831	6	35.903213593	31.942306485	26.083578274
6	28.484072001	21.524620213	31.889860479	7	36.066906616	33.084130465	26.766013504
7	27.812006417	22.780994197	31.797537285	1	35.342371060	33.807238855	26.810718996
6	28.619942413	23.948438850	31.555221228	1	37.017334467	33.332392173	27.052663703
6	26.445544413	22.913426614	31.905150146	7	36.949893615	31.157719334	25.819801683
7	25.923377112	24.124097385	31.864275527	1	36.786167815	30.308514709	25.270980893
6	25.660136212	21.732329146	32.058332640	1	37.916748610	31.434085713	26.000808105
6	26.291773405	20.545091995	32.260547819	26	41.095966171	29.967759242	26.517693794
7	27.660309371	20.443383805	32.230895467	6	39.798328115	32.330492066	27.576931579
1	28.561937702	24.769786521	32.555899676	8	38.946615205	33.179821492	27.815446640
1	28.243875082	24.546842833	30.713363567	8	39.839629325	31.554557603	26.542425496
1	26.499647680	24.927909816	32.121449240	6	40.992412724	32.105112417	28.541867396
1	25.725110907	19.637924643	32.477905628	8	41.892536266	31.362418514	28.135550197
1	24.574071908	21.805131288	32.102678392	6	41.048021739	32.862309184	29.840968363
1	29.676305141	23.682582179	31.470929965	6	42.082413165	32.355451123	30.852514921
1	24.907453744	24.260062907	31.971390829	6	42.010613009	33.097943838	32.213062665
8	26.682418369	29.392115500	36.595580094	8	41.533337841	32.456391615	33.183836323
1	27.497766917	29.879320574	36.303756087	8	42.442443124	34.278504641	32.248606109
1	26.628314118	28.610053313	36.015929628	1	43.092929553	32.488826735	30.433171718
8	31.829454431	26.581084678	32.566225279	1	41.920777816	31.280719828	31.019393893
1	31.598352000	27.519697530	32.622290090	1	40.028214734	32.852938730	30.259891209
1	32.738846491	26.550161004	32.952819661	1	41.233353968	33.925318537	29.591677798
1	27.266107500	20.915713648	36.443902040	8	40.084527131	29.368527763	28.270174635
1	23.326717268	26.191969820	35.351638785	8	39.563639534	30.184155446	29.083592892
1	29.182748485	25.821010588	40.452309055	8	44.872894760	35.313321097	23.973951458
1	26.247677880	32.975167123	30.540667440	6	44.094829628	34.718441608	23.251651279
1	28.094795272	19.591406455	32.523006902	7	42.741775145	34.593958751	23.622222946

Dioxygen activation step reaction states cartesian coordinates for AlkB-dsDNA

RC1

QM/MM (BS1) = -3412.915331 a.u.

QM/MM (BS2+ZPE) = -3414.926892 a.u.

6	44.351819855	30.348043233	23.773765187
7	44.848874081	31.121427882	24.804058722
1	45.801263582	31.507500225	24.871066448
6	43.869955417	31.282940584	25.716041460
1	43.991825758	31.830645466	26.647504646
7	42.760615755	30.655116255	25.328300790
6	43.050390983	30.066504828	24.111726364
1	42.309251115	29.479193405	23.574289214
6	38.799762279	27.301256167	23.895628902
1	38.525344584	26.344675885	24.369584637
1	37.863991083	27.722202651	23.495658671
6	39.192737115	28.236747487	25.049625229
8	40.374618437	28.780152196	25.105501754
8	38.332156714	28.432115817	25.909685428
6	44.121528266	27.420440304	28.292152647
7	43.569308094	26.579396692	27.347673410
1	43.847022436	25.617777018	27.120093416

TS1

QM/MM (BS1) = -3412.895796 a.u.

QM/MM (BS2+ZPE) = -3414.905834 a.u.

6	44.364245735	30.329393640	23.759372661
7	44.846202514	31.122683524	24.783071203

1	45.794526129	31.519036157	24.848011010
6	43.863657769	31.279775469	25.690958776
1	43.960334473	31.840426746	26.617985356
7	42.767769591	30.626690949	25.304468489
6	43.067808017	30.027742441	24.096917942
1	42.336843232	29.423470866	23.565275420
6	38.826579929	27.354731349	23.935751804
1	38.542236531	26.397547571	24.403399455
1	37.895057729	27.782736813	23.532224698
6	39.215930340	28.281184946	25.103012636
8	40.407297884	28.795209141	25.199419322
8	38.338787754	28.489319761	25.942831895
6	44.170759213	27.396924122	28.306512538
7	43.614882162	26.553426742	27.365408002
1	43.882291428	25.587644691	27.144706148
6	42.631485325	27.225438953	26.738908554
1	42.024395187	26.825503066	25.933430035
7	42.518694279	28.445898297	27.235375155
6	43.468272737	28.572908309	28.220164517
1	43.574479585	29.496802387	28.783722740
6	33.327509115	32.045771655	25.906301335
1	33.286637274	33.142167594	25.851753834
1	32.656202091	31.677372281	25.117010020
7	34.644615333	31.523855697	25.618061667
1	34.690881750	30.636590717	25.100458874
6	35.848719258	31.973904865	26.012252500
7	36.008799017	33.119356324	26.689252481
1	35.276148242	33.833828066	26.750869097
1	36.956663920	33.380706600	26.968295270
7	36.898190823	31.196861839	25.735789535
1	36.727906680	30.348798438	25.186972877
1	37.869005688	31.478726233	25.879960082
26	41.176522803	29.995391169	26.581367285
6	39.665951605	32.269524036	27.536665006
8	38.894100803	33.174876479	27.802518840
8	39.755821058	31.561437923	26.469273436
6	40.795767220	31.709803147	28.627546383
8	41.859057116	31.316236294	27.977305662
6	40.918849694	32.586359225	29.873170296
6	42.071354705	32.225740434	30.824088297
6	42.015027067	33.017483612	32.161579836
8	41.485141049	32.423805007	33.138018977
8	42.491639071	34.180160701	32.179006172
1	43.028496936	32.435919202	30.321666107
1	42.028451945	31.149559426	31.046809794
1	39.951763365	32.540889352	30.399531089
1	41.022148776	33.626797670	29.525533224
8	40.287975125	29.421252560	28.295940545
8	39.998245538	30.467679345	29.049142078
8	44.897381034	35.309794617	23.986222095
6	44.115188744	34.718287300	23.265765008
7	42.764824328	34.589139984	23.644167334
6	42.376066252	35.299433237	24.863481639
6	41.849960538	33.837255177	22.952797925
7	40.616497918	33.721998414	23.415749319
6	42.268083898	33.189108696	21.759719128
6	43.551362582	33.348473001	21.343605705
7	44.436997002	34.123473599	22.052732836
1	43.035594801	36.164022103	24.975493487
1	42.463738693	34.643296835	25.744543148
1	40.333649646	34.086626780	24.315375238
1	43.912299059	32.829628817	20.452777066

1	41.574491209	32.576469664	21.187882948
1	41.347820675	35.661786448	24.763095381
1	39.920715715	33.159948352	22.902585058
1	44.985827154	29.952211094	22.947315284
1	39.484865748	27.114759341	23.100802378
1	45.072967464	27.168286990	28.873797873
1	32.902129460	31.708941297	26.851639786
1	45.377902129	34.209704503	21.725266392

IMI

QM/MM (BS1) = -3412.989066 a.u.

QM/MM (BS2+ZPE) = -3414.994183 a.u.

6	44.403438222	30.402143188	23.709171192
7	44.904872459	31.169541873	24.741349382
1	45.864401047	31.531520215	24.822957843
6	43.910514726	31.365776805	25.633447443
1	44.033171832	31.921771847	26.560725610
7	42.791584689	30.772039265	25.230655147
6	43.087215243	30.165926904	24.025236079
1	42.338947701	29.589682228	23.484598819
6	38.777161172	27.278493920	23.840535973
1	38.488878615	26.337601441	24.336101973
1	37.846025790	27.720654924	23.451185927
6	39.258450843	28.230269739	24.950526566
8	40.402074529	28.800382605	24.868890651
8	38.473935755	28.402976339	25.904336394
6	43.967767894	27.479422056	28.235891109
7	43.439868963	26.650815200	27.267239669
1	43.756579149	25.711412291	27.004763378
6	42.401616930	27.295473985	26.696241378
1	41.822655580	26.897511881	25.867675121
7	42.214864103	28.483504035	27.255122468
6	43.191673811	28.612985585	28.218463546
1	43.267671199	29.513864453	28.820901913
6	33.358158585	31.888372544	25.944919494
1	33.333439578	32.982371167	25.835969895
1	32.706043365	31.489941071	25.154816242
7	34.676436148	31.333431634	25.722476959
1	34.738908004	30.461433508	25.179485940
6	35.856463365	31.753060985	26.205097321
7	35.949630688	32.908015890	28.93562150
1	35.233888814	33.640629464	26.842235386
1	36.852253348	33.195018219	27.248965607
7	36.921179436	30.977089580	26.031993642
1	36.813246074	30.125409744	25.473797398
1	37.886582448	31.240963926	26.298539476
26	41.075496675	30.095369860	26.320679554
6	38.786072385	35.058234003	26.710541584
8	38.084899173	34.993403700	27.636880630
8	39.497906824	35.122210485	25.796721024
6	40.728587713	31.833741380	28.760557122
8	41.699817998	31.257117226	28.285479309
6	40.617589933	32.347548618	30.179406345
6	41.839431636	33.121985768	30.678298875
6	41.831125130	33.410347681	32.199998205
8	41.301322695	32.561858609	32.960578680
8	42.394166289	34.473838977	32.561222803
1	41.950028485	34.081680026	30.151213258
1	42.750359448	32.536717049	30.460833231
1	40.486366067	31.464955983	30.828330637
1	39.699400058	32.946802085	30.268691930

8	39.636265571	31.469194640	26.743808550
8	39.613085168	32.030941394	28.068989446
8	45.020920813	35.299577824	23.849431522
6	44.237755667	34.696136501	23.138029701
7	42.884816730	34.594090252	23.503455818
6	42.483084164	35.356143919	24.683353455
6	41.966987854	33.830014074	22.828955367
7	40.725543304	33.761210173	23.275633756
6	42.392783390	33.127262729	21.670882931
6	43.676880574	33.272861214	21.255304739
7	44.561452358	34.067578860	21.944622914
1	43.205143668	36.163345921	24.824506041
1	42.457827751	34.710203583	25.575659322
1	40.424882476	34.200906142	24.136716331
1	44.037826036	32.731666064	20.379326729
1	41.700101013	32.496276831	21.118626124
1	41.496256586	35.791033176	24.510909285
1	40.026860311	33.184198582	22.783348025
1	45.017326361	29.996414598	22.905061131
1	39.423512906	27.024083189	23.000552679
1	44.865123114	27.253750396	28.811992865
1	32.899289593	31.606015079	26.892432468
1	45.502863309	34.152520662	21.618275230

TS2

QM/MM (BS1) = -3412.976382 a.u.

QM/MM (BS2+ZPE) = -3414.994860 a.u.

6	44.388843439	30.385732597	23.715280443
7	44.880767070	31.157011173	24.749903474
1	45.837592648	31.527723834	24.832617508
6	43.886492143	31.343164183	25.641019726
1	43.999936558	31.898538473	26.569568818
7	42.774288102	30.734685923	25.234330537
6	43.076301677	30.130673714	24.028503039
1	42.334006646	29.547520285	23.487633873
6	38.808986056	27.298401182	23.833422243
1	38.500004720	26.356315043	24.313920583
1	37.887892087	27.762797224	23.445710165
6	39.291286011	28.217622302	24.971650888
8	40.451911606	28.767110623	24.932847505
8	38.493042462	28.374831941	25.911726767
6	43.950358820	27.472008410	28.259174892
7	43.431804894	26.650280207	27.278931216
1	43.758062640	25.717128739	27.005427569
6	42.382663357	27.285262584	26.720112575
1	41.809909642	26.892071627	25.885649505
7	42.178817406	28.461968447	27.298300834
6	43.155687551	28.592609869	28.262568977
1	43.212922976	29.485506495	28.878857247
6	33.361671746	31.914914948	25.941458045
1	33.348795958	33.010356823	25.848849116
1	32.700255891	31.536953236	25.148885414
7	34.671553980	31.348343791	25.699996102
1	34.717023323	30.482862784	25.146128331
6	35.860000831	31.721852143	26.203173497
7	35.984625190	32.857704998	26.917724055
1	35.291956592	33.612781368	26.877041734
1	36.891620236	33.099521083	27.296630941
7	36.898588288	30.915697558	26.015905865
1	36.754843496	30.090361525	25.426231512
1	37.878774639	31.135232799	26.272578585

26	41.085800502	30.110035520	26.366911235
6	38.780023709	35.022617543	26.752551410
8	38.066755088	34.997026992	27.670537732
8	39.499960476	35.053394810	25.842337262
6	40.691354458	31.873958460	28.728519419
8	41.637977763	31.183020933	28.305224722
6	40.635326161	32.397419345	30.161535706
6	41.898703631	33.088810509	30.674822922
6	41.876332372	33.391960041	32.194846474
8	41.329463246	32.556222474	32.957725605
8	42.441284427	34.455742787	32.554990280
1	42.079581866	34.036696240	30.146357903
1	42.772006708	32.442198282	28.472797226
1	40.439763401	31.519479544	30.801266534
1	39.760347529	33.057529323	30.254663441
8	39.644126086	31.181931230	26.588518602
8	39.645344708	32.159470567	28.030222625
8	45.005185251	35.303043887	23.853542086
6	44.221681029	34.702322615	23.140459894
7	42.868090771	34.602394276	23.504666199
6	42.466155387	35.367155145	24.683274402
6	41.949640842	33.839329282	22.829421006
7	40.708423139	33.769242824	23.275804469
6	42.376180020	33.136756010	21.670912988
6	43.660987989	33.280298482	21.256635366
7	44.546314423	34.073167797	21.947298609
1	43.180452067	36.182742098	24.816244145
1	42.451375022	34.726939269	25.579753457
1	40.406904679	34.202442598	24.140307900
1	44.022279829	32.738145066	20.381218453
1	41.682825381	32.507991106	21.116920628
1	41.473629544	35.790312976	24.514580823
1	40.010267561	33.194009724	22.780386464
1	45.008399389	29.986843962	22.912095781
1	39.452227905	27.038553398	22.992716369
1	44.853863747	27.250623509	28.827272514
1	32.904623705	31.623066932	26.886973327
1	45.488170872	34.156588066	21.621845097

IM2

QM/MM (BS1) = -3412.986491 a.u.

QM/MM (BS2+ZPE) = -3414.995616 a.u.

6	44.400980310	30.385265503	23.704762098
7	44.885473652	31.161639161	24.738407887
1	45.841088996	31.536668184	24.823504325
6	43.888188902	31.350778895	25.623909187
1	43.995139402	31.916259587	26.547075160
7	42.780849360	30.735544497	25.212366046
6	43.088208847	30.126535966	24.010761959
1	42.351067950	29.543645099	23.463156181
6	38.808465382	27.318969058	23.863555459
1	38.491882844	26.379265238	24.343321438
1	37.892016437	27.790197578	23.471709707
6	39.290132902	28.237639400	24.997229024
8	40.439728533	28.821593987	24.927721238
8	38.525923679	28.387964495	25.960951586
6	43.918311402	27.519890034	28.211569493
7	43.409919997	26.687902508	27.234297692
1	43.729199074	25.745461180	26.985602319
6	42.388910045	27.332434121	26.635538858
1	41.826086680	26.927751477	25.800756631

7	42.192738991	28.523674255	27.184458652	1	43.798722789	31.692787754	26.636500008
6	43.142346839	28.653442535	28.174561895	7	42.654265204	30.454638962	25.306535767
1	43.187170290	29.550348769	28.785837205	6	42.976070002	29.897301954	24.086163002
6	33.368101651	31.945583309	25.937752080	1	42.262084240	29.288850889	23.537105003
1	33.344483534	33.041313475	25.852160284	6	38.787634256	27.318088830	23.890803086
1	32.708364812	31.565702970	25.144554093	1	38.595952017	26.369163202	24.419866472
7	34.683906077	31.395907417	25.688384974	1	37.818653827	27.642765102	23.484679180
1	34.735066563	30.527820488	25.139839404	6	39.108747303	28.356137516	24.981139983
6	35.876441151	31.809246427	26.149113188	8	40.299517549	28.871005458	25.072768944
7	35.994629926	32.942799489	26.862588315	8	38.169883357	28.627560407	25.737521796
1	35.284297297	33.682207952	26.853413980	6	44.117195119	27.396625052	28.330335267
1	36.902835105	33.191933899	27.235795978	7	43.574172641	26.552075329	27.385882045
7	36.932797057	33.070737686	25.924563178	1	43.870756639	25.599452425	25.99450056
1	36.779436865	30.208667286	25.332058129	6	42.551214581	27.195507037	26.792855512
1	37.916809994	31.325576627	26.051005065	1	41.953439387	26.778380054	25.987604069
26	41.032119497	30.208313626	26.276412612	7	42.399921150	28.400812670	27.317029369
6	38.813187390	35.057623883	26.832810035	6	43.368992661	28.547962057	28.278552554
8	38.025997988	35.072184105	27.688003693	1	43.464488675	29.463814477	28.856532666
8	39.597141338	35.065537819	25.976400709	6	33.797652001	31.930035500	26.077982833
6	40.464990243	31.835646635	28.658750791	1	33.748908183	33.016330414	25.913566123
8	41.276903393	30.956098891	28.194114603	1	33.310060760	31.462128758	25.211572793
6	40.552398286	32.154465217	30.157348078	7	35.161354144	31.421212773	26.100112867
6	41.746822421	33.026172729	30.573519706	1	35.326780419	30.611667898	25.479218713
6	41.829487909	33.341626003	32.093963049	6	36.233795489	31.957122305	26.696090494
8	41.327374345	32.520218001	32.901432385	7	36.155368007	33.153111736	27.317420363
8	42.430808051	34.402100629	32.404151480	1	35.408126789	33.830673059	27.130329011
1	41.742759838	33.987635386	30.036571769	1	36.967485891	33.498654161	27.814374617
1	42.690174177	32.522988868	30.293537871	7	37.389253917	31.291122563	26.719167120
1	40.611243664	31.197829202	30.696439818	1	37.497960021	30.347451449	26.329064727
1	39.614558858	32.650610381	30.447802643	1	38.220487990	31.698745825	27.162575564
8	39.759151530	31.437049598	26.011910847	26	41.065550709	29.866127270	26.587475154
8	39.597723089	32.422495140	27.978918086	6	38.962295780	35.099117873	26.918021543
8	44.999865686	35.292559764	23.891003951	8	38.382818858	35.328798346	27.898613756
6	44.210267660	34.692279096	23.183903632	8	39.538610762	34.880049985	25.933718500
7	42.867178305	34.565322679	23.575145370	6	40.800569726	32.084191971	28.483269001
6	42.470791472	35.326152539	24.758798060	8	41.529299626	31.435707282	27.609793386
6	41.948771081	33.786032888	22.917563002	6	41.473169255	32.280503294	29.844410460
7	40.733431712	33.654364677	23.416133644	6	41.138664949	33.573661130	30.591485019
6	42.353315573	33.134653150	21.719971545	6	41.598032723	33.586706165	32.071661604
6	43.626583149	33.305438201	21.280712004	8	41.281388964	32.606237519	32.793236186
7	44.519720461	34.088790163	21.973036520	8	42.232801307	34.602259611	32.460731509
1	43.170938127	36.156572589	24.874744595	1	40.043314204	33.703657670	30.586316757
1	42.482601089	34.691475492	25.659094188	1	41.575831271	34.446950591	30.082219472
1	40.465630124	34.006220832	24.329040066	1	42.560993407	32.160367904	29.719682546
1	43.975444034	32.786597726	20.386214368	1	41.138540688	31.426106800	30.462449629
1	41.657380597	32.508403367	21.166104547	8	39.881262445	29.486163035	27.622565253
1	41.465728197	35.725143649	24.605216175	8	39.659594879	32.492117186	28.259071756
1	40.032964666	33.078571083	22.924776974	8	44.979344224	35.291298820	23.862795380
1	45.022874017	29.986191248	22.903478579	6	44.192341061	34.690798278	23.153805628
1	39.453249995	27.059695680	23.023854661	7	42.839826863	34.594763222	23.522081269
1	44.806860011	27.293291965	28.800807990	6	42.444726444	35.358253415	24.704311182
1	32.915526185	31.643002436	26.882044189	6	41.917915052	33.833570119	22.850173766
1	45.459568704	34.173343956	21.642115940	7	40.676216173	33.772855396	23.296751897

IM3

QM/MM (BS1) = -3413.001422 a.u.

QM/MM (BS2+ZPE) = -3415.021109 a.u.

6	44.263701153	30.249137449	23.755945757	1	40.373725488	34.222099670	24.152556379
7	44.719185792	31.032952796	24.798491661	1	43.984122895	32.711911078	20.405462471
1	45.654498706	31.454000902	24.876537786	1	41.644966284	32.490906545	21.146349969
6	43.726867477	31.137128909	25.705508557	1	41.452632944	35.784610578	24.540111000

1	39.976086590	33.201209900	22.800480181
1	44.906061309	29.905159114	22.945316581
1	39.453309358	27.085429903	23.059650994
1	45.029109767	27.177567801	28.885756655
1	33.190914233	31.669082699	26.945070046
1	45.452516142	34.139529339	21.632156004

IM4

QM/MM (BS1) = -3413.006828 a.u.

QM/MM (BS2+ZPE) = -3415.027170 a.u.

6	44.433352135	30.356812060	23.684492641
7	44.926587676	31.121621079	24.720577529
1	45.876241579	31.512774148	24.793694347
6	43.945153473	31.273008197	25.633090190
1	44.063505362	31.826713674	26.561966149
7	42.844812613	30.643417532	25.234512796
6	43.131755266	30.068332162	24.014903782
1	42.392837271	29.486863533	23.468152456
6	38.788849523	27.292539099	23.894143920
1	38.513319497	26.347493584	24.389895217
1	37.852005488	27.728674817	23.513564902
6	39.253552276	28.242810319	25.006949524
8	40.455785385	28.701945117	24.997368008
8	38.441330494	28.512448268	25.908546613
6	43.953634883	27.509564479	28.172570083
7	43.442077341	26.659125860	27.212981650
1	43.748121960	25.704670616	26.992314382
6	42.443262719	27.303020698	26.580306718
1	41.876384861	26.889014210	25.753750874
7	42.266797939	28.513528229	27.091743406
6	43.203413465	28.657215489	28.090806514
1	43.261664926	29.570273435	28.676279142
6	33.663549760	31.939604289	26.037076749
1	33.609503581	33.028953191	25.895833621
1	33.132121529	31.491631416	25.185858414
7	35.023593378	31.430613099	25.986566273
1	35.169624872	30.608067153	25.380002847
6	36.122254540	31.929636749	26.566517862
7	36.092045912	33.105542776	27.225877429
1	35.357199554	33.806372139	27.079806871
1	36.924274213	33.408499826	27.718357025
7	37.257567862	31.232559851	26.534253470
1	37.329417787	30.333035608	26.057037797
1	38.133924911	31.625170163	26.895685706
26	41.083984927	30.089515651	26.267987655
6	38.957587065	35.035715130	26.992872109
8	38.341077642	35.208879246	27.963520605
8	39.571509781	34.876853686	26.020543485
6	40.396514130	31.643621859	28.746997680
8	41.078755782	30.742835517	28.085697520
6	40.875540029	31.825808214	30.195025440
6	41.229606965	33.260458601	30.604563095
6	41.601654359	33.443428048	32.101691323
8	41.239870262	32.557928341	32.918313648
8	42.226606763	34.495842061	32.393465730
1	40.370329207	33.924091756	30.400465177
1	42.066052767	33.655164074	30.005599575
1	41.722024689	31.149422861	30.380802284
1	40.052380862	31.482519725	30.844587089
8	40.158375732	31.253517074	25.644967722
8	39.428040118	32.267950956	28.313281726

8	44.974918313	35.298236735	23.887851399
6	44.190554750	34.695043951	23.176978945
7	42.842715367	34.576619026	23.554928254
6	42.442305231	35.341671128	24.734415112
6	41.926777754	33.799847410	22.889666857
7	40.700884252	33.688749139	23.364128946
6	42.344869057	33.129778120	21.707068521
6	43.623215645	33.292006635	21.280487702
7	44.510767714	34.080871856	21.974747895
1	43.129509930	36.184572215	24.838954718
1	42.471392363	34.715163228	25.639902580
1	40.420398519	34.055762734	24.266043023
1	43.980718984	32.764757295	20.394265191
1	41.652053676	32.500520198	21.152671653
1	41.430179308	35.725059124	24.584534118
1	40.004940815	33.109019211	22.870506979
1	45.050123496	29.962621767	22.876857561
1	39.431427265	27.043428772	23.049688348
1	44.833277122	27.284296370	28.775522096
1	33.100786721	31.661725838	26.928226927
1	45.451449093	34.167068337	21.646630230

2OG Rearrangement Coordinates for AlkB-dsDNA

ES1

QM/MM (BS1) = -3269.997721 a.u.

QM/MM (BS2+ZPE) = -3271.827539 a.u.

6	31.621630967	27.064892502	30.383328851
7	31.290609156	28.283254955	30.937978508
1	30.455212897	28.506277606	31.492304826
6	32.242764866	29.172789475	30.605992482
1	32.209514944	30.218875533	30.900156606
7	33.185627254	28.596320020	29.867525478
6	32.807341411	27.275346458	29.719890402
1	33.407468094	26.583483338	29.136043475
6	36.059488890	26.076296070	26.055058722
1	35.926350111	26.212964154	24.970603831
1	37.092688836	25.735600200	26.199046099
6	35.963643174	27.452846404	26.725924396
8	34.978828936	27.678311917	27.515598634
8	36.848151193	28.283939488	26.461746773
6	31.135259935	30.671443003	26.365917382
7	31.442302021	29.475351658	25.755019539
1	30.862070016	28.947175257	25.091511826
6	32.641230783	29.071596397	26.212502474
1	33.116329636	28.136198910	25.929676491
7	33.137275059	29.950262960	27.077962122
6	32.201396180	30.955704750	27.185220958
1	32.357511131	31.798837225	27.852794547
6	42.559020644	28.450845263	29.156063981
1	42.716478970	28.607381386	30.228772439
1	42.949226364	27.443958047	28.942641685
7	41.160705224	28.471248951	28.794057910
1	40.901073032	27.863304229	28.005773779
6	40.109645672	28.973376363	29.465771221
7	40.252895933	29.829089249	30.493192515
1	41.146156157	29.969660391	30.971966874
1	39.404996851	30.125913770	30.978888957
7	38.895976530	28.642439469	29.026931577
1	38.821152481	27.797918173	28.448147903
1	38.040510293	28.970608142	29.486364852

26	34.629653768	29.375192639	28.534618207
6	36.483869284	31.011270827	30.208305159
8	37.389588219	31.327876352	30.986370084
8	36.312646937	29.894915703	29.622080761
6	35.404945481	32.073748579	29.826822011
8	34.419353686	31.685959304	29.215607968
6	35.632782968	33.497685814	30.234483214
6	34.817011433	34.552394043	29.492816327
6	35.050913836	35.984172251	30.009846138
8	35.273999989	36.137062983	31.238518731
8	34.989024170	36.921996195	29.164935352
1	33.740379751	34.334444757	29.607161916
1	35.017608124	34.525964190	28.411113973
1	36.716789741	33.692351920	30.188557264
1	35.402222171	33.541618480	31.314738548
8	33.153910968	28.118377443	35.391288723
6	33.445972946	27.159572536	34.705137611
7	34.641517355	27.157427744	33.943602468
6	35.506816541	28.334237304	34.076400965
6	34.996582504	26.149427228	33.075441851
7	36.047032121	26.282825600	32.291085437
6	34.196018995	24.975235524	33.064442907
6	33.065127525	24.949836402	33.805682483
7	32.674244850	26.010807428	34.584553615
1	35.083528009	28.979228958	34.851128263
1	35.563534055	28.881199481	33.122422662
1	36.652253823	27.110601166	32.260053652
1	32.421361224	24.079850505	33.794397741
1	34.482691202	24.121940776	32.459041576
1	36.516981963	28.018646645	34.373711090
1	36.285566899	25.578814353	31.579813217
1	30.969532273	26.192002242	30.413282390
1	35.370647445	25.291660790	26.367968076
1	30.186981755	31.192316334	26.233528570
1	43.171432294	29.151480047	28.588498833
1	31.775401880	25.960891561	35.019941050

TS for 2OG rearrangement
QM/MM (BS1) = -3269.991780 a.u.
QM/MM (BS2+ZPE) = -3271.820336 a.u.

6	31.586386090	27.132211019	30.369041013
7	31.251395084	28.366857271	30.883251838
1	30.416884012	28.598178660	31.437217284
6	32.196090707	29.250820952	30.511399731
1	32.168695661	30.306614650	30.768748243
7	33.133894553	28.653826712	29.782679934
6	32.764237405	27.327169649	29.686828942
1	33.361365807	26.621806989	29.116311260
6	36.096829727	26.043363777	26.065189222
1	35.922290734	26.199775205	24.988897563
1	37.124949270	25.671786060	26.160088451
6	36.073288864	27.411826743	26.756591117
8	35.100667769	27.688190286	27.546207045
8	37.006108570	28.190291467	26.497757348
6	31.177435557	30.649315948	26.379680282
7	31.488303495	29.463462336	25.751813387
1	30.909323448	28.943899132	25.080537341
6	32.689153001	29.055811388	26.207476539
1	33.166586938	28.126990787	25.905148601
7	33.181448675	29.921115406	27.086685016

6	32.242771851	30.922451415	27.205196362
1	32.390102777	31.755336892	27.888465830
6	42.608503898	28.404804582	29.043989675
1	42.744752318	28.513321813	30.125779729
1	43.002177602	27.408441188	28.796071811
7	41.221330759	28.440005194	28.649641830
1	40.955123085	27.817357251	27.876321365
6	40.191244677	29.069191191	29.235660225
7	40.366897196	29.895663901	30.281460834
1	41.214058187	29.854205150	30.855378395
1	39.528423354	30.227790090	30.759873141
7	38.982714973	28.897054441	28.704738543
1	38.844193859	28.228330024	27.94730580
1	38.143450572	29.406769466	29.001019683
26	34.704917235	29.367303125	28.558092886
6	36.617992348	31.281649275	29.699149765
8	37.600770619	31.562969558	30.389822624
8	36.494111145	30.322352921	28.868865391
6	35.347146149	32.157376666	29.795554461
8	34.277613814	31.631401013	29.517192099
6	35.514373150	33.580028218	30.240487142
6	34.663537384	34.626655275	29.519472022
6	34.972976241	36.054750012	30.008414698
8	35.258342893	36.206825256	31.224409733
8	34.921899772	36.983700601	29.153154586
1	33.591830627	34.430292737	29.698709474
1	34.811836757	34.585973154	28.429557568
1	36.584354196	33.827043300	30.187429551
1	35.264356612	33.600517484	31.315999821
8	32.945365776	28.112147344	35.361265794
6	33.198053601	27.103254630	34.736938438
7	34.289887889	27.071719408	33.832257315
6	35.111146706	28.283599682	33.742257822
6	34.531024897	26.022315535	32.980426303
7	35.378180003	26.126032138	31.977103953
6	33.843701736	24.803663633	33.217329242
6	32.842286578	24.796106326	34.119949739
7	32.480396635	25.916296588	34.823066062
1	34.859290663	28.924905182	34.591769714
1	34.915150307	28.817632630	32.799488611
1	35.860921329	26.990820679	31.714620523
1	32.286260288	23.887978883	34.297685332
1	34.103128448	23.904346843	32.669842741
1	36.174300689	28.007480100	33.785070071
1	35.346252607	25.383069048	31.264650286
1	30.940940985	26.255645792	30.424730737
1	35.398602636	25.273875233	26.394481846
1	30.235182040	31.180079713	26.243608751
1	43.227952716	29.131498790	28.518379546
1	31.576144764	25.900170520	35.249728682

ES2
QM/MM (BS1) = -3269.999004 a.u.
QM/MM (BS2+ZPE) = -3271.830009 a.u.

6	31.653611334	27.117420980	30.345688939
7	31.321170396	28.344856558	30.879582989
1	30.477979193	28.572994252	31.421989245
6	32.280738482	29.226887530	30.538111720
1	32.255249728	30.278807682	30.811252982
7	33.226431837	28.635415297	29.814895133
6	32.843367073	27.315236464	29.685026125

1	33.437859966	26.615379766	29.104469395
6	36.127778267	26.029331410	26.043909983
1	35.965839614	26.183108254	24.965439500
1	37.152687328	25.654388087	26.153381246
6	36.099483000	27.398879278	26.729883769
8	35.117766963	27.684699256	27.503019392
8	37.038417169	28.173724446	26.481082957
6	31.214984070	30.649302613	26.377394946
7	31.525414251	29.466529220	25.743935980
1	30.943290532	28.947391622	25.075111919
6	32.724271732	29.054886709	26.201045712
1	33.200513180	28.125639194	25.899367700
7	33.216352825	29.915503058	27.085022971
6	32.278891892	30.917310649	27.206349614
1	32.425565352	31.746169171	27.894545203
6	42.607166408	28.407886855	29.074248368
1	42.742556936	28.547399912	30.152730186
1	43.023652282	27.414353506	28.854494466
7	41.219618823	28.387276602	28.681193293
1	40.964687536	27.722490603	27.940135987
6	40.187457663	29.098144425	29.159219809
7	40.339166239	30.000642364	30.144851827
1	41.141064890	29.967967553	30.779819726
1	39.494174177	30.474358700	30.467937340
7	39.001219497	28.922713478	28.582030329
1	38.884848001	28.221387478	27.853423506
1	38.159678687	29.464167777	28.809828916
26	34.761631383	29.361127187	28.533666889
6	36.688914075	31.353910984	29.556494406
8	37.711800891	31.675494120	30.175167889
8	36.548877349	30.395996688	28.735059733
6	35.390648477	32.172311175	29.760025654
8	34.329296714	31.615431867	29.514104361
6	35.524289085	33.582609983	30.252439113
6	34.681757131	34.632078283	29.523709203
6	34.986358059	36.056458551	30.024853647
8	35.273107547	36.198930265	31.240927678
8	34.931892168	36.990540916	29.174541189
1	33.607696218	34.433819201	29.685777700
1	34.846442695	34.597927369	28.436039285
1	36.590072295	33.848480042	30.231241267
1	35.236235207	33.577918446	31.318277649
8	32.878833448	28.107698307	35.307865491
6	33.133225927	27.091310174	34.696287063
7	34.203844436	27.060141734	33.767815999
6	35.005660625	28.280756413	33.633963090
6	34.451061780	25.994918907	32.939254493
7	35.277518351	26.094946938	31.916580374
6	33.800350583	24.767866687	33.222468172
6	32.811345875	24.764384679	34.140127828
7	32.437446847	25.893803692	34.821063391
1	34.786496353	28.923203555	34.491697195
1	34.760699158	28.808833428	32.698941526
1	35.649693674	26.986008950	31.577092727
1	32.273628546	23.850992055	34.343924179
1	34.064494402	23.863522755	32.685155702
1	36.071662882	28.013997849	33.629409885
1	35.233525078	25.339821667	31.216573496
1	31.003672180	26.243050162	30.379186462
1	35.424259800	25.262499123	26.368097174
1	30.273735280	31.181886002	26.241479627
1	43.212770197	29.131972144	28.529260420

1	31.536542144	25.877689298	35.254749383
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Substrate hydroxylation step reaction states cartesian coordinates for AlkB-dsDNA

Snapshot 1

RC2

QM/MM (BS1) = -3375.982529 a.u.

QM/MM (BS2+ZPE) = -3377.931323 a.u.

6	27.513498642	22.629163518	37.006586909
7	27.067532430	23.585801841	37.891787747
1	26.274960111	23.489520226	38.536976848
6	27.893289656	24.641015571	37.845554246
1	27.754109097	25.543113378	38.434624120
7	28.866604148	24.4122289781	36.972199008
6	28.660234260	23.153007899	36.454852215
1	29.361204744	22.709916326	35.757497679
6	31.459532509	24.418974189	32.197653092
1	30.988141812	25.296891850	31.737316088
1	32.508067451	24.349266120	31.873235720
6	31.498535661	24.510642474	33.712235284
8	30.704245896	25.443262415	34.214181802
8	32.270499707	23.830301452	34.363428218
6	26.399296206	27.450541292	34.872800151
7	26.664435656	26.626605526	33.799122336
1	26.045748970	26.424118640	33.006263060
6	27.890105300	26.094460979	33.983858336
1	28.372308633	25.413398593	33.288954552
7	28.425092661	26.534698254	35.114663084
6	27.507270315	27.383523147	35.682001977
1	27.715320203	27.885073089	36.624344613
6	35.714964168	27.862752652	35.916142526
1	34.657037023	28.166793817	35.999336111
1	36.012711198	27.502203253	36.913939344
7	35.880640315	26.854135053	34.875885662
1	36.406904782	27.079165831	34.022698935
6	35.109657289	25.751696264	34.795354563
7	34.206266819	25.456190633	35.727279171
1	33.885209240	26.140022823	36.411493659
1	33.573424784	24.66378792	35.563031062
7	35.211816608	24.987286096	33.688303645
1	36.094298418	25.030201376	33.163205999
1	34.773835105	24.058668164	33.661741683
26	30.183773317	25.714738827	36.050047632
8	31.436353741	25.027006490	36.794326437
8	32.578597597	27.629576852	37.280597100
6	31.426872213	28.065347040	37.330509829
8	30.380026891	27.487034615	36.828978074
6	31.125008306	29.442254140	37.914703795
6	31.961812308	29.889972118	39.118212369
6	31.711888317	31.382772459	39.357705614
8	30.884369392	31.707227578	40.249859540
8	32.311007675	32.191381580	38.591952887
1	33.026447690	29.707227688	38.917674507
1	31.672424871	29.315045930	40.012228978
1	30.050284424	29.488113894	38.145564233
1	31.310163552	30.146215422	37.083234391
8	29.117790850	21.875809588	41.428275000
6	29.567584707	21.217007123	40.506056170
7	30.758324641	21.605413429	39.862559607

6	31.469557544	22.757280071	40.417076921
6	31.245512813	21.011718577	38.716864420
7	32.328833386	21.478355235	38.139916097
6	30.532872686	19.890540278	38.195135647
6	29.451972490	19.429673726	38.867818850
7	28.983983499	20.062814392	39.999976635
1	31.395331248	23.619205049	39.732831682
1	32.527006599	22.498066094	40.568200254
1	32.782500513	22.311469549	38.494550040
1	28.917501103	18.549974495	38.513560633
1	30.890409182	19.388533090	37.299046680
1	31.018701412	23.005588177	41.381253765
1	32.623907044	21.152844800	37.155177732
8	34.786376219	28.164111248	38.930001050
1	34.554419585	27.952840364	39.857753100
1	33.985446445	27.925572082	38.426915917
8	32.742523633	21.039239292	35.655893001
1	33.385513842	20.652654457	35.021367944
1	31.838857672	20.799279683	35.293645774
1	26.900753372	21.777642737	36.710744187
1	30.928542928	23.543028264	31.825045897
1	25.443338849	27.950291492	35.029205361
1	36.277928549	28.767427949	35.686575481
1	28.144514491	19.731491156	40.430661197

TS7

QM/MM (BS1) = -3375.952287 a.u.

QM/MM (BS2+ZPE) = -3377.893800 a.u.

6	27.399831014	22.422807490	36.932698112
7	26.992417768	23.324799826	37.889399814
1	26.204323452	23.214975798	38.535258932
6	27.857786271	24.346160045	37.923822164
1	27.758844593	25.199474325	38.588952182
7	28.818475398	24.151869883	37.031633402
6	28.563036237	22.946033421	36.416855680
1	29.247148197	22.530268254	35.685191910
6	31.426533968	24.247394774	32.421369627
1	31.007101397	25.175894351	32.012221854
1	32.472730661	24.147782020	32.092342184
6	31.474578521	24.266708421	33.942112416
8	30.898750000	25.326525882	34.483418381
8	32.085926132	23.423529119	34.580248933
6	26.445927416	27.376078809	34.944827594
7	26.740438918	26.559404937	33.874237544
1	26.138906454	26.358435335	33.070646362
6	27.953750496	26.008536643	34.105465215
1	28.443656924	25.323373886	33.419404041
7	28.454056644	26.425763948	35.257904153
6	27.524025729	27.280197913	35.794774517
1	27.695363252	27.764352714	36.754421831
6	35.721150187	27.751503301	35.896838118
1	34.663595524	28.047352812	36.002560229
1	36.043462810	27.393861662	36.888063963
7	35.865084351	26.738717235	34.854533265
1	36.395360150	26.960121096	34.001310681
6	35.099114428	25.635328975	34.785752261
7	34.204709143	25.340684363	35.729182272
1	33.895473956	26.011681957	36.433239266
1	33.604546963	24.521728023	35.605507802
7	35.181669058	24.862731959	33.676379224
1	36.062156409	24.920601402	33.147592804

1	34.809001018	23.902077387	33.704325767
26	30.300965170	25.467282554	36.335188802
8	31.508946149	24.612446662	37.264647550
8	32.661998413	27.519123150	37.297521273
6	31.502047223	27.916170439	37.449424037
8	30.443782526	27.260114583	37.103778793
6	31.207328870	29.316553418	37.980920003
6	32.083526843	29.830254000	39.129988642
6	31.786677986	31.319381406	39.342622602
8	30.936715631	31.627691793	40.219150268
8	32.369738163	32.138295556	38.575637326
1	33.143380410	29.674547209	38.887963871
1	31.853352208	29.273215537	40.052167149
1	30.143305169	29.359333837	38.256755703
1	31.352083650	29.985193892	37.112152780
8	29.561006520	22.207467857	40.485555897
6	29.885819929	21.383502447	39.657829417
7	30.981686612	21.642381465	38.774730095
6	31.764810789	22.807120339	39.042046014
6	31.297403522	20.835482958	37.684619649
7	32.221893781	21.217700678	36.834533171
6	30.590729926	19.605251155	37.561596331
6	29.630660127	19.289248923	38.466296632
7	29.278412645	20.142540331	39.491890661
1	31.590256831	23.725032196	38.168725718
1	32.841890531	22.603112778	38.961116969
1	32.532827585	22.184717273	36.806014026
1	29.097372689	18.346228231	38.384366537
1	30.811688113	18.933876930	36.734977647
1	31.467210786	23.261616454	39.990677350
1	32.505652598	20.638511734	35.978170756
8	34.877187147	28.102502104	38.918323087
1	34.640147680	27.893463586	39.844787395
1	34.083414272	27.845828548	38.413113599
8	32.855582897	20.104090905	34.488730262
1	32.904338875	19.108891595	34.409875581
1	31.878336613	20.213125332	34.291837781
1	26.755324531	21.614295335	36.587753451
1	30.861025282	23.424017385	31.985116353
1	25.493290716	27.893748400	35.056938408
1	36.272299844	28.660275081	35.655104310
1	28.489542265	19.917606255	40.063782849

Snapshot 2

RC2

QM/MM (BS1) = -3528.063820 a.u.

QM/MM (BS2+ZPE) = -3530.159254 a.u.

6	27.871007140	21.612468272	41.928123500
7	27.900134029	22.615105189	42.873033905
1	27.596506486	22.535973156	43.851587029
6	28.398035458	23.724078830	42.295826418
1	28.515861472	24.672075656	42.814111961
7	28.691520198	23.488139989	41.023065163
6	28.373652579	22.168375676	40.776960843
1	28.499560564	21.723543047	39.794174269
6	28.916651647	22.926306439	35.728216460
1	28.225006627	23.391707077	35.009958825
1	29.914530065	22.975595696	35.262996388
6	28.974914062	23.787229398	36.974894790
8	28.728027083	23.281822326	38.124685873
8	29.289691720	24.999181440	36.903898032

6	24.970855058	25.764235325	40.069949642
7	24.806850450	24.746505516	39.152053926
1	23.924953842	24.334653599	38.823136721
6	26.030607965	24.344843389	38.759650411
1	26.207850752	23.538743516	38.055748608
7	26.972172880	25.063914899	39.357901256
6	26.323685011	25.954938725	40.182848259
1	26.871837831	26.680600809	40.774597431
6	34.557709834	27.283698061	36.418512645
1	33.681079831	27.846317576	36.782073946
1	35.207613798	27.114480369	37.293372900
7	34.148424401	26.039611471	35.793446981
1	34.508716853	25.815229628	34.865918878
6	33.301187643	25.161812092	36.362785983
7	32.923921662	25.322416398	37.631987267
1	33.367365423	25.979888580	38.294059413
1	32.147841405	24.776801231	38.008751393
7	32.798643446	24.155928746	35.637261776
1	33.106741580	24.062658208	34.659819633
1	32.566558830	23.261280771	36.111594031
26	29.084190095	24.788734898	39.378270506
8	30.689559164	24.557981581	39.409698941
8	28.663610421	28.704027408	39.059470778
6	29.440695041	27.768828834	39.286950494
8	29.045996452	26.664593525	39.841832570
6	30.906729056	27.903070254	38.934734398
6	31.312726457	29.314610465	38.531545171
6	31.162698373	30.402003961	39.613826620
8	31.153877798	30.059099612	40.825990136
8	31.097238946	31.592627418	39.194169450
1	30.743526178	29.648852574	37.651250515
1	32.374542050	29.309941714	38.226093241
1	31.108328163	27.191961544	38.116819409
1	31.496147923	27.529913630	39.783151565
8	31.652253380	21.730879296	44.099143121
6	31.545515286	20.861791074	43.257241221
7	32.007218065	21.068674374	41.931542059
6	32.649310986	22.356236383	41.652452523
6	31.854868004	20.157172659	40.913927356
7	32.291795773	20.444164521	39.697817442
6	31.227479167	18.919519653	41.208135947
6	30.829595990	18.681882762	42.482991659
7	30.980974397	19.610947579	43.483188693
1	32.764273474	22.881634444	42.604884468
1	32.030586813	22.963449242	40.970463796
1	32.677502714	21.339949836	39.423313396
1	30.369820337	17.736584130	42.743996700
1	31.083068395	18.162876188	40.437831385
1	33.640959813	22.184003556	41.207841873
1	32.149111939	19.780579198	38.926020563
8	32.780654621	21.581776917	36.674533577
1	33.318427571	21.405634047	35.862041126
1	32.217445512	20.769352010	36.786609138
8	28.300252827	29.894343609	41.847029468
1	29.119404407	29.613180592	41.401182273
1	27.608878041	29.664799150	41.202834327
8	26.093335980	29.127539243	39.662668695
1	26.125553048	30.073198344	39.433111901
1	26.977820535	28.807029595	39.354588422
8	34.136887792	26.830958963	39.643562195
1	34.539609591	26.066163554	40.132080872
1	33.801310500	27.438968482	40.345098332

1	27.357377092	20.661201283	42.067201229
1	28.626680268	21.884103516	35.861621806
1	24.166690127	26.224234751	40.644220148
1	35.093028413	27.917982638	35.711982805
1	30.619090752	19.391316509	44.389154982

TS7

QM/MM (BS1) = -3528.029559 a.u.

QM/MM (BS2+ZPE) = -3530.125014 a.u.

6	27.799647387	21.462995257	41.977020298
7	27.848875481	22.460587687	42.926188178
1	27.542133714	22.389649958	43.903336521
6	28.386493420	23.555674240	42.360724737
1	28.538286003	24.493019215	42.889732543
7	28.683333778	23.318187815	41.090005582
6	28.326834030	22.010806911	40.834434445
1	28.440198015	21.569602327	39.848644801
6	28.931794176	22.842701186	35.752125799
1	28.227380024	23.365845650	35.086972228
1	29.914930605	22.891562497	35.257981106
6	29.048316487	23.597087567	37.060353693
8	28.723682565	23.050722027	38.159632426
8	29.493613305	24.783666676	37.101174310
6	25.065399993	25.730832514	40.090944728
7	24.877494126	24.728069288	39.161869201
1	23.987462481	24.327641361	38.843066039
6	26.095395003	24.306458946	38.763670952
1	26.248726074	23.500108787	38.053746678
7	27.056433657	24.993937521	39.365151900
6	26.426705476	25.887644005	40.200104353
1	26.992272948	26.590743205	40.805317854
6	34.521594175	27.254171727	36.437195750
1	33.661431056	27.837681515	36.809768861
1	35.173089899	27.066013332	37.306857749
7	34.084592560	26.020695464	35.809729161
1	34.370983440	25.832534143	34.849352630
6	33.283188849	25.113614829	36.403780429
7	32.964581721	25.232473040	37.692779737
1	33.395966400	25.920611880	38.329371961
1	32.267910940	24.616083406	38.123714462
7	32.770472404	24.119139349	35.668857865
1	33.089984653	24.024231092	34.695351552
1	32.503695028	23.228527900	36.127618836
26	29.288597058	24.539982257	39.429061600
8	30.976635731	23.940287588	39.593544764
8	28.661514731	28.385707015	39.209995347
6	29.579979858	27.570911405	39.352194582
8	29.437106854	26.410236178	39.909176439
6	30.977548160	27.903400244	38.863737184
6	31.183240775	29.354526749	38.459331956
6	31.120506510	30.408347251	39.583617626
8	31.153777397	30.036572552	40.783859938
8	31.066809963	31.611465906	39.193178952
1	30.442529667	29.649290134	37.700509249
1	32.169445659	29.466482319	37.973904303
1	31.169228256	27.233319704	38.008127371
1	31.690417083	27.581632118	39.633288081
8	31.282132027	21.980933681	43.794571827
6	31.267643107	21.049374285	43.018289451
7	31.696157926	21.228436108	41.663726591
6	32.219175340	22.519415856	41.302580756

6	31.641754371	20.224204054	40.713137420
7	32.030383789	20.484566654	39.477925324
6	31.182559829	18.944256927	41.112704905
6	30.827542444	18.745749016	42.408754695
7	30.873428102	19.754319492	43.342893433
1	32.275029358	23.157969364	42.187641987
1	31.498457215	23.162124813	40.488645318
1	32.208199346	21.418283299	39.118354294
1	30.479242334	17.771290564	42.737698533
1	31.106218926	18.128033221	40.395172629
1	33.178242591	22.430427176	40.772841187
1	31.964034773	19.759254948	38.752864131
8	32.630282534	21.518492049	36.606642237
1	33.233853511	21.368780688	35.835585756
1	32.081492278	20.689650805	36.659274503
8	28.245047045	29.891569440	41.820154958
1	29.022278035	29.536356058	41.355214747
1	27.511572421	29.649772839	41.227958440
8	26.118179793	30.085176212	39.682545503
1	26.237027553	30.005439679	39.389692363
1	26.972252183	28.658521567	39.432477460
8	34.154162207	26.799781903	39.679118578
1	34.519628753	26.025468278	40.182656004
1	33.829892723	27.427252413	40.368366393
1	27.249437633	20.529603511	42.095832751
1	28.614141186	21.804024239	35.843307500
1	24.258132590	26.201847611	40.651775757
1	35.067763613	27.879819121	35.731269691
1	30.548017230	19.556315251	44.267487713

**Snapshot 3
RC2**

QM/MM (BS1) = -3453.536340 a.u.

QM/MM (BS2+ZPE) = -3455.550390 a.u.

6	29.743526712	21.863207163	45.728228760
7	30.202554378	22.989525843	46.378482468
1	30.619257765	23.020710480	47.318835382
6	30.027438350	24.050857450	45.572083519
1	30.265929106	25.080985220	45.837575317
7	29.486359074	23.653045325	44.424099704
6	29.302573555	22.290506314	44.500758384
1	28.860408546	21.714677529	43.690637415
6	25.935071453	22.473129124	40.389531642
1	25.144928205	23.167540381	40.698542278
1	26.019133603	22.511340150	39.297841057
6	27.291575981	22.836629591	40.988835492
8	27.214863028	23.715028348	41.984959629
8	28.327453760	22.374405382	40.560416993
6	26.103374626	25.814580344	46.107095593
7	25.371799668	24.789316485	45.543616318
1	24.511276032	24.357383334	45.904150863
6	26.012678837	24.385616655	44.433568458
1	25.668573737	23.597489546	43.770199965
7	27.113310855	25.104186679	44.251837693
6	27.194621400	25.999942493	45.293318289
1	28.053280751	26.665789106	45.392294284
6	31.306993933	26.555017327	37.088426620
1	31.278556816	26.818351225	38.160682250

1	32.333220218	26.228448680	36.856345492
7	30.342412237	25.527220741	36.756007728
1	29.434497735	25.837899243	36.389993674
6	30.420575325	24.233021108	37.107659059
7	31.474584103	23.760469164	37.777763978
1	32.110618733	24.372188861	38.306642612
1	31.463466301	22.777174336	38.031640769
7	29.394139069	23.435072898	36.786660146
1	28.699491962	23.804212278	36.122217339
1	29.514308411	22.416309854	36.659221728
26	28.604369335	24.667177549	42.862470226
8	29.839802972	24.304128005	41.856606502
8	30.904368524	27.202632991	42.6711106233
6	29.820887277	27.148651487	42.080488177
8	28.758047721	26.594263551	42.584172841
6	29.636365250	27.809698590	40.714876969
6	29.214584471	29.280245387	40.826475635
6	30.268012170	30.183838490	41.488452815
8	29.839513332	31.021518588	42.336412582
8	31.464050703	30.044120409	41.141112209
1	28.275141710	29.392458566	41.382918160
1	29.034837083	29.671703135	39.807796498
1	28.898832593	27.231026430	40.148003286
1	30.583090765	27.769305908	40.163114287
8	34.282201468	22.268058477	45.174578926
6	33.593980473	21.446253174	44.601921998
7	32.885124682	21.782541257	43.423458446
6	33.034004833	23.160520983	42.935534369
6	32.079584557	20.902476930	42.735747128
7	31.361051236	21.337833698	41.715476766
6	32.045567683	19.546372957	43.169909147
6	32.683240493	19.210209220	44.320765749
7	33.427687719	20.127841825	45.029473725
1	33.305860347	23.157765821	41.869208514
1	33.828283956	23.633820628	43.519296769
1	30.820256774	20.686865761	41.119927963
1	32.585080722	18.203475476	44.728387724
1	31.449404400	18.809603199	42.634689170
1	32.095582834	23.723658774	43.056978372
1	31.184504307	22.326114789	41.547187007
8	28.771433514	24.945555242	39.376055502
1	28.627456349	24.103842978	38.914865925
1	29.232996997	24.665415961	40.194042665
8	33.243572793	25.313062110	39.492962329
1	33.172596513	26.139519877	40.028319871
1	34.192669805	25.144732928	39.406271200
8	30.302348074	27.452958669	45.429579616
1	29.901690849	28.329089335	45.252349090
1	30.622837390	27.211218532	44.533523642
1	29.560204266	20.906940365	46.218141015
1	25.620151706	21.476004339	40.697159734
1	25.848800448	26.274854630	47.061771922
1	31.081685707	27.454643622	36.515734676
1	33.734182540	19.892586289	45.951801348

TS7

QM/MM (BS1) = -3453.499251 a.u.

QM/MM (BS2+ZPE) = -3455.515109 a.u.

6	29.673496258	21.777341079	45.862805282
7	30.165934138	22.887367228	46.514824552
1	30.604268851	22.905673083	47.444379154

1	28.274906020	29.442508362	41.460338749
1	28.958478097	29.835869952	39.877471837
1	28.905475677	27.393830049	40.019269215
1	30.583206300	27.950411059	40.085992455
8	34.373293712	22.273623321	45.159893496
6	33.666424537	21.471345219	44.587162556
7	33.000970536	21.844872479	43.367373844
6	33.289245367	23.114517154	42.887614771
6	32.123827686	20.996393255	42.689815480
7	31.400635679	21.483755087	41.697068822
6	32.058016493	19.643350112	43.121529207
6	32.671515973	19.276484644	44.278974177
7	33.431783058	20.169394960	45.007398472
1	33.039622902	23.357597936	41.857240530
1	33.974139731	23.702505417	43.489918870
1	30.850452104	20.844966253	41.094861096
1	32.535724746	18.272079470	44.684095970
1	31.434811919	18.929189791	42.585130752
1	31.010049380	24.855239873	42.004138378
1	31.163534701	22.485122381	41.612403155
8	28.983533883	25.040993322	39.441219082
1	28.733401572	24.148419631	39.144945398
1	29.567589035	24.812909238	40.202852789
8	33.129797536	25.254047814	39.657993229
1	33.115067998	26.141759662	40.090588306
1	34.068946159	25.041464014	39.553291118
8	30.313049250	27.427591219	45.294251546
1	29.918649514	28.310920151	45.138223703
1	30.632031347	27.192299831	44.397976917
1	29.539760567	20.844063821	46.232669640
1	25.584351283	21.464588144	40.657421475
1	25.851638934	26.266165306	47.032673709
1	31.058252934	27.420427217	36.511040943
1	33.727133767	19.918072598	45.929123764

TSS

QM/MM (BS1) = -3453.514459 a.u.

QM/MM (BS2+ZPE) = -3455.525257 a.u.

6	29.681312153	21.665218559	45.884433068
7	30.197430545	22.766727319	46.531857122
1	30.629420355	22.785758899	47.463536112
6	30.047969612	23.837025596	45.732525362
1	30.339613402	24.852852527	45.994738203
7	29.463566187	23.476035117	44.597930970
6	29.227247809	22.124648697	44.674212367
1	28.730173955	21.576506709	43.878371886
6	26.072706561	22.389111895	40.354567604
1	25.314944002	23.122106466	40.661022045
1	26.143030433	22.393478677	39.261964474
6	27.441509596	22.741310301	40.928288957
8	27.429104263	23.462717324	42.016005733
8	28.472819840	22.404353894	40.348640602
6	26.114436208	25.821386590	46.119539889
7	25.402738614	24.788383884	45.547923863
1	24.547069623	24.343838206	45.903030378
6	26.057119549	24.411402896	44.430385388
1	25.730700241	23.614072103	43.767385383
7	27.143025365	25.149776247	44.249702552
6	27.199900092	26.032999687	45.300817752
1	28.046790006	26.711448916	45.407992253
6	31.272235159	26.512655265	37.072299954
1	31.246646576	26.765783122	38.146940448

1	32.297111544	26.187043195	36.831279371
7	30.304855167	25.491573472	36.730880815
1	29.400693686	25.804883621	36.361263308
6	30.387394425	24.186605035	37.050866662
7	31.458855522	23.704631206	37.691686933
1	32.071707399	24.308780753	38.252069208
1	31.453055538	22.716293071	37.922080790
7	29.375222998	23.393036661	36.709146569
1	28.661416871	23.765461359	36.069644410
1	29.475411275	22.369052109	36.612822932
26	28.793165352	24.511041797	42.917000565
8	30.580435211	24.199993627	42.111794144
8	31.057150722	26.978511392	42.366983284
6	29.911058631	27.085382769	41.863872100
8	28.885969410	26.489912851	42.327365964
6	29.696496063	27.940362147	40.612985916
6	29.219008557	29.364426745	40.898036873
6	30.282338570	30.273401486	41.533455895
8	29.858340120	31.126111698	42.369833846
8	31.474198058	30.128160799	41.177153053
1	28.329610681	29.379191050	41.542553119
1	28.921179123	29.835018633	39.942211641
1	28.970404937	27.407883674	39.989920029
1	30.635719231	28.004156555	40.050517201
8	33.525449035	22.543502491	45.102002372
6	33.025946083	21.607202196	44.522677223
7	32.367471792	21.822210727	43.251177877
6	32.451481040	23.091341884	42.700057504
6	31.684842740	20.809936683	42.567086105
7	30.963840352	21.144795341	41.520122745
6	31.805878992	19.485654292	43.065792857
6	32.464999286	19.261374321	44.234267828
7	33.066197231	20.282258572	44.946082037
1	32.591546374	23.160379195	41.623149528
1	32.865305158	23.848635819	43.360044173
1	30.505127547	20.426329179	40.930286284
1	32.493873017	18.258226679	44.661604762
1	31.312317996	18.661336015	42.554110504
1	31.088262073	25.026635981	42.232525928
1	30.675886309	22.110295753	41.337382574
8	29.181415964	24.929053230	39.588026461
1	28.923654625	24.000613610	39.421600497
1	29.787123694	24.794616512	40.342477169
8	33.188752088	25.201717952	39.525883134
1	33.176050194	26.090708541	39.955450741
1	34.127117540	24.989964029	39.412037862
8	30.406870291	27.381976394	45.192840309
1	30.003632835	28.259019119	45.025784687
1	30.738159707	27.133690085	44.306372308
1	29.446843551	20.717741909	46.369592623
1	25.712504968	21.416886726	40.690871563
1	25.848278594	26.275034868	47.074228681
1	31.048725887	27.419241945	36.509973074
1	33.449987777	20.085867115	45.848361209

PD

QM/MM (BS1) = -3453.609297 a.u.

QM/MM (BS2+ZPE) = -3455.604508 a.u.

6	29.782674594	21.702401093	45.631315212
7	30.220690415	22.849663343	46.260875920
1	30.590031893	22.916538991	47.218408954

6	30.116568960	23.871731829	45.391619710
1	30.355444020	24.904858273	45.642250565
7	29.643395010	23.442415502	44.223545607
6	29.436841434	22.083744576	44.357955384
1	29.050599718	21.473513835	43.543529807
6	26.278122522	22.211502294	40.139318377
1	25.422670800	22.883352402	39.973682532
1	26.764686667	22.002773080	39.177420932
6	27.237213110	22.920949424	41.075200378
8	26.735550395	23.623478790	42.025445281
8	28.479019723	22.909663412	40.915518132
6	26.052816735	25.943401772	46.179259849
7	25.262657755	24.957886241	45.627909412
1	24.362365347	24.599932319	45.967403086
6	25.890562571	24.493240681	44.533182244
1	25.488885955	23.730982439	43.870245179
7	27.041366234	25.129863280	44.348557726
6	27.165601786	26.035755119	45.377038512
1	28.057170262	26.659597478	45.480651226
6	31.349914235	26.549620799	37.048837140
1	31.353238151	26.803570865	38.125385688
1	32.358756396	26.194576954	36.776177393
7	30.341299986	25.567513048	36.721722937
1	29.468493177	25.906239490	36.299797973
6	30.348266006	24.276544842	37.090893348
7	31.378218344	23.767198346	37.794958831
1	31.933888201	24.370561260	38.398180254
1	31.295278505	22.796817544	38.088114825
7	29.337981916	23.505710600	36.720938480
1	28.645089742	23.868947426	36.054518487
1	29.406354983	22.473522525	36.742388976
26	28.416150508	24.423871444	42.854268529
8	33.178849187	23.772602188	42.359226149
8	30.495400189	27.561698217	42.741531337
6	29.765450859	27.134418418	41.834221309
8	29.142586604	26.015209590	41.846432371
6	29.571739669	27.979345630	40.563422577
6	29.148759525	29.416469354	40.861251180
6	30.220319144	30.287728790	41.533185766
8	29.807886043	31.127696314	42.384320094
8	31.411973026	30.151641828	41.163402769
1	28.241420736	29.451240818	41.482540365
1	28.893853702	29.913213049	39.905639355
1	28.846412670	27.483216865	39.906728518
1	30.526668024	28.013408319	40.015260735
8	34.854171276	22.115466630	45.192050359
6	34.137547121	21.355030229	44.570718088
7	33.685826646	21.665866500	43.265271899
6	34.227013356	22.887173104	42.638685787
6	32.807525665	20.874196724	42.549663097
7	32.347672340	21.320845500	41.394744785
6	32.448955367	19.608514983	43.082722623
6	32.902905186	19.270010383	44.315182405
7	33.703784588	20.119361929	45.047013199
1	34.754101413	22.569854443	41.720501536
1	34.954806950	23.295210203	43.352772611
1	31.680207005	20.765911348	40.832201857
1	32.613896169	18.320140951	44.766231825
1	31.789317252	18.940767644	42.531778959
1	33.389300598	24.340505802	41.584572285
1	32.393104905	22.324707775	41.229470998
8	28.851234020	25.078332703	39.318110551

1	28.783914249	24.114301944	39.449870844
1	29.056397320	25.376841436	40.227288924
8	33.312348600	25.397595884	40.081368308
1	33.133478826	26.299643859	40.465583996
1	34.178223774	25.479987104	39.653954723
8	30.102558786	27.621271928	45.488786496
1	29.722051731	28.512040341	45.341957706
1	30.346549985	27.387673564	44.567326289
1	29.574081411	20.766418331	46.149477817
1	25.870559301	21.280487252	40.533235296
1	25.837885622	26.406020276	47.142512702
1	31.139302119	27.461368396	36.489886183
1	33.919598544	19.865012503	45.989723756

Snapshot 4
RC2
QM/MM (BS1) = -3387.649551 a.u.
QM/MM (BS2+ZPE) = -3389.601928 a.u.

6	28.147647136	43.730064062	43.113309518
7	29.412446532	43.278708386	43.408698698
1	30.052598939	43.655280431	44.123849237
6	29.691071329	42.259639563	42.579589182
1	30.631143705	41.713879185	42.594106689
7	28.670312531	42.030694016	41.765234270
6	27.693176056	42.942850276	42.081938848
1	26.764334986	42.999031749	41.519358840
6	25.885963190	42.097265350	37.195442225
1	26.395165549	42.499997447	36.307275158
1	25.267421954	41.251756747	36.860492612
6	26.935677240	41.543949443	38.143210490
8	27.005108354	41.983973343	39.346881463
8	27.746154917	40.687080061	37.747134553
6	31.468356518	43.859757897	38.754516656
7	30.294490062	44.402947209	38.287671402
1	30.161278288	45.323400185	37.851606234
6	29.304782870	43.541164146	38.565178047
1	28.262211576	43.733031921	38.348039090
7	29.772589492	42.458171616	39.164817612
6	31.127981975	42.641053908	39.299541780
1	31.744889208	41.892615897	39.790121882
6	22.610906892	38.892616784	34.069814105
1	21.526553800	38.968449545	33.869426074
1	23.062084955	39.849250222	33.757533524
7	22.904868569	38.613091105	35.456701048
1	23.334612349	37.721475040	35.725800030
6	22.764562556	39.523282477	36.438398840
7	22.237524865	40.733488556	36.205120305
1	21.633674103	40.938154885	35.403168165
1	22.087002307	41.290333330	37.055197792
7	23.188521248	39.245276039	37.660453584
1	23.599371438	38.355537357	37.966402454
1	23.039171363	39.970090747	38.372323410
26	28.558360750	40.869029106	39.989604539
8	27.568350240	39.762843705	40.625857624
8	29.377001722	37.744913126	39.591015259
6	30.289436255	38.555548376	39.659146476
8	30.159267642	39.840435902	39.865622590
6	31.739229630	38.109719258	39.526760886
6	32.239880786	37.493421019	40.832363917
6	33.578202127	36.756572180	40.736558673
8	34.210249529	36.781154839	39.648496784

8	33.947164990	36.139919561	41.767887428	1	23.146327745	39.838245600	33.664015368
1	31.500656323	36.770285777	41.212742673	7	22.976244319	38.583629876	35.347393968
1	32.326915325	38.259197083	41.622215303	1	23.373546714	37.672785758	35.603278103
1	32.366575921	38.959920615	39.225849276	6	22.857651798	39.484305275	36.337326139
1	31.792426666	37.359513208	38.725045309	7	22.362822401	40.709517017	36.109804968
8	26.467207845	41.248784835	45.453745834	1	21.745447360	40.920882142	35.319446800
6	25.603062387	42.077191535	45.287985881	1	22.221461981	41.263027905	36.963430467
7	24.599877337	41.897484841	44.299452665	7	23.276566775	39.181026592	37.556510483
6	24.646285309	40.626301503	43.562382767	1	23.634621644	38.263630821	37.848415073
6	23.631613213	42.825251047	44.030250022	1	23.124205681	39.888376207	38.283940480
7	22.804979886	42.654059222	43.010379320	26	28.202000376	40.775971435	40.506818493
6	23.520714637	43.960346020	44.892449997	8	26.952278504	39.962160327	41.495802404
6	24.454782270	44.146015700	45.860568243	8	29.044409169	37.617359601	39.873499082
7	25.499668942	43.269147985	46.015606059	6	29.940141821	38.441242883	40.028437920
1	25.107477876	40.759181408	42.573099527	8	29.767658782	39.657574608	40.463198650
1	23.629246700	40.230270923	43.449490125	6	31.397972637	38.077238639	39.756703561
1	22.098223569	43.365231719	42.836105551	6	32.064715253	37.530529468	41.022335116
1	24.402935584	45.005375115	46.534057774	6	33.385781976	36.779177405	40.823721770
1	22.687523752	44.649925656	44.774784806	8	33.967253902	36.825306489	39.708297443
1	25.248551578	39.922552029	44.144741139	8	33.799770822	36.129681114	41.818238119
1	22.857831908	41.883044356	42.331376482	1	31.386403790	36.834890551	41.539726878
8	24.239346708	37.166931886	39.227323992	1	32.243008414	38.344266596	41.745159699
1	23.513389242	37.026848322	39.858225296	1	31.939757650	38.959332303	39.383010114
1	24.647337583	38.002921838	39.589011218	1	31.419780698	37.314477928	38.966950963
8	24.831880978	39.642420421	39.992912140	8	26.810320029	40.969369066	45.590165506
1	24.104532903	40.161445870	40.424494653	6	25.937203339	41.729659668	45.253906475
1	25.698100520	39.921583899	40.346809040	7	25.088673774	41.408783936	44.141536373
1	27.750721505	44.676124332	43.481395555	6	25.366858867	40.153762534	43.493342112
1	25.242409581	42.872970346	37.610397444	6	24.075120290	42.245661669	43.724361595
1	32.378278592	44.459094502	38.784596202	7	23.348940300	41.968876895	42.660073300
1	23.025895756	38.107529967	33.437761692	6	23.803523872	43.424870566	44.483651370
1	26.218220430	43.458748991	46.684715707	6	24.601072436	43.744248695	45.534790684
				7	25.671110120	42.956604064	45.873440845
				1	26.200651872	40.216037340	42.532886845
				1	24.468260980	39.705208328	43.055846108
				1	22.707260407	42.689239010	42.300907795
				1	24.405344176	44.637064183	46.134933745
				1	22.941031590	44.042475255	44.231379361
				1	25.876426051	39.477997721	44.187810405
				1	23.432556830	41.151191337	42.050566103
				8	24.151741203	36.914203885	39.026360798
				1	23.404390968	36.782790045	39.630984895
				1	24.616006480	37.702662878	39.441553622
				8	24.892523389	39.226792486	39.921873127
				1	24.076726136	39.685577260	40.258534989
				1	25.650953754	39.470781997	40.508761499
				1	27.715572610	44.926003099	43.611942725
				1	25.238113138	42.862693999	37.759388235
				1	32.278765609	44.347375163	38.840908679
				1	23.085086337	38.096316696	33.330180508
				1	26.311203079	43.254975977	46.581415212

TS7

QM/MM (BS1) = -3387.608678 a.u.

QM/MM (BS2+ZPE) = -3389.562261 a.u.

6	28.084061499	43.949678208	43.297184139	6	30.556341623	22.656880214	48.650120925
7	29.345598920	43.483807550	43.583351453	7	31.469747296	23.627821023	48.995964055
1	30.015170275	43.871134964	44.262760027	1	32.202435574	23.543577365	49.713515694
6	29.583560981	42.421508930	42.801741532	6	31.253901807	24.702055204	48.216952802
1	30.513223969	41.859073743	42.813389591				
7	28.535881978	42.175979852	42.030709172				
6	27.586997742	43.125553711	42.319192715				
1	26.651235160	43.179749410	41.768155334				
6	25.880942314	42.034255823	37.461851421				
1	26.534943470	42.368587818	36.641522252				
1	25.275560917	41.200418400	37.079084372				
6	26.741009297	41.501137823	38.597637102				
8	26.792037621	42.106657389	39.713781915				
8	27.452980773	40.476677228	38.435004037				
6	31.367509395	43.750222656	38.873898255				
7	30.186104205	44.290052873	38.426459497				
1	30.054937718	45.204757926	37.978335676				
6	29.199156705	43.440059292	38.761737550				
1	28.152306684	43.644606312	38.580449542				
7	29.667348970	42.369637129	39.380114625				
6	31.027350470	42.548790960	39.465529807				
1	31.661545717	41.817580045	39.962721790				
6	22.681893258	38.885030377	33.965344567				
1	21.597777464	38.977139948	33.769379659				

Snapshot 5

RC2

QM/MM (BS1) = -3454.993953 a.u.

QM/MM (BS2+ZPE) = -3457.012097 a.u.

6	30.556341623	22.656880214	48.650120925
7	31.469747296	23.627821023	48.995964055
1	32.202435574	23.543577365	49.713515694
6	31.253901807	24.702055204	48.216952802

1	31.830220261	25.620774738	48.284393585	1	28.530283049	22.995805129	41.885558964
7	30.244817950	24.477971113	47.382675743	8	28.421972447	27.145117372	42.699053994
6	29.797310414	23.196950830	47.635419052	1	28.518917169	26.752177250	41.812397563
1	28.983609905	22.754182585	47.061798905	1	28.941775438	26.564507481	43.288608319
6	25.489304614	24.019734720	45.195384191	8	31.875955178	25.751465908	43.001536065
1	24.921444450	24.898513427	45.524752932	1	31.130238874	25.133409397	43.033280873
1	25.311598623	23.867061004	44.120344586	1	31.736885730	26.323415977	43.788319772
6	26.992506209	24.219456755	45.385449376	1	30.427151035	21.740243675	49.225581239
8	27.320269670	25.298291524	46.073103358	1	25.100149083	23.149409097	45.723738808
8	27.811193166	23.435846741	44.931969187	1	28.287639786	27.641411197	51.324392799
6	28.130104746	27.238075658	50.324107598	1	29.690993652	27.910839645	36.987181238
7	27.124923333	26.336502165	50.040853172	1	33.861309140	19.648763437	47.097410369
1	26.386274884	26.020826113	50.675770529	TS7			
6	27.296824541	25.907753921	48.779178652	QM/MM (BS1) = -3454.951357 a.u.			
1	26.658510400	25.198075138	48.268672523	QM/MM (BS2+ZPE) = -3456.971787 a.u.			
7	28.349876688	26.489938998	48.228231051	6	30.615522303	22.506379447	48.834224712
6	28.88522987	27.322002429	49.180889717	7	31.555510000	23.449714698	49.176680557
1	29.778866391	27.906701018	48.970707049	1	32.285088086	23.356638807	49.894128900
6	29.868800525	27.324628000	37.888739861	6	31.385186508	24.520469634	48.387150927
1	29.572792446	27.932971081	38.759108470	1	31.996562827	25.415655497	48.450708358
1	30.959839196	27.164388769	37.960880442	7	30.374848532	24.322209150	47.551376439
7	29.145929300	26.065657173	37.873987347	6	29.880983413	23.060736765	47.810577129
1	28.795941660	25.721655189	36.979276320	1	29.053256627	22.642195572	47.238338452
6	28.957584857	25.264685604	38.940413629	6	25.639088192	24.000174414	45.247697633
7	29.512340010	25.574831966	40.138510778	1	25.128063712	24.907823433	45.589827319
1	30.344792428	26.174472770	40.182185105	1	25.423596675	23.873376877	44.174535252
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7	28.219473465	24.171820325	38.826563609	8	27.601514265	25.287292771	45.797967913
1	27.565888015	24.035094836	38.043958978	8	27.900177189	23.186484445	45.089302944
1	27.997139606	23.609741724	39.658737771	6	28.224692999	27.189549623	50.248301084
26	29.115549155	25.957557337	46.315840640	7	27.203225558	26.327742816	49.909613933
8	29.624153167	25.618133445	44.808557379	1	26.430007154	26.028572538	50.510315007
8	31.714996651	27.639001573	45.045321615	6	27.429757363	25.901650475	48.648580189
6	30.922241893	28.244607161	45.756408714	1	26.780952369	25.221556913	48.108369086
8	29.932871449	27.695027192	46.427953026	7	28.532557638	26.438660802	48.155084012
6	31.030557977	29.758157140	45.931010583	6	29.043571979	27.244908358	49.142450647
6	32.442835073	30.255385038	46.244205328	1	29.968041924	27.799152463	48.997325644
6	32.748149961	31.716325865	45.810167423	6	29.874800601	27.309336317	37.885038811
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8	34.067300640	22.045261261	46.280494489	1	30.392762166	26.115552259	40.151756820
6	33.306547801	21.193337638	45.860974006	1	29.549762012	24.751838876	40.800247896
7	32.358476885	21.501621370	44.857637209	7	28.250425687	24.128839994	38.779048102
6	32.353136529	22.877233668	44.350756547	1	27.579992705	24.017093475	38.006763401
6	31.448806583	20.602096227	44.350015233	1	28.024633831	23.555981930	39.602281470
7	30.594866811	20.963923293	43.418006582	26	29.481454511	25.699001545	46.184249625
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7	33.284674895	19.869537889	46.310820208	6	31.171822961	28.246756568	45.685576217
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8	29.277530660	23.370967038	42.459366678				
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1	29.697176384	27.900989122	36.987005445
1	33.651224947	19.892976038	47.122698369

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