Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

A Computational Study of the Phosphoryl Transfer Reaction between ATP and Dha in Aqueous Solution

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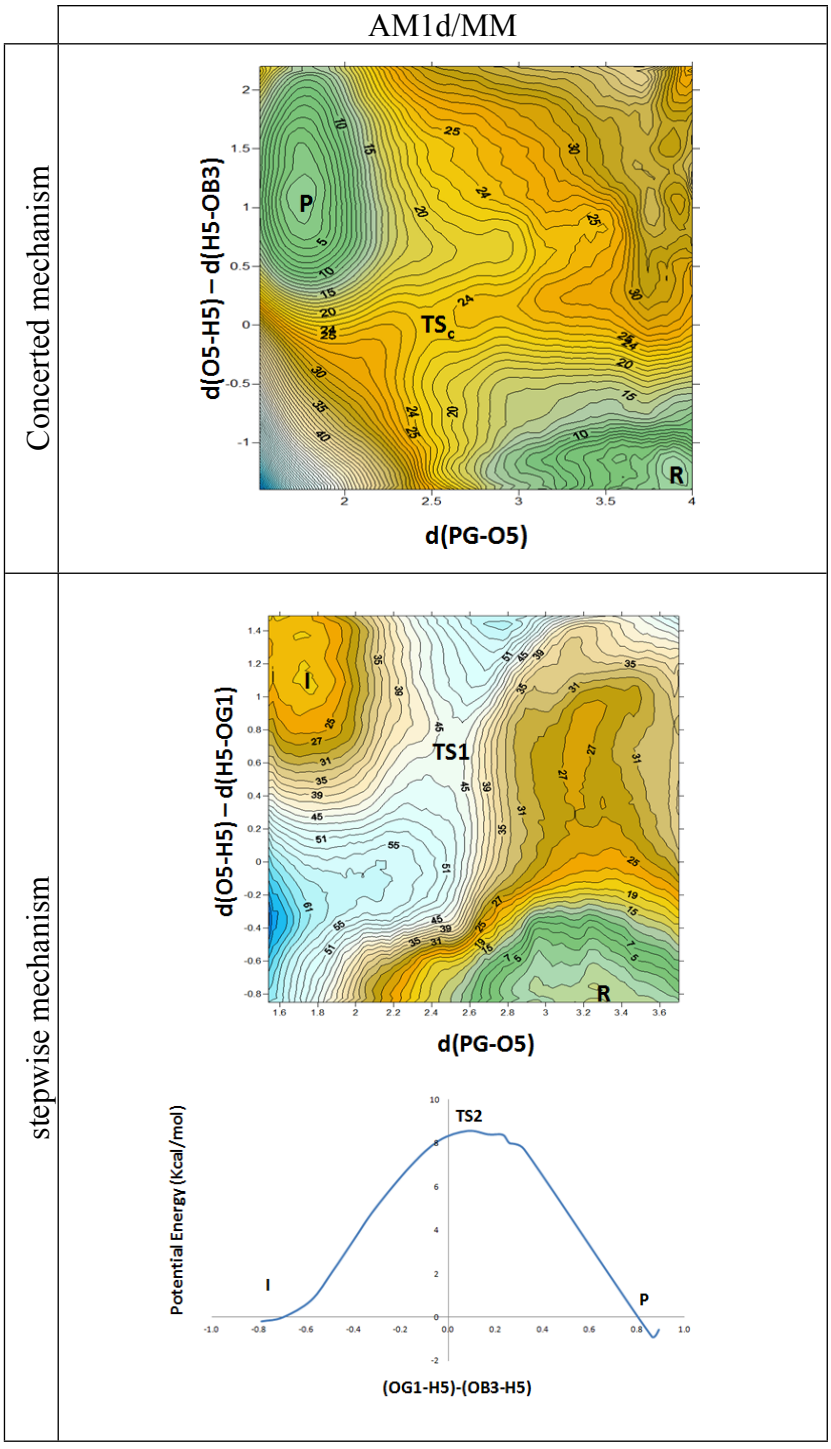

Figure S1. PES of the concerted and stepwise mechanisms of the phosphoryl transfer reaction from ATP to Dha in aqueous solution obtained at AM1d/MM level. Energies are given in kcal·mol^{-1} and distances in Å.

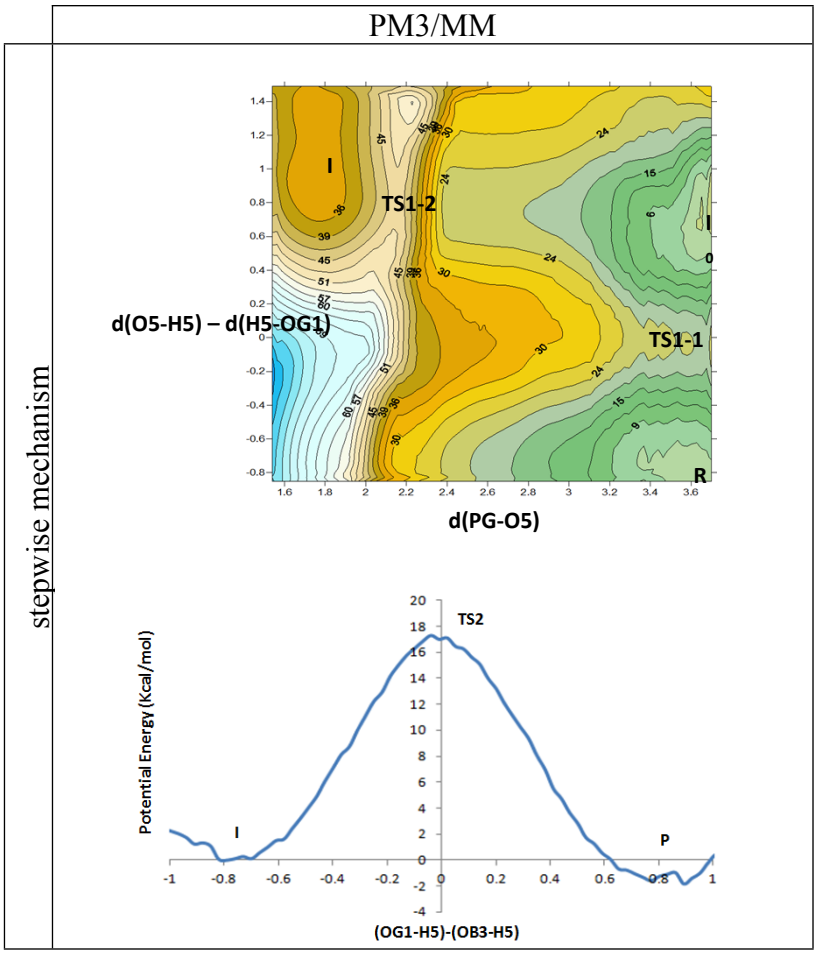

Figure S2. PES and potential energy profile of the stepwise mechanism of the phosphoryl transfer reaction from ATP to Dha in aqueous solution obtained at PM3/MM level. Energies are given in kcal·mol^{-1} and distances in Å.

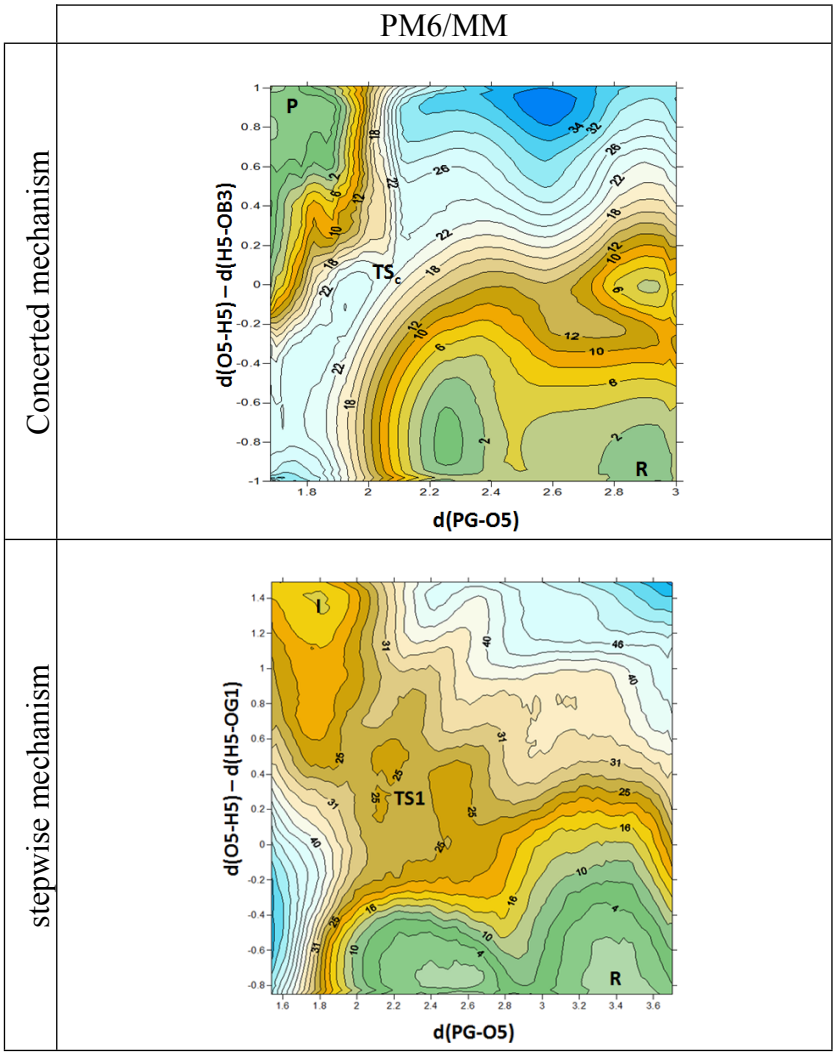

Figure S3. PES of the concerted and stepwise mechanisms of the phosphoryl transfer reaction from ATP to Dha in aqueous solution obtained at PM6/MM level. Energies are given in kcal·mol^{-1} and distances in Å.

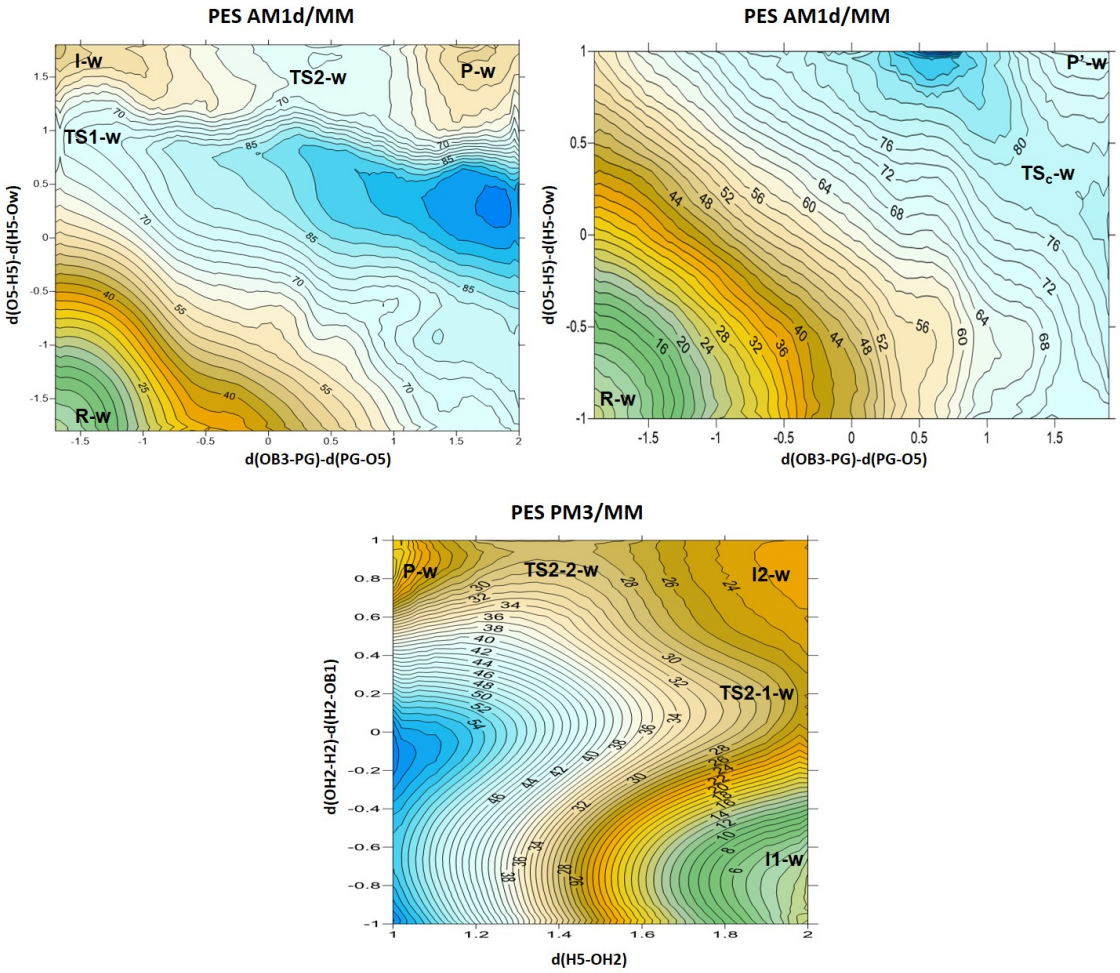

Figure S4. PES of the stepwise solvent-assisted mechanisms of the phosphoryl transfer reaction from ATP to Dha in aqueous solution obtained at AM1d/MM level for the concerted and stepwise mechanisms (on the top) and PM3/MM level (down part). Energies are given in kcal·mol^{-1} and distances in Å.

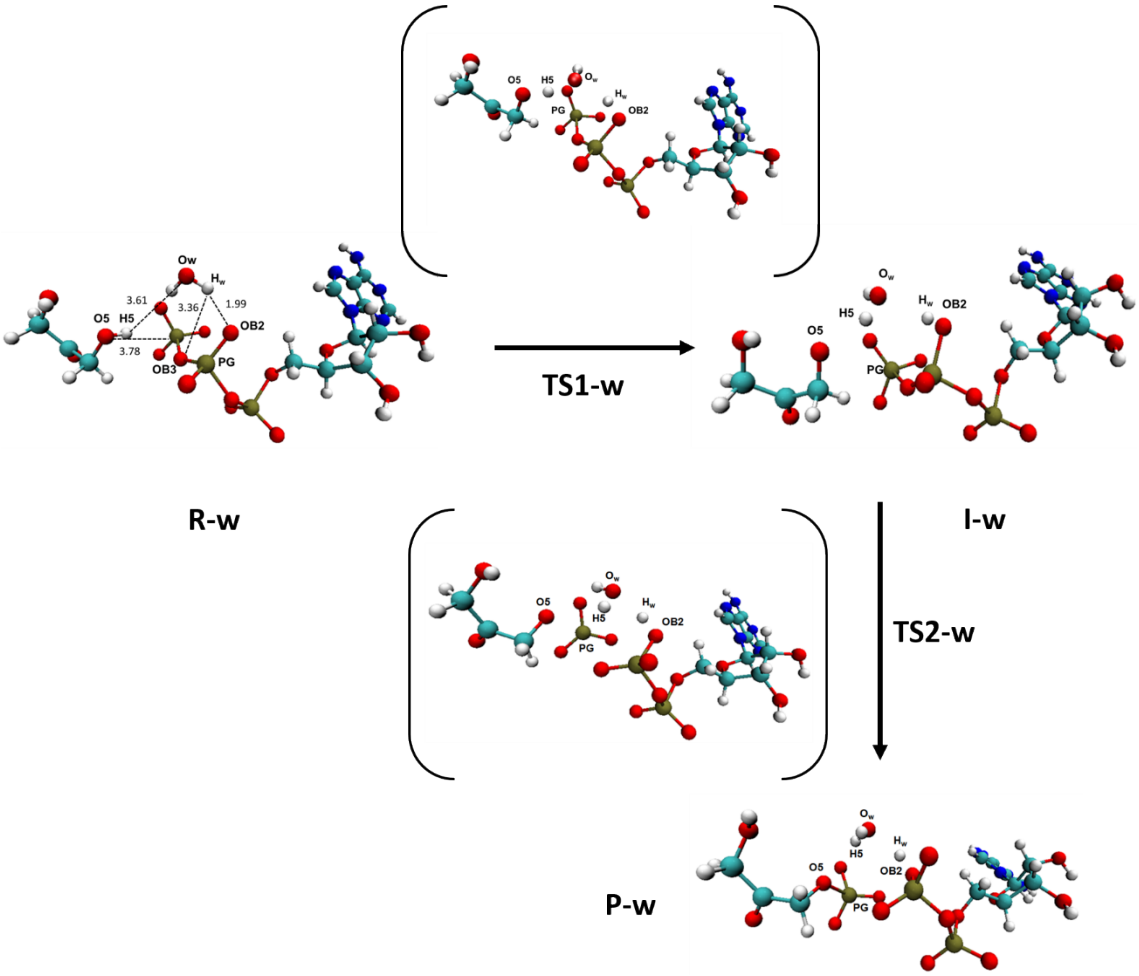

Figure S5. Geometries of the stationary points of the stepwise solvent-assisted mechanisms of the phosphoryl transfer reaction from ATP to Dha in aqueous solution obtained at AM1d/MM level. Distances in Å.

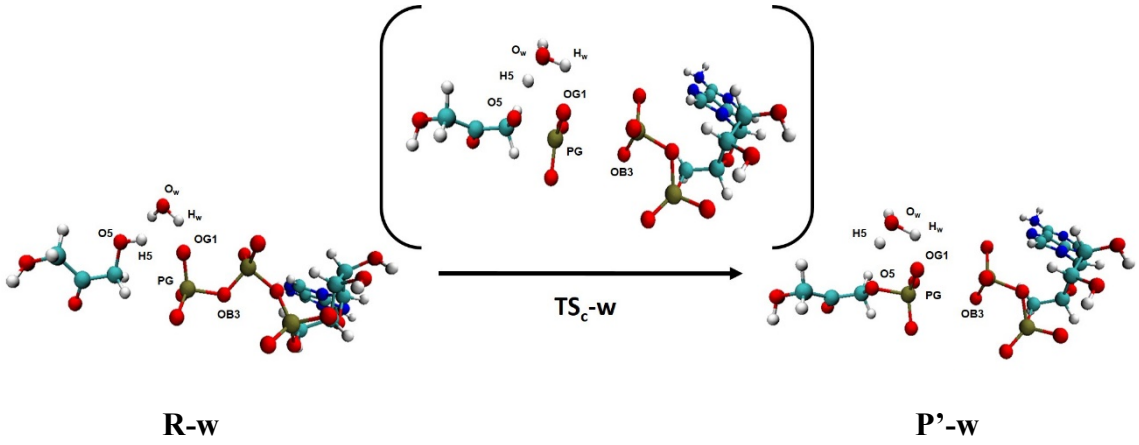

Figure S6. Geometries of the stationary points of the concerted solvent-assisted mechanisms of the phosphoryl transfer reaction from ATP to Dha in aqueous solution obtained at AM1d/MM level. It must be pointed out that **P'-w** correspond to a stationary state previous to the final **P-w**.

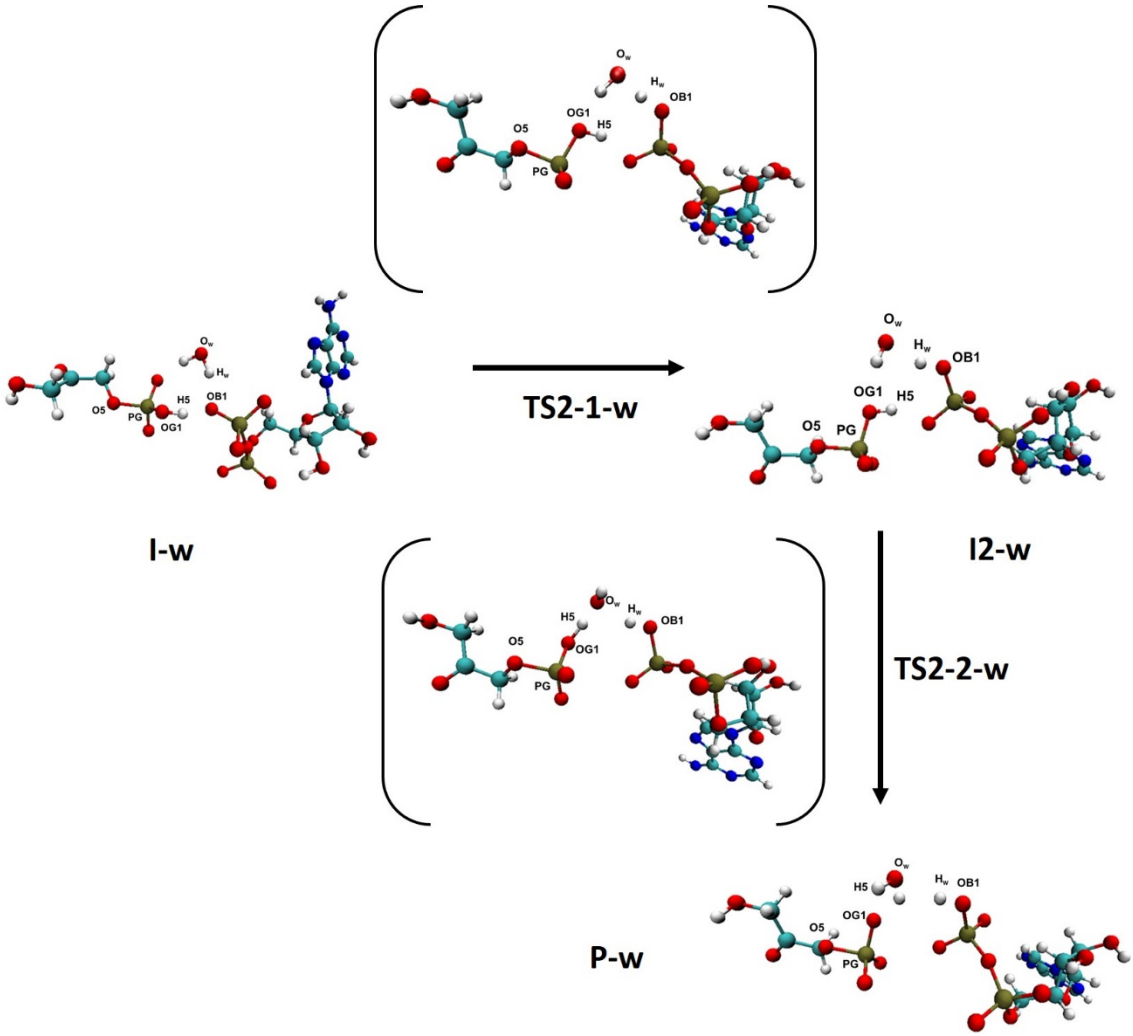

Figure S7. Geometries of the stationary points of the stepwise solvent-assisted mechanisms of the phosphoryl transfer reaction from ATP to Dha in aqueous solution obtained at PM3/MM level.

Table S1. QM/MM free energies relative to reactants of the two possible reaction mechanisms corresponding to the phosphoryl transfer from ATP to Dha. Table shows the results from QM/MM calculations with the QM region treated by AM1d/MM, PM3/MM and PM6/MM. Energies are given in kcal·mol^{-1}.

Table S2. QM/MM free energies relative to reactants of the two possible reaction mechanisms corresponding to the phosphoryl transfer from ATP to Dha. Table shows the results from QM/MM calculations with the QM region treated by AM1d:B3LYP/MM, PM3:B3LYP/MM and PM6:B3LYP/MM. Energies are given in kcal·mol^{-1}

AM1d/MM		**PM3/MM**		**PM6/MM**	
Concerted mechanism		Stepwise mechanism		Concerted mechanism	
R	0.00	**R**	0.00	**R**	0.00
TS_c	34.59	**TS1-1**	13.24	**TS_c**	14.0
P	11.63	**I_0**	-1.45	**P**	0.51
Stepwise mechanism		**TS1-2**	14.09	Stepwise mechanism	
R	0.00	**I (TS1-2)**	-2.82	**R**	0.00
TS1	26.40	**I (TS2)**	-2.82	**TS1**	11.69
I (TS1)	8.29	**TS2**	15.91	**I**	-3.39
I (TS2)	8.29	**P**	-0.26		
TS2	15.49				
P	14.13				

AM1d:B3LYP/MM		**PM3:B3LYP/MM**		**PM6:B3LYP/MM**	
Concerted mechanism		Stepwise mechanism		Concerted mechanism	
R	0.00	**R**	0.00	**R**	0.00
TS_c	34.22	**TS1**	30.92	**TS_c**	55.32
P	13.62	**I (TS1)**	-9.70	**P**	25.42
Stepwise mechanism		**I (TS2)**	-9.70	Stepwise mechanism	
R	0.00	**TS2**	5.75	**R**	0.00
TS1	37.28	**P**	1.25	**TS1**	45.01
I	20.36			**I**	7.22
Iprofile	20.36				
TS2	33.44				
P	28.51				

Tables S4: Cartesian coordinates of the QM atoms of the localized stationary points.

AM1d/MM Concerted mechanism	R	TS_c	P
C1 DHA	-7.599 0.988 -0.198	-7.248 0.940 -0.229	-7.174 0.875 -0.172
C2 DHA	-6.364 1.796 -0.459	-6.100 1.865 -0.590	-5.916 1.683 -0.475
H21 DHA	-6.650 2.843 -0.777	-6.360 2.346 -1.578	-6.107 2.268 -1.420
H22 DHA	-5.689 1.834 0.459	-6.073 2.658 0.212	-5.767 2.399 0.383
C3 DHA	-8.423 0.359 -1.289	-8.170 0.423 -1.319	-8.151 0.510 -1.277
H31 DHA	-9.117 -0.428 -0.874	-8.933 -0.274 -0.871	-9.010 -0.072 -0.835
H32 DHA	-9.014 1.164 -1.816	-8.701 1.306 -1.770	-8.542 1.465 -1.723
O4 DHA	-8.032 0.879 1.004	-7.583 0.738 0.948	-7.523 0.634 0.994
O5 DHA	-5.643 1.243 -1.572	-4.849 1.267 -0.722	-4.764 0.924 -0.705
H5 DHA	-4.871 0.692 -1.227	-3.995 2.254 -0.670	-2.630 2.575 0.540
O6 DHA	-7.605 -0.338 -2.240	-7.490 -0.326 -2.296	-7.581 -0.328 -2.256
H6 DHA	-7.295 0.307 -2.959	-7.290 0.270 -3.049	-7.395 0.224 -3.043
C1' ATP	5.252 1.568 0.113	5.209 1.531 0.075	5.253 1.546 0.124
H1' ATP	5.987 2.255 0.635	5.984 2.194 0.559	6.041 2.199 0.605
C2' ATP	5.167 1.934 -1.381	5.152 1.903 -1.418	5.230 1.865 -1.383
H2' ATP	4.803 1.100 -2.048	4.750 1.074 -2.061	4.868 1.001 -2.003
O2' ATP	6.470 2.229 -1.894	6.434 2.172 -1.918	6.521 2.143 -1.858
HT2 ATP	6.865 3.035 -1.443	6.807 2.937 -1.440	6.858 2.940 -1.408
C3' ATP	4.186 3.127 -1.401	4.182 3.104 -1.426	4.236 3.042 -1.480
H3' ATP	3.611 3.212 -2.366	3.548 3.126 -2.349	3.588 2.962 -2.390
O3' ATP	4.968 4.330 -1.232	4.957 4.282 -1.313	4.992 4.236 -1.518
HT3 ATP	4.390 5.116 -1.430	4.401 5.019 -1.610	4.368 4.957 -1.695
C4' ATP	3.296 2.927 -0.155	3.342 2.916 -0.145	3.408 2.948 -0.182
O4' ATP	3.942 1.888 0.669	3.944 1.867 0.647	3.994 1.940 0.671
H4' ATP	3.273 3.841 0.509	3.370 3.849 0.481	3.455 3.910 0.391
C5' ATP	1.884 2.469 -0.508	1.902 2.504 -0.431	1.965 2.527 -0.439
H51 ATP	1.790 1.358 -0.664	1.839 1.401 -0.643	1.901 1.418 -0.610
H52 ATP	1.493 3.012 -1.419	1.513 3.061 -1.327	1.570 3.052 -1.352
O5' ATP	1.043 2.740 0.651	1.136 2.748 0.730	1.201 2.805 0.718
PA ATP	0.033 4.078 0.663	0.045 4.218 0.719	0.153 4.299 0.689
OA1 ATP	0.897 5.286 0.349	0.997 5.437 0.455	1.101 5.529 0.492
OA2 ATP	-0.753 3.976 1.945	-0.875 4.032 1.964	-0.822 4.064 1.893
OA3 ATP	-0.896 3.860 -0.639	-0.757 4.073 -0.812	-0.588 4.171 -0.894
PB ATP	-1.777 2.572 -1.228	-1.826 2.759 -1.482	-1.671 2.864 -1.535
OB1 ATP	-2.466 3.321 -2.362	-2.369 3.580 -2.717	-2.330 3.499 -2.804
OB2 ATP	-0.826 1.468 -1.651	-0.923 1.498 -1.748	-0.847 1.537 -1.647
OB3 ATP	-2.807 2.187 -0.069	-3.023 2.724 -0.306	-2.844 3.086 -0.259
PG ATP	-3.120 0.672 0.683	-3.627 0.201 0.838	-3.825 0.163 0.744
OG1 ATP	-3.545 -0.286 -0.458	-3.861 -1.022 -0.133	-4.010 -1.301 0.127
OG2 ATP	-1.813 0.280 1.371	-2.096 0.417 1.120	-2.279 0.573 0.826
OG3 ATP	-4.280 0.978 1.621	-4.670 0.704 1.870	-4.660 0.650 1.991

AM1d/MM Stepwise mechanism	TS1	I	TS2
C1 DHA	-7.263 -0.755 0.837	-7.387 -0.818 0.841	-7.402 -0.852 0.840
C2 DHA	-5.771 -0.546 0.799	-5.881 -0.724 0.855	-5.905 -0.813 0.858
H21 DHA	-5.401 -0.439 1.861	-5.530 -0.805 1.924	-5.536 -0.731 1.926
H22 DHA	-5.332 -1.472 0.319	-5.487 -1.615 0.282	-5.505 -1.753 0.363
C3 DHA	-8.143 -0.109 -0.182	-8.174 -0.042 -0.175	-8.199 -0.106 -0.174
H31 DHA	-8.092 1.013 -0.091	-8.030 1.057 0.007	-8.088 1.008 -0.031
H32 DHA	-7.835 -0.436 -1.217	-7.808 -0.303 -1.206	-7.879 -0.402 -1.218
O4 DHA	-7.790 -1.535 1.723	-7.961 -1.577 1.646	-7.989 -1.603 1.707
O5 DHA	-5.392 0.579 0.056	-5.459 0.467 0.265	-5.433 0.315 0.077
H5 DHA	-4.593 1.701 -1.204	-4.740 1.898 -1.255	-2.264 2.091 -0.193
O6 DHA	-9.512 -0.554 -0.077	-9.538 -0.406 -0.156	-9.587 -0.486 -0.121
H6 DHA	-9.937 -0.153 0.722	-9.943 -0.006 0.626	-10.039 -0.054 0.648
C1' ATP	6.187 2.151 -0.333	6.211 2.141 -0.276	6.204 2.150 -0.330
H1' ATP	7.235 2.583 -0.309	7.273 2.528 -0.279	7.258 2.570 -0.321
C2' ATP	5.325 2.907 -1.365	5.390 2.954 -1.297	5.338 2.926 -1.344
H2' ATP	4.996 2.282 -2.244	4.966 2.322 -2.121	4.977 2.309 -2.216
O2' ATP	6.123 3.921 -1.996	6.213 3.885 -1.963	6.148 3.923 -1.988
HT2 ATP	6.134 4.751 -1.450	6.435 4.598 -1.346	6.177 4.755 -1.446
C3' ATP	4.128 3.486 -0.576	4.272 3.620 -0.463	4.171 3.530 -0.531
H3' ATP	3.131 3.132 -0.981	3.247 3.356 -0.845	3.156 3.208 -0.926
O3' ATP	4.183 4.916 -0.746	4.487 5.013 -0.590	4.263 4.961 -0.689
HT3 ATP	3.391 5.317 -0.265	3.874 5.459 0.012	3.525 5.387 -0.146
C4' ATP	4.350 3.114 0.906	4.470 3.129 0.988	4.408 3.139 0.944
O4' ATP	5.650 2.445 0.989	5.708 2.400 1.037	5.695 2.444 1.002
H4' ATP	4.467 4.025 1.568	4.594 3.998 1.692	4.550 4.041 1.614
C5' ATP	3.313 2.146 1.494	3.376 2.190 1.527	3.365 2.184 1.543
H51 ATP	3.778 1.541 2.324	3.854 1.467 2.247	3.825 1.582 2.377
H52 ATP	2.830 1.485 0.721	2.900 1.616 0.686	2.874 1.521 0.776
O5' ATP	2.266 2.883 2.178	2.410 2.877 2.284	2.323 2.935 2.223
PA ATP	1.209 3.853 1.307	1.243 3.960 1.376	1.340 3.976 1.354
OA1 ATP	1.980 5.072 0.818	2.096 5.203 0.889	2.130 5.227 0.990
OA2 ATP	0.058 4.133 2.239	0.055 4.267 2.360	0.120 4.200 2.213
OA3 ATP	0.895 2.794 0.135	0.937 2.857 0.118	1.191 3.067 0.028
PB ATP	-0.471 2.304 -0.721	-0.578 2.252 -0.802	-0.152 2.472 -0.772
OB1 ATP	-0.921 3.548 -1.470	-1.033 3.557 -1.589	-0.701 3.647 -1.572
OB2 ATP	0.135 1.147 -1.514	0.135 1.083 -1.617	0.401 1.254 -1.507
OB3 ATP	-1.487 1.807 0.374	-1.582 1.707 0.346	-1.169 2.089 0.356
PG ATP	-3.209 1.165 0.396	-3.657 0.949 0.512	-3.865 0.808 0.451
OG1 ATP	-3.583 1.714 -1.083	-3.834 1.579 -1.152	-3.381 1.637 -0.791
OG2 ATP	-2.755 -0.273 0.445	-2.902 -0.434 0.586	-3.014 -0.462 0.580
OG3 ATP	-3.621 1.980 1.588	-3.826 2.005 1.669	-3.957 1.703 1.687

PM3/MM Stepwise mechanism	R			TS1-1			I_0			TS1-2		
C1 DHA	-7.895	-0.842	0.948	-7.854	-0.838	0.958	-7.916	-0.874	0.950	-7.562	-0.871	0.973
C2 DHA	-6.437	-0.424	0.907	-6.389	-0.425	1.017	-6.471	-0.366	0.985	-6.038	-0.772	1.010
H21 DHA	-5.918	-0.677	1.853	-5.969	-0.662	2.015	-6.003	-0.666	1.949	-5.670	-1.010	2.028
H22 DHA	-5.934	-0.995	0.099	-5.858	-1.068	0.284	-5.952	-0.950	0.191	-5.662	-1.564	0.330
C3 DHA	-8.839	-0.197	-0.044	-8.710	-0.234	-0.133	-8.798	-0.323	-0.147	-8.322	-0.100	-0.087
H31 DHA	-8.856	0.900	0.124	-8.618	0.871	-0.111	-8.736	0.786	-0.138	-8.137	0.984	0.048
H32 DHA	-8.472	-0.379	-1.071	-8.340	-0.582	-1.114	-8.416	-0.670	-1.125	-7.955	-0.384	-1.090
O4 DHA	-8.277	-1.695	1.748	-8.308	-1.670	1.748	-8.336	-1.707	1.759	-8.148	-1.619	1.759
O5 DHA	-6.356	0.958	0.695	-6.217	0.915	0.752	-6.393	0.958	0.789	-5.566	0.460	0.618
H5 DHA	-5.517	1.118	0.201	-5.255	1.071	0.156	-4.943	1.236	-0.054	-5.172	1.344	-0.935
O6 DHA	-10.133	-0.739	-0.029	-10.055	-0.639	-0.098	-10.133	-0.765	-0.113	-9.696	-0.391	-0.131
H6 DHA	-10.562	-0.413	0.753	-10.467	-0.163	0.613	-10.531	-0.374	0.656	-10.102	0.059	0.601
C1' ATP	6.279	2.243	-0.250	6.275	2.240	-0.246	6.287	2.231	-0.221	6.244	2.225	-0.271
H1' ATP	7.323	2.606	-0.133	7.318	2.604	-0.121	7.334	2.580	-0.085	7.283	2.601	-0.150
C2' ATP	5.531	3.110	-1.287	5.530	3.106	-1.285	5.567	3.106	-1.270	5.485	3.103	-1.291
H2' ATP	5.245	2.530	-2.192	5.249	2.524	-2.190	5.300	2.529	-2.183	5.158	2.524	-2.182
O2' ATP	6.335	4.111	-1.858	6.334	4.108	-1.853	6.383	4.106	-1.822	6.298	4.079	-1.894
HT2 ATP	6.589	4.706	-1.163	6.591	4.698	-1.154	6.650	4.683	-1.116	6.573	4.682	-1.213
C3' ATP	4.277	3.618	-0.523	4.271	3.610	-0.527	4.299	3.610	-0.531	4.265	3.648	-0.501
H3' ATP	3.366	3.124	-0.939	3.365	3.104	-0.940	3.398	3.114	-0.967	3.325	3.214	-0.920
O3' ATP	4.131	5.009	-0.670	4.116	4.997	-0.688	4.158	5.000	-0.678	4.186	5.048	-0.601
HT3 ATP	3.355	5.224	-0.128	3.337	5.214	-0.153	3.367	5.216	-0.164	3.409	5.276	-0.064
C4' ATP	4.496	3.207	0.964	4.491	3.212	0.964	4.487	3.193	0.959	4.477	3.187	0.971
O4' ATP	5.706	2.452	1.042	5.697	2.449	1.043	5.696	2.443	1.062	5.671	2.404	1.026
H4' ATP	4.678	4.091	1.617	4.676	4.102	1.607	4.653	4.072	1.623	4.675	4.045	1.654
C5' ATP	3.335	2.358	1.557	3.331	2.371	1.571	3.317	2.335	1.518	3.290	2.349	1.531
H51 ATP	3.734	1.626	2.286	3.733	1.656	2.316	3.699	1.592	2.246	3.663	1.590	2.245
H52 ATP	2.827	1.779	0.760	2.825	1.776	0.786	2.823	1.767	0.705	2.775	1.805	0.715
O5' ATP	2.409	3.089	2.298	2.400	3.105	2.301	2.378	3.057	2.250	2.380	3.093	2.273
PA ATP	1.226	4.135	1.528	1.210	4.135	1.529	1.217	4.136	1.511	1.220	4.162	1.482
OA1 ATP	2.021	5.333	0.991	2.008	5.321	0.973	2.011	5.310	0.949	2.061	5.369	1.015
OA2 ATP	0.139	4.439	2.546	0.132	4.447	2.548	0.153	4.426	2.546	0.141	4.490	2.502
OA3 ATP	0.686	3.185	0.303	0.628	3.152	0.338	0.616	3.205	0.279	0.623	3.243	0.290
PB ATP	-0.360	2.396	-0.822	-0.371	2.401	-0.842	-0.376	2.445	-0.864	-0.492	2.326	-0.734
OB1 ATP	-1.028	3.551	-1.581	-1.032	3.559	-1.591	-1.136	3.557	-1.595	-1.124	3.462	-1.577
OB2 ATP	0.471	1.351	-1.586	0.485	1.361	-1.577	0.437	1.387	-1.594	0.420	1.343	-1.533
OB3 ATP	-1.371	1.489	0.087	-1.465	1.461	-0.046	-1.431	1.505	0.035	-1.496	1.513	0.180
PG ATP	-2.977	0.996	0.654	-2.977	0.990	0.695	-2.876	1.003	0.771	-3.782	0.849	0.660
OG1 ATP	-3.989	1.180	-0.532	-4.173	1.165	-0.386	-4.039	1.305	-0.422	-4.217	1.364	-0.907
OG2 ATP	-2.630	-0.505	0.920	-2.624	-0.505	0.899	-2.606	-0.491	0.905	-3.141	-0.515	0.720
OG3 ATP	-3.231	1.908	1.887	-3.127	1.934	1.896	-3.125	1.901	1.967	-3.801	1.880	1.758

PM3/MM Stepwise mechanism	I	TS2	P
C1 DHA	-7.736 -0.982 0.962	-7.702 -0.961 0.973	-7.757 -1.018 0.963
C2 DHA	-6.217 -0.881 0.950	-6.185 -0.837 0.985	-6.240 -0.900 0.873
H21 DHA	-5.789 -1.241 1.908	-5.784 -1.093 1.987	-5.756 -1.386 1.744
H22 DHA	-5.840 -1.547 0.148	-5.790 -1.592 0.273	-5.918 -1.450 -0.034
C3 DHA	-8.517 -0.211 -0.080	-8.489 -0.215 -0.082	-8.596 -0.208 -0.002
H31 DHA	-8.320 0.874 0.044	-8.314 0.874 0.034	-8.459 0.870 0.225
H32 DHA	-8.173 -0.500 -1.092	-8.137 -0.507 -1.089	-8.252 -0.377 -1.040
O4 DHA	-8.283 -1.718 1.782	-8.259 -1.700 1.787	-8.268 -1.781 1.785
O5 DHA	-5.825 0.429 0.717	-5.789 0.433 0.615	-5.881 0.428 0.795
H5 DHA	-2.816 1.587 -0.612	-2.492 1.626 -0.444	-2.160 1.672 -0.213
O6 DHA	-9.891 -0.495 -0.084	-9.859 -0.523 -0.089	-9.954 -0.563 -0.026
H6 DHA	-10.276 -0.040 0.656	-10.254 -0.071 0.647	-10.328 -0.311 0.812
C1' ATP	6.235 2.222 -0.224	6.243 2.231 -0.276	6.236 2.209 -0.217
H1' ATP	7.279 2.577 -0.090	7.283 2.605 -0.160	7.280 2.569 -0.088
C2' ATP	5.512 3.096 -1.274	5.484 3.104 -1.301	5.505 3.081 -1.261
H2' ATP	5.227 2.509 -2.176	5.168 2.525 -2.197	5.203 2.495 -2.158
O2' ATP	6.342 4.073 -1.848	6.290 4.090 -1.895	6.327 4.056 -1.847
HT2 ATP	6.586 4.682 -1.161	6.559 4.691 -1.210	6.603 4.652 -1.161
C3' ATP	4.257 3.627 -0.531	4.253 3.637 -0.518	4.263 3.625 -0.504
H3' ATP	3.343 3.156 -0.971	3.321 3.183 -0.936	3.338 3.174 -0.943
O3' ATP	4.139 5.023 -0.655	4.151 5.035 -0.631	4.171 5.023 -0.617
HT3 ATP	3.363 5.242 -0.112	3.382 5.261 -0.085	3.395 5.254 -0.084
C4' ATP	4.437 3.193 0.955	4.470 3.190 0.958	4.444 3.175 0.976
O4' ATP	5.645 2.437 1.060	5.671 2.421 1.020	5.649 2.417 1.070
H4' ATP	4.609 4.062 1.630	4.661 4.055 1.634	4.619 4.035 1.663
C5' ATP	3.240 2.345 1.476	3.292 2.346 1.526	3.249 2.325 1.495
H51 ATP	3.591 1.545 2.156	3.671 1.590 2.241	3.593 1.534 2.187
H52 ATP	2.720 1.845 0.634	2.776 1.795 0.715	2.735 1.813 0.657
O5' ATP	2.345 3.078 2.245	2.378 3.084 2.275	2.345 3.064 2.252
PA ATP	1.202 4.195 1.490	1.226 4.166 1.512	1.226 4.196 1.523
OA1 ATP	2.062 5.394 1.059	2.040 5.369 1.022	2.052 5.390 1.053
OA2 ATP	0.089 4.432 2.502	0.116 4.445 2.505	0.093 4.402 2.496
OA3 ATP	0.679 3.408 0.183	0.686 3.276 0.248	0.710 3.385 0.183
PB ATP	-0.260 2.454 -0.928	-0.352 2.481 -0.862	-0.201 2.566 -0.963
OB1 ATP	-1.069 3.556 -1.701	-1.014 3.618 -1.662	-1.044 3.626 -1.683
OB2 ATP	0.749 1.586 -1.700	0.471 1.402 -1.577	0.662 1.548 -1.666
OB3 ATP	-1.177 1.496 -0.091	-1.452 1.658 -0.008	-1.206 1.569 -0.051
PG ATP	-4.120 0.727 0.910	-4.057 0.748 0.785	-4.139 0.768 0.801
OG1 ATP	-3.778 1.406 -0.603	-3.635 1.352 -0.659	-3.857 1.426 -0.593
OG2 ATP	-3.372 -0.592 0.981	-3.336 -0.601 0.971	-3.373 -0.592 0.916
OG3 ATP	-4.015 1.759 2.006	-3.977 1.776 1.927	-3.988 1.730 2.008

PM6/MM Concerted mechanism	R	TS_c	P
C1 DHA	-7.037 1.692 0.836	-6.738 1.630 0.844	-6.365 1.528 0.872
C2 DHA	-5.962 0.622 0.700	-5.690 0.516 0.738	-5.279 0.478 0.670
H21 DHA	-6.021 -0.021 1.606	-5.869 -0.089 1.657	-5.427 -0.317 1.431
H22 DHA	-6.105 0.005 -0.208	-5.915 -0.121 -0.138	-5.364 0.026 -0.339
C3 DHA	-8.299 1.527 -0.009	-8.048 1.487 0.054	-7.672 1.382 0.081
H31 DHA	-9.213 1.584 0.615	-8.933 1.558 0.717	-8.547 1.456 0.756
H32 DHA	-8.341 2.338 -0.773	-8.114 2.308 -0.697	-7.745 2.202 -0.671
O4 DHA	-6.964 2.641 1.587	-6.647 2.611 1.557	-6.286 2.478 1.623
O5 DHA	-4.657 1.229 0.702	-4.341 0.935 0.795	-4.010 1.102 0.839
H5 DHA	-4.098 0.802 -0.051	-3.795 1.199 -0.397	-3.387 1.478 -0.946
O6 DHA	-8.254 0.317 -0.758	-8.082 0.287 -0.713	-7.714 0.179 -0.681
H6 DHA	-8.763 -0.413 -0.271	-8.648 -0.408 -0.241	-8.316 -0.491 -0.221
C1' ATP	5.102 1.618 -0.240	5.089 1.619 -0.248	5.070 1.634 -0.265
H1' ATP	5.933 2.167 0.263	5.924 2.169 0.245	5.909 2.190 0.217
C2' ATP	4.790 2.221 -1.619	4.769 2.218 -1.627	4.737 2.222 -1.645
H2' ATP	5.005 1.543 -2.474	4.978 1.535 -2.480	4.929 1.530 -2.495
O2' ATP	5.537 3.391 -1.926	5.522 3.381 -1.942	5.497 3.376 -1.975
HT2 ATP	5.992 3.809 -1.137	5.977 3.802 -1.156	5.960 3.799 -1.194
C3' ATP	3.287 2.627 -1.538	3.268 2.631 -1.537	3.241 2.649 -1.544
H3' ATP	2.627 1.944 -2.121	2.604 1.952 -2.119	2.565 1.984 -2.130
O3' ATP	3.083 3.890 -2.135	3.069 3.898 -2.127	3.051 3.926 -2.118
HT3 ATP	3.849 4.506 -1.961	3.847 4.505 -1.967	3.849 4.514 -1.982
C4' ATP	2.940 2.645 -0.031	2.926 2.645 -0.029	2.903 2.651 -0.037
O4' ATP	3.946 1.799 0.612	3.937 1.802 0.610	3.927 1.823 0.602
H4' ATP	3.051 3.665 0.397	3.036 3.664 0.399	2.992 3.668 0.399
C5' ATP	1.609 1.988 0.347	1.599 1.983 0.358	1.588 1.958 0.341
H51 ATP	1.753 0.991 0.816	1.756 0.994 0.838	1.783 0.972 0.811
H52 ATP	0.950 1.837 -0.541	0.938 1.828 -0.528	0.928 1.796 -0.541
O5' ATP	0.972 2.743 1.368	0.957 2.744 1.373	0.926 2.692 1.362
PA ATP	0.048 4.068 0.919	0.028 4.061 0.914	-0.013 4.005 0.904
OA1 ATP	1.000 5.059 0.283	0.981 5.054 0.284	0.916 4.979 0.217
OA2 ATP	-0.735 4.337 2.154	-0.772 4.342 2.135	-0.789 4.324 2.128
OA3 ATP	-1.002 3.638 -0.283	-1.032 3.598 -0.277	-1.132 3.491 -0.195
PB ATP	-1.544 2.400 -1.245	-1.611 2.398 -1.254	-1.528 2.514 -1.435
OB1 ATP	-2.684 2.957 -2.052	-2.681 3.026 -2.102	-2.560 3.314 -2.197
OB2 ATP	-0.327 1.880 -2.000	-0.378 1.836 -1.942	-0.286 1.967 -2.105
OB3 ATP	-2.204 1.278 -0.296	-2.507 1.275 -0.442	-2.466 1.257 -0.897
PG ATP	-1.880 0.317 1.099	-2.272 0.294 1.117	-2.650 0.160 1.308
OG1 ATP	-2.806 -0.845 0.685	-2.979 -0.984 0.661	-3.307 -1.245 1.204
OG2 ATP	-0.396 -0.085 1.025	-0.758 -0.021 1.086	-1.267 0.075 0.644
OG3 ATP	-2.266 1.099 2.330	-2.598 1.203 2.269	-2.536 0.821 2.685

PM6/MM Stepwise mechanism	TS1	I
C1 DHA	-7.585 -0.858 0.855	-7.602 -0.872 0.860
C2 DHA	-6.073 -0.702 0.815	-6.086 -0.786 0.875
H21 DHA	-5.714 -0.750 1.876	-5.743 -0.799 1.927
H22 DHA	-5.670 -1.625 0.315	-5.692 -1.670 0.318
C3 DHA	-8.397 -0.125 -0.180	-8.399 -0.130 -0.182
H31 DHA	-8.273 0.970 -0.062	-8.276 0.964 -0.048
H32 DHA	-8.076 -0.416 -1.207	-8.074 -0.426 -1.206
O4 DHA	-8.110 -1.593 1.682	-8.138 -1.602 1.685
O5 DHA	-5.700 0.495 0.073	-5.691 0.413 0.219
H5 DHA	-5.083 1.811 -1.128	-4.827 2.067 -1.350
O6 DHA	-9.764 -0.515 -0.104	-9.769 -0.511 -0.113
H6 DHA	-10.216 -0.049 0.647	-10.208 -0.049 0.649
C1' ATP	6.203 2.142 -0.304	6.212 2.141 -0.305
H1' ATP	7.252 2.526 -0.295	7.262 2.524 -0.303
C2' ATP	5.370 2.950 -1.332	5.376 2.942 -1.330
H2' ATP	4.973 2.335 -2.168	4.966 2.323 -2.154
O2' ATP	6.209 3.882 -1.988	6.211 3.873 -1.996
HT2 ATP	6.421 4.646 -1.387	6.435 4.627 -1.385
C3' ATP	4.245 3.618 -0.500	4.258 3.612 -0.495
H3' ATP	3.222 3.375 -0.886	3.235 3.362 -0.875
O3' ATP	4.456 5.024 -0.617	4.474 5.016 -0.629
HT3 ATP	3.764 5.481 -0.023	3.800 5.480 -0.028
C4' ATP	4.448 3.169 0.963	4.461 3.166 0.968
O4' ATP	5.693 2.407 1.023	5.712 2.413 1.024
H4' ATP	4.613 4.026 1.656	4.612 4.026 1.658
C5' ATP	3.340 2.239 1.493	3.356 2.234 1.503
H51 ATP	3.785 1.541 2.236	3.821 1.521 2.224
H52 ATP	2.860 1.655 0.686	2.878 1.661 0.687
O5' ATP	2.366 2.965 2.230	2.384 2.965 2.238
PA ATP	1.316 4.009 1.353	1.306 4.024 1.364
OA1 ATP	2.155 5.241 0.998	2.118 5.282 1.036
OA2 ATP	0.163 4.247 2.300	0.149 4.257 2.315
OA3 ATP	1.053 3.153 0.023	1.064 3.181 0.028
PB ATP	-0.364 2.294 -0.724	-0.394 2.279 -0.749
OB1 ATP	-0.971 3.440 -1.532	-1.001 3.425 -1.554
OB2 ATP	0.318 1.196 -1.562	0.288 1.182 -1.589
OB3 ATP	-1.119 1.735 0.465	-1.107 1.736 0.461
PG ATP	-3.861 0.885 0.420	-3.989 0.863 0.414
OG1 ATP	-3.934 1.495 -1.114	-4.024 1.504 -1.136
OG2 ATP	-3.101 -0.396 0.458	-3.139 -0.369 0.436
OG3 ATP	-3.978 1.901 1.510	-4.002 1.902 1.493

AM1d/MM Solvent-assisted	R-w			TS1-w			I-w		
C1 DHA	-7.493	0.924	-0.260	-7.358	0.812	-0.442	-7.560	0.937	-0.227
C2 DHA	-6.207	1.638	-0.543	-6.010	1.321	-0.916	-6.283	1.654	-0.577
H21 DHA	-6.449	2.690	-0.883	-6.192	2.385	-1.253	-6.545	2.725	-0.837
H22 DHA	-5.540	1.671	0.381	-5.302	1.340	-0.044	-5.567	1.629	0.300
C3 DHA	-8.370	0.325	-1.324	-8.359	0.323	-1.464	-8.412	0.307	-1.301
H31 DHA	-9.077	-0.437	-0.886	-9.126	-0.337	-0.971	-9.122	-0.452	-0.877
H32 DHA	-8.956	1.150	-1.828	-8.874	1.222	-1.901	-8.977	1.128	-1.831
O4 DHA	-7.945	0.910	0.944	-7.690	0.863	0.756	-7.993	0.874	0.986
O5 DHA	-5.524	1.032	-1.655	-5.527	0.583	-1.985	-5.724	1.056	-1.690
H5 DHA	-4.645	0.644	-1.353	-4.449	0.297	-1.924	-3.264	0.171	-2.273
O6 DHA	-7.612	-0.395	-2.305	-7.768	-0.462	-2.469	-7.659	-0.415	-2.288
H6 DHA	-7.284	0.246	-3.019	-7.350	0.144	-3.113	-7.081	0.251	-2.799
C1' ATP	5.246	1.569	0.126	5.323	1.575	0.135	5.241	1.568	0.133
H1' ATP	5.984	2.254	0.647	6.118	2.220	0.613	5.972	2.256	0.659
C2' ATP	5.162	1.933	-1.367	5.279	1.914	-1.367	5.161	1.934	-1.361
H2' ATP	4.801	1.098	-2.036	4.896	1.062	-1.992	4.800	1.100	-2.030
O2' ATP	6.467	2.227	-1.879	6.563	2.185	-1.860	6.465	2.228	-1.871
HT2 ATP	6.860	3.036	-1.432	6.915	2.975	-1.408	6.860	3.037	-1.423
C3' ATP	4.181	3.125	-1.389	4.293	3.101	-1.428	4.181	3.128	-1.383
H3' ATP	3.607	3.210	-2.355	3.645	3.056	-2.341	3.611	3.218	-2.351
O3' ATP	4.964	4.328	-1.218	5.052	4.294	-1.410	4.962	4.329	-1.203
HT3 ATP	4.388	5.115	-1.418	4.468	5.006	-1.711	4.392	5.118	-1.416
C4' ATP	3.289	2.925	-0.144	3.469	2.974	-0.131	3.286	2.921	-0.142
O4' ATP	3.938	1.891	0.684	4.070	1.961	0.703	3.929	1.884	0.685
H4' ATP	3.262	3.841	0.519	3.500	3.927	0.459	3.252	3.836	0.523
C5' ATP	1.880	2.461	-0.502	2.029	2.547	-0.392	1.884	2.449	-0.508
H51 ATP	1.789	1.350	-0.664	1.982	1.450	-0.630	1.812	1.341	-0.688
H52 ATP	1.491	3.003	-1.415	1.614	3.124	-1.264	1.491	3.015	-1.405
O5' ATP	1.029	2.721	0.653	1.286	2.750	0.795	1.040	2.670	0.660
PA ATP	0.018	4.050	0.687	0.091	4.132	0.763	0.030	3.999	0.708
OA1 ATP	0.863	5.262	0.341	0.905	5.406	0.350	0.832	5.221	0.322
OA2 ATP	-0.755	3.944	1.976	-0.786	3.989	2.044	-0.764	3.917	1.978
OA3 ATP	-0.994	3.845	-0.561	-0.726	3.638	-0.715	-0.862	3.679	-0.625
PB ATP	-1.696	2.528	-1.281	-2.022	2.523	-1.209	-1.851	2.542	-1.217
OB1 ATP	-2.401	3.267	-2.409	-2.636	3.444	-2.316	-2.350	3.255	-2.452
OB2 ATP	-0.615	1.531	-1.646	-1.076	1.228	-1.891	-0.864	1.345	-1.691
OB3 ATP	-2.799	1.833	-0.373	-2.905	1.974	0.026	-2.922	2.092	-0.203
PG ATP	-3.085	0.574	0.738	-3.158	0.290	1.194	-3.174	0.529	0.803
OG1 ATP	-3.662	-0.515	-0.198	-3.783	-0.811	0.258	-3.558	-0.638	-0.096
OG2 ATP	-1.743	0.236	1.379	-1.653	0.078	1.650	-1.729	0.370	1.283
OG3 ATP	-4.151	1.070	1.702	-4.099	1.045	2.184	-4.148	1.012	1.836
Ow HOH	-2.304	-0.540	-2.443	-3.276	-0.250	-2.351	-2.628	-0.510	-2.371
Hw HOH	-1.844	0.227	-1.984	-1.650	0.416	-1.929	-1.314	0.443	-1.846
Hw HOH	-2.921	-0.901	-1.755	-3.234	-1.061	-1.873	-2.796	-1.151	-1.611

AM1d/MM Solvent-assisted	TS2-w			P-w		
C1 DHA	-7.446	0.907	-0.203	-7.250	0.869	-0.152
C2 DHA	-6.076	1.505	-0.429	-5.903	1.562	-0.291
H21 DHA	-6.141	2.285	-1.242	-5.871	2.133	-1.263
H22 DHA	-5.700	1.974	0.528	-5.723	2.236	0.595
C3 DHA	-8.322	0.340	-1.292	-8.158	0.371	-1.257
H31 DHA	-9.043	-0.413	-0.866	-8.902	-0.370	-0.837
H32 DHA	-8.876	1.193	-1.779	-8.708	1.249	-1.706
O4 DHA	-7.955	0.882	0.980	-7.777	0.807	1.017
O5 DHA	-5.242	0.458	-0.773	-4.869	0.582	-0.320
H5 DHA	-3.332	0.650	-2.095	-3.434	0.449	-2.477
O6 DHA	-7.613	-0.394	-2.304	-7.498	-0.359	-2.302
H6 DHA	-7.279	0.243	-3.011	-7.299	0.253	-3.083
C1' ATP	5.235	1.569	0.134	5.236	1.570	0.134
H1' ATP	5.964	2.259	0.660	5.964	2.259	0.663
C2' ATP	5.156	1.935	-1.360	5.160	1.936	-1.360
H2' ATP	4.796	1.100	-2.028	4.799	1.101	-2.028
O2' ATP	6.461	2.228	-1.870	6.466	2.228	-1.868
HT2 ATP	6.854	3.040	-1.425	6.857	3.040	-1.422
C3' ATP	4.176	3.128	-1.382	4.181	3.129	-1.384
H3' ATP	3.607	3.219	-2.351	3.616	3.222	-2.355
O3' ATP	4.956	4.329	-1.199	4.960	4.331	-1.199
HT3 ATP	4.382	5.118	-1.403	4.380	5.119	-1.389
C4' ATP	3.276	2.919	-0.145	3.277	2.917	-0.151
O4' ATP	3.920	1.882	0.683	3.921	1.883	0.681
H4' ATP	3.238	3.833	0.520	3.231	3.830	0.515
C5' ATP	1.876	2.447	-0.523	1.879	2.440	-0.535
H51 ATP	1.803	1.337	-0.685	1.806	1.327	-0.677
H52 ATP	1.499	2.997	-1.437	1.512	2.974	-1.461
O5' ATP	1.007	2.695	0.618	1.003	2.715	0.593
PA ATP	0.031	4.057	0.638	0.034	4.078	0.584
OA1 ATP	0.907	5.267	0.383	0.932	5.283	0.373
OA2 ATP	-0.798	3.932	1.887	-0.837	3.956	1.802
OA3 ATP	-0.761	3.901	-0.774	-0.728	3.966	-0.860
PB ATP	-1.818	2.806	-1.394	-1.812	2.871	-1.451
OB1 ATP	-1.985	3.317	-2.820	-1.691	3.075	-2.968
OB2 ATP	-0.872	1.486	-1.547	-1.065	1.475	-1.176
OB3 ATP	-3.064	2.725	-0.572	-3.187	3.160	-0.923
PG ATP	-3.403	0.121	1.006	-3.665	0.122	0.936
OG1 ATP	-3.679	-1.123	0.217	-3.848	-1.305	0.379
OG2 ATP	-1.925	0.290	1.259	-2.155	0.357	1.041
OG3 ATP	-4.342	0.814	1.917	-4.432	0.708	2.105
Ow HOH	-2.873	-0.147	-2.196	-2.885	-0.320	-2.217
Hw HOH	-1.373	0.615	-1.629	-1.608	0.668	-1.455
Hw HOH	-3.255	-0.853	-1.587	-3.288	-0.818	-1.424

AM1d/MM Solvent-assisted	R-w	TS_c-w	P´-w
C1 DHA	-7.334 -0.667 0.597	-7.354 -0.687 0.608	-7.371 -0.688 0.639
C2 DHA	-5.922 -0.355 0.186	-5.910 -0.390 0.395	-5.905 -0.424 0.533
H21 DHA	-5.466 0.364 0.929	-5.567 0.013 1.406	-5.566 -0.149 1.580
H22 DHA	-5.328 -1.318 0.136	-5.350 -1.327 0.088	-5.390 -1.350 0.126
C3 DHA	-8.513 -0.126 -0.149	-8.479 -0.113 -0.183	-8.471 -0.104 -0.186
H31 DHA	-8.622 0.984 0.010	-8.560 1.002 -0.023	-8.551 1.011 -0.030
H32 DHA	-8.421 -0.361 -1.251	-8.365 -0.356 -1.279	-8.353 -0.351 -1.281
O4 DHA	-7.523 -1.415 1.625	-7.619 -1.483 1.587	-7.696 -1.516 1.575
O5 DHA	-5.903 0.239 -1.126	-5.563 0.680 -0.482	-5.482 0.700 -0.243
H5 DHA	-5.048 0.753 -1.296	-4.964 0.443 -1.809	-4.890 0.420 -2.092
O6 DHA	-9.725 -0.795 0.255	-9.718 -0.752 0.188	-9.725 -0.729 0.164
H6 DHA	-10.100 -0.377 1.075	-10.068 -0.367 1.037	-10.067 -0.369 1.027
C1' ATP	6.139 2.145 -0.346	6.155 2.143 -0.344	6.159 2.142 -0.344
H1' ATP	7.179 2.594 -0.328	7.199 2.584 -0.330	7.203 2.581 -0.329
C2' ATP	5.263 2.886 -1.377	5.281 2.888 -1.370	5.287 2.889 -1.371
H2' ATP	4.950 2.259 -2.263	4.957 2.264 -2.251	4.964 2.265 -2.252
O2' ATP	6.043 3.915 -2.008	6.063 3.924 -1.989	6.071 3.925 -1.988
HT2 ATP	6.066 4.750 -1.472	6.016 4.758 -1.451	6.017 4.762 -1.454
C3' ATP	4.052 3.432 -0.586	4.079 3.440 -0.577	4.084 3.442 -0.579
H3' ATP	3.064 3.048 -0.993	3.086 3.053 -0.976	3.090 3.056 -0.977
O3' ATP	4.069 4.865 -0.739	4.087 4.870 -0.757	4.096 4.872 -0.762
HT3 ATP	3.262 5.244 -0.267	3.279 5.251 -0.264	3.293 5.258 -0.265
C4' ATP	4.296 3.080 0.895	4.327 3.091 0.907	4.331 3.095 0.905
O4' ATP	5.599 2.419 0.977	5.629 2.426 0.982	5.631 2.425 0.982
H4' ATP	4.395 4.004 1.549	4.447 4.019 1.548	4.456 4.022 1.546
C5' ATP	3.280 2.126 1.526	3.298 2.144 1.543	3.298 2.152 1.540
H51 ATP	3.763 1.573 2.378	3.771 1.566 2.387	3.765 1.574 2.386
H52 ATP	2.772 1.409 0.821	2.793 1.454 0.811	2.792 1.463 0.807
O5' ATP	2.269 2.909 2.214	2.276 2.933 2.203	2.276 2.943 2.197
PA ATP	1.184 3.837 1.352	1.321 3.973 1.285	1.326 3.988 1.277
OA1 ATP	1.861 5.139 0.944	2.109 5.262 1.028	2.133 5.269 1.027
OA2 ATP	-0.031 3.966 2.236	0.081 4.206 2.123	0.090 4.232 2.115
OA3 ATP	1.093 2.831 0.084	1.294 3.245 -0.152	1.271 3.245 -0.142
PB ATP	-0.271 2.361 -0.755	-0.094 2.281 -0.585	-0.118 2.264 -0.582
OB1 ATP	-0.717 3.632 -1.455	-0.906 3.398 -1.247	-0.933 3.384 -1.230
OB2 ATP	0.224 1.157 -1.549	0.321 1.167 -1.569	0.365 1.188 -1.577
OB3 ATP	-1.144 1.900 0.492	-0.266 1.676 0.807	-0.357 1.625 0.780
PG ATP	-2.785 1.295 0.448	-3.701 1.115 0.244	-3.773 1.094 0.200
OG1 ATP	-3.287 1.693 -0.936	-3.526 1.737 -1.126	-3.499 1.683 -1.221
OG2 ATP	-2.476 -0.196 0.633	-3.097 -0.268 0.396	-3.084 -0.257 0.344
OG3 ATP	-3.407 1.987 1.657	-3.968 1.884 1.504	-3.933 1.940 1.441
Ow HOH	-4.106 0.360 -3.045	-4.269 0.267 -2.787	-4.257 0.212 -2.814
Hw HOH	-3.330 0.658 -2.489	-3.323 0.670 -2.586	-3.322 0.804 -2.408
Hw HOH	-4.384 -0.541 -2.757	-4.165 -0.709 -2.961	-4.164 -0.777 -2.948

PM3/MM Solvent-assisted	I1-w	TS2-1-w	I2-w
C1 DHA	-7.783 -0.980 0.976	-7.784 -0.987 0.989	-7.799 -0.988 0.955
C2 DHA	-6.263 -0.877 0.944	-6.264 -0.890 0.956	-6.277 -0.908 0.895
H21 DHA	-5.818 -1.322 1.857	-5.818 -1.350 1.862	-5.816 -1.494 1.715
H22 DHA	-5.902 -1.466 0.077	-5.906 -1.464 0.079	-5.942 -1.349 -0.064
C3 DHA	-8.578 -0.194 -0.044	-8.582 -0.186 -0.017	-8.591 -0.190 -0.058
H31 DHA	-8.404 0.889 0.117	-8.419 0.895 0.172	-8.400 0.891 0.104
H32 DHA	-8.227 -0.444 -1.063	-8.224 -0.407 -1.040	-8.249 -0.442 -1.080
O4 DHA	-8.318 -1.729 1.792	-8.321 -1.741 1.800	-8.334 -1.722 1.784
O5 DHA	-5.876 0.450 0.824	-5.880 0.439 0.863	-5.882 0.418 0.985
H5 DHA	-2.867 1.593 -0.571	-2.955 1.664 -0.615	-2.947 1.542 -0.580
O6 DHA	-9.945 -0.508 -0.062	-9.945 -0.514 -0.049	-9.962 -0.487 -0.067
H6 DHA	-10.339 -0.109 0.704	-10.349 -0.124 0.717	-10.353 -0.050 0.680
C1' ATP	6.225 2.217 -0.175	6.229 2.218 -0.189	6.222 2.224 -0.189
H1' ATP	7.264 2.575 -0.014	7.267 2.579 -0.024	7.260 2.585 -0.029
C2' ATP	5.524 3.099 -1.235	5.530 3.107 -1.246	5.521 3.102 -1.255
H2' ATP	5.249 2.517 -2.142	5.258 2.530 -2.157	5.253 2.517 -2.162
O2' ATP	6.371 4.070 -1.793	6.376 4.084 -1.795	6.362 4.079 -1.811
HT2 ATP	6.581 4.695 -1.110	6.565 4.719 -1.114	6.570 4.706 -1.129
C3' ATP	4.259 3.638 -0.514	4.262 3.641 -0.526	4.250 3.637 -0.541
H3' ATP	3.348 3.178 -0.974	3.354 3.181 -0.991	3.345 3.167 -1.001
O3' ATP	4.152 5.036 -0.631	4.151 5.039 -0.639	4.133 5.033 -0.670
HT3 ATP	3.373 5.257 -0.093	3.373 5.260 -0.102	3.355 5.259 -0.135
C4' ATP	4.406 3.190 0.971	4.405 3.188 0.958	4.398 3.203 0.948
O4' ATP	5.603 2.420 1.096	5.602 2.416 1.082	5.597 2.436 1.080
H4' ATP	4.570 4.052 1.658	4.568 4.048 1.648	4.558 4.073 1.626
C5' ATP	3.186 2.351 1.453	3.183 2.348 1.430	3.186 2.360 1.437
H51 ATP	3.513 1.527 2.116	3.506 1.517 2.086	3.516 1.539 2.101
H52 ATP	2.670 1.886 0.589	2.668 1.893 0.559	2.668 1.891 0.575
O5' ATP	2.291 3.079 2.225	2.284 3.067 2.207	2.283 3.078 2.212
PA ATP	1.159 4.217 1.485	1.160 4.223 1.499	1.166 4.234 1.508
OA1 ATP	2.043 5.400 1.052	2.045 5.391 1.053	2.041 5.393 1.043
OA2 ATP	0.073 4.467 2.526	0.087 4.463 2.544	0.080 4.463 2.533
OA3 ATP	0.564 3.456 0.193	0.519 3.473 0.194	0.534 3.459 0.199
PB ATP	-0.256 2.464 -0.985	-0.282 2.451 -0.929	-0.220 2.413 -0.898
OB1 ATP	-1.082 3.544 -1.785	-1.160 3.549 -1.783	-1.111 3.532 -1.775
OB2 ATP	0.847 1.700 -1.732	0.802 1.707 -1.698	0.852 1.717 -1.704
OB3 ATP	-1.175 1.460 -0.200	-1.234 1.495 -0.177	-1.188 1.471 -0.177
PG ATP	-4.167 0.737 0.999	-4.168 0.732 0.980	-4.168 0.686 1.051
OG1 ATP	-3.826 1.399 -0.523	-3.885 1.383 -0.552	-3.858 1.220 -0.510
OG2 ATP	-3.427 -0.588 1.069	-3.415 -0.591 1.046	-3.408 -0.629 1.157
OG3 ATP	-4.043 1.768 2.092	-4.029 1.761 2.077	-4.010 1.770 2.093
Ow HOH	-3.751 3.480 -2.211	-3.484 3.507 -2.319	-3.624 3.594 -2.469
Hw HOH	-4.024 2.907 -1.482	-3.836 2.938 -1.646	-3.940 3.382 -1.613
Hw HOH	-2.777 3.514 -2.158	-2.239 3.471 -1.978	-2.084 3.388 -1.913

PM3/MM Solvent-assisted	TS2-2-w	P-w
C1 DHA	-7.784 -1.040 0.998	-7.805 -1.009 0.987
C2 DHA	-6.266 -0.905 1.056	-6.287 -0.909 1.027
H21 DHA	-5.860 -1.411 1.954	-5.871 -1.322 1.965
H22 DHA	-5.849 -1.420 0.167	-5.885 -1.519 0.188
C3 DHA	-8.524 -0.316 -0.105	-8.553 -0.222 -0.070
H31 DHA	-8.290 0.767 -0.055	-8.346 0.861 0.057
H32 DHA	-8.179 -0.688 -1.089	-8.200 -0.505 -1.079
O4 DHA	-8.366 -1.759 1.811	-8.391 -1.732 1.796
O5 DHA	-5.919 0.429 1.082	-5.924 0.408 0.951
H5 DHA	-3.995 2.202 -1.171	-3.343 2.180 -1.560
O6 DHA	-9.909 -0.548 -0.114	-9.934 -0.480 -0.100
H6 DHA	-10.279 -0.073 0.620	-10.309 -0.071 0.671
C1' ATP	6.239 2.212 -0.180	6.253 2.217 -0.201
H1' ATP	7.279 2.569 -0.023	7.295 2.576 -0.055
C2' ATP	5.536 3.081 -1.248	5.539 3.101 -1.251
H2' ATP	5.269 2.489 -2.152	5.269 2.520 -2.161
O2' ATP	6.374 4.056 -1.811	6.368 4.089 -1.807
HT2 ATP	6.582 4.685 -1.131	6.464 4.785 -1.168
C3' ATP	4.265 3.614 -0.534	4.274 3.621 -0.517
H3' ATP	3.362 3.134 -0.987	3.367 3.140 -0.961
O3' ATP	4.142 5.009 -0.677	4.145 5.016 -0.653
HT3 ATP	3.373 5.239 -0.132	3.388 5.243 -0.092
C4' ATP	4.423 3.196 0.960	4.450 3.191 0.970
O4' ATP	5.618 2.425 1.091	5.644 2.416 1.079
H4' ATP	4.593 4.073 1.626	4.633 4.060 1.644
C5' ATP	3.213 2.366 1.476	3.239 2.363 1.489
H51 ATP	3.546 1.569 2.168	3.571 1.553 2.164
H52 ATP	2.696 1.864 0.634	2.710 1.879 0.643
O5' ATP	2.309 3.106 2.229	2.346 3.101 2.258
PA ATP	1.203 4.261 1.505	1.220 4.245 1.553
OA1 ATP	2.076 5.430 1.060	2.069 5.412 1.064
OA2 ATP	0.085 4.466 2.502	0.109 4.469 2.547
OA3 ATP	0.636 3.542 0.131	0.637 3.487 0.209
PB ATP	-0.036 2.354 -0.874	-0.093 2.388 -0.818
OB1 ATP	-1.124 3.385 -1.716	-0.970 3.595 -1.706
OB2 ATP	1.024 1.813 -1.805	0.883 1.734 -1.750
OB3 ATP	-0.763 1.320 -0.067	-1.009 1.477 -0.078
PG ATP	-4.199 0.789 0.875	-4.163 0.695 0.915
OG1 ATP	-4.200 1.264 -0.667	-4.150 1.103 -0.574
OG2 ATP	-3.426 -0.541 1.018	-3.359 -0.630 1.135
OG3 ATP	-3.983 1.848 1.967	-4.009 1.754 2.053
Ow HOH	-3.813 3.129 -1.925	-3.739 2.934 -2.067
Hw HOH	-3.927 3.885 -1.373	-4.300 3.364 -1.431
Hw HOH	-2.057 3.126 -1.676	-1.894 3.412 -1.704