Supporting Information for:

Roles of Closed- and Open-loop Conformations in Large-scale Structural Transitions of L-Lactate Dehydrogenase

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Contents:

Figure S1. Illustration of distance between key residues, C*α*-Glu103 and C*α*-Tyr238, O3-pyruvate and CZ-Arg105, O1-pyruvate and CZ-Arg105, and CZ-Arg105 and CZ-Arg168, respectively. The notations of *o* and *c* in parenthesis refer to open- and closed- loop conformations, respectively. Blue and yellow arrows refer to distances in closed- and open-loop conformations, respectively.

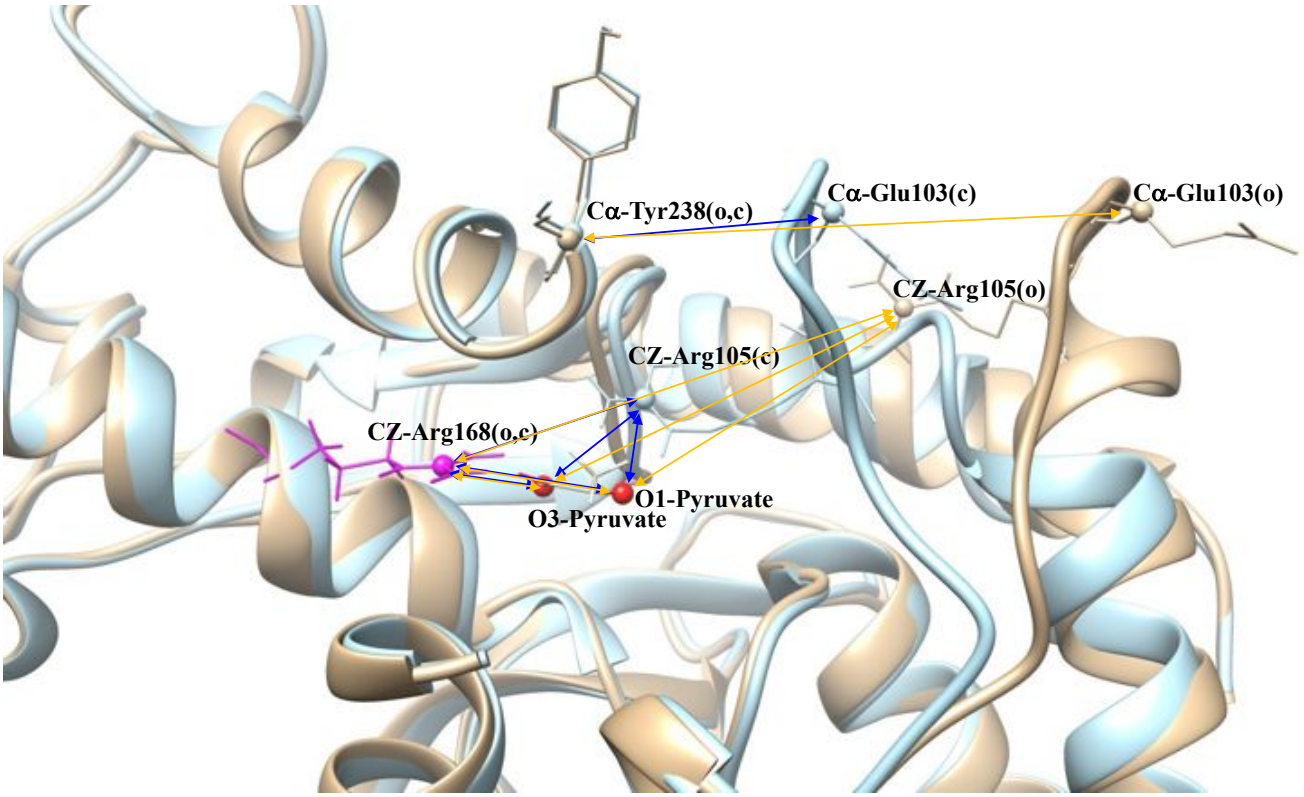
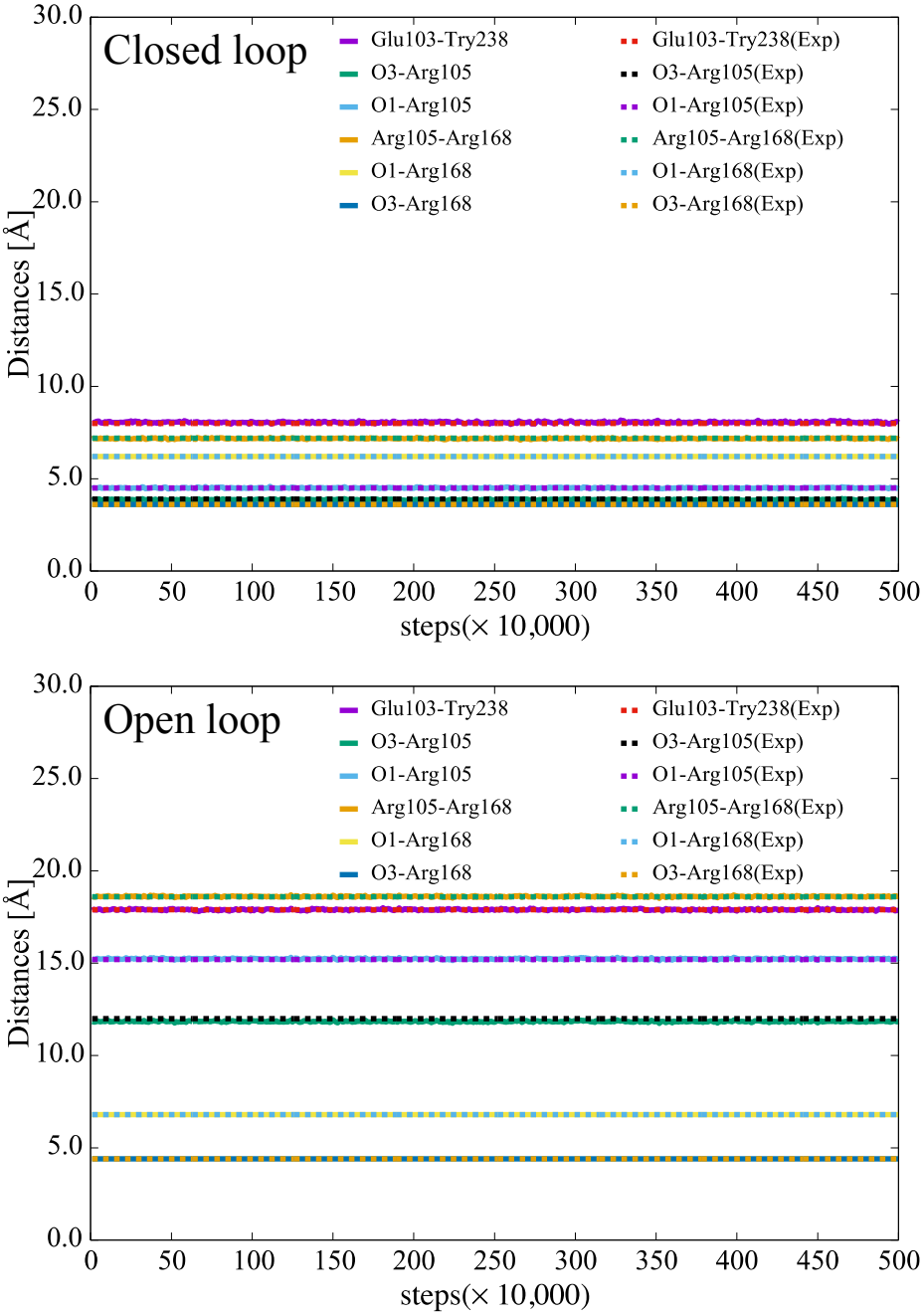


Table S1. Distances between C*α*-Glu103 and C*α*-Tyr238, O3-pyruvate and CZ-Arg105, O1-pyruvate and CZ-Arg105, and CZ-Arg105 and CZ-Arg168, and O1-pyruvate and CZ-Arg168, and O3-pyruvate and CZ-Arg168 at stationary points. Unit in (Å)

	Glu103_Try238	O3_Arg105	O1_Arg105	Arg105_Arg168	O1_Arg168
Exp(Closed)	8.0	3.9	4.5	7.2	6.2
Exp(Open)	17.9	12.0	15.2	18.6	6.8
*c*EQ1	8.2	3.7	3.6	5.9	6.1
m(*o*)EQ1	15.6	11.8	13.3	15.8	6.1
*c*TS1	8.4	3.9	3.4	6.2	6.2
*m*SSTS1	8.5	3.9	3.6	6.3	6.1
	14.7	11.8	12.9	15.7	
m(*c*)EQ2	8.5	4.0	3.4	6.3	6.1
m(*c*)TS2	8.5	4.2	3.4	6.3	6.2
*o*TS2	15.5	10.4	11.5	14.6	6.2
m(*c*)EQ3	8.6	4.3	3.4	6.2	6.1
*c*TS3	8.6	4.4	3.3	6.2	6.1
*m*SSTS3	8.6	4.2	3.4	6.1	6.1
	13.1	12.1	12.9	15.6	
*c*EQ4	8.5	4.3	3.3	6.2	6.1
m(*o*)EQ4	15.5	10.6	12.2	14.8	6.2

Figure S2. Distances during replica-exchange MD in a) closed- and b) open-loop conformations. Distances were defined in Figure S1. Unit in (Å)



Cartesian coordinates of the reaction center for all structures described in Figure 4:

REMARK o(m)EQ1

ATOM	1	C1	PYA	1	-0.325	-17.524	21.547	1.00	0.00
ATOM	2	O1	PYA	1	-1.152	-18.428	21.504	1.00	0.00
ATOM	3	C2	PYA	1	0.843	-17.478	20.523	1.00	0.00
ATOM	4	O2	PYA	1	1.791	-16.692	20.774	1.00	0.00
ATOM	5	O3	PYA	1	0.684	-18.194	19.492	1.00	0.00
ATOM	6	C3	PYA	1	-0.409	-16.392	22.522	1.00	0.00
ATOM	7	H1	PYA	1	0.518	-16.306	23.094	1.00	0.00
ATOM	8	H2	PYA	1	-0.515	-15.462	21.954	1.00	0.00
ATOM	9	H3	PYA	1	-1.281	-16.514	23.162	1.00	0.00
ATOM	10	C1	NAD	2	-3.176	-15.676	19.694	1.00	0.00
ATOM	11	H1	NAD	2	-3.261	-15.143	18.744	1.00	0.00
ATOM	12	H2	NAD	2	-2.213	-16.208	19.628	1.00	0.00
ATOM	13	C2	NAD	2	-4.304	-16.679	19.844	1.00	0.00
ATOM	14	C3	NAD	2	-4.547	-17.617	18.730	1.00	0.00
ATOM	15	O1	NAD	2	-4.119	-17.396	17.594	1.00	0.00
ATOM	16	N1	NAD	2	-5.342	-18.738	18.945	1.00	0.00
ATOM	17	H3	NAD	2	-5.378	-19.116	19.892	1.00	0.00
ATOM	18	H4	NAD	2	-5.202	-19.462	18.255	1.00	0.00
ATOM	19	C4	NAD	2	-3.176	-14.719	20.864	1.00	0.00
ATOM	20	H5	NAD	2	-2.404	-13.960	20.915	1.00	0.00
ATOM	21	C5	NAD	2	-5.163	-16.620	20.887	1.00	0.00
ATOM	22	H6	NAD	2	-5.962	-17.343	20.966	1.00	0.00
ATOM	23	C6	NAD	2	-4.090	-14.741	21.841	1.00	0.00
ATOM	24	H7	NAD	2	-4.077	-14.062	22.685	1.00	0.00
ATOM	25	N2	NAD	2	-5.134	-15.676	21.880	1.00	0.00
ATOM	26	C7	NAD	2	-6.271	-15.512	22.770	1.00	0.00
ATOM	2713	CD	ARG	170	4.143	-18.797	15.544	1.00	0.00
ATOM	2716	NE	ARG	170	4.404	-17.968	16.737	1.00	0.00
ATOM	2717	HE	ARG	170	5.338	-18.099	17.117	1.00	0.00
ATOM	2718	CZ	ARG	170	3.467	-17.634	17.668	1.00	0.00
ATOM	2719	NH1	ARG	170	3.886	-17.253	18.885	1.00	0.00
ATOM	2720	HH11	ARG	170	4.784	-17.669	19.135	1.00	0.00
ATOM	2721	HH12	ARG	170	3.173	-17.158	19.628	1.00	0.00
ATOM	2722	NH2	ARG	170	2.169	-17.546	17.348	1.00	0.00
ATOM	2723	HH21	ARG	170	1.977	-18.048	16.485	1.00	0.00

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ATOM   2724 HH22 ARG   170       1.518 -17.795  18.139  1.00  0.00
ATOM   3096  CB  HIP   194      -3.491 -22.949  17.933  1.00  0.00
ATOM   3099  CG  HIP   194      -2.598 -21.820  18.358  1.00  0.00
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ATOM   3103  HE1 HIP   194       0.135 -20.068  18.099  1.00  0.00
ATOM   3104  NE2 HIP   194      -1.524 -20.233  19.459  1.00  0.00
ATOM   3105  HE2 HIP   194      -1.258 -19.518  20.180  1.00  0.00
ATOM   3106  CD2 HIP   194      -2.643 -21.039  19.474  1.00  0.00
ATOM   3107  HD2 HIP   194      -3.361 -21.018  20.269  1.00  0.00
END
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REMARK oTS2

ATOM	1	C1	PYA	1	-0.892	-17.371	21.236	1.00	0.00
ATOM	2	O1	PYA	1	-1.567	-18.499	21.271	1.00	0.00
ATOM	3	C2	PYA	1	0.388	-17.218	20.376	1.00	0.00
ATOM	4	O2	PYA	1	1.057	-16.170	20.569	1.00	0.00
ATOM	5	O3	PYA	1	0.607	-18.184	19.601	1.00	0.00
ATOM	6	C3	PYA	1	-0.855	-16.609	22.525	1.00	0.00
ATOM	7	H1	PYA	1	0.015	-16.957	23.086	1.00	0.00
ATOM	8	H2	PYA	1	-0.707	-15.559	22.292	1.00	0.00
ATOM	9	H3	PYA	1	-1.756	-16.762	23.119	1.00	0.00
ATOM	10	C1	NAD	2	-2.655	-15.760	20.048	1.00	0.00
ATOM	11	H1	NAD	2	-2.197	-15.529	19.087	1.00	0.00
ATOM	12	H2	NAD	2	-1.701	-16.482	20.485	1.00	0.00
ATOM	13	C2	NAD	2	-3.810	-16.660	19.973	1.00	0.00
ATOM	14	C3	NAD	2	-3.908	-17.555	18.775	1.00	0.00
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ATOM	18	H4	NAD	2	-4.528	-19.371	18.159	1.00	0.00
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ATOM	21	C5	NAD	2	-4.782	-16.587	20.922	1.00	0.00
ATOM	22	H6	NAD	2	-5.599	-17.291	20.936	1.00	0.00
ATOM	23	C6	NAD	2	-3.849	-14.649	21.882	1.00	0.00
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ATOM	26	C7	NAD	2	-6.004	-15.471	22.742	1.00	0.00
ATOM	2713	CD	ARG	170	4.416	-18.685	15.600	1.00	0.00
ATOM	2716	NE	ARG	170	4.332	-17.719	16.715	1.00	0.00
ATOM	2717	HE	ARG	170	5.228	-17.358	17.010	1.00	0.00
ATOM	2718	CZ	ARG	170	3.298	-17.616	17.595	1.00	0.00
ATOM	2719	NH1	ARG	170	3.353	-16.685	18.552	1.00	0.00
ATOM	2720	HH11	ARG	170	4.204	-16.164	18.663	1.00	0.00
ATOM	2721	HH12	ARG	170	2.671	-16.727	19.313	1.00	0.00
ATOM	2722	NH2	ARG	170	2.186	-18.341	17.459	1.00	0.00
ATOM	2723	HH21	ARG	170	2.389	-19.264	17.047	1.00	0.00
ATOM	2724	HH22	ARG	170	1.539	-18.362	18.278	1.00	0.00
ATOM	3096	CB	HIP	194	-3.586	-23.303	17.897	1.00	0.00

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ATOM   3101  HD1 HIP   194      -1.196 -22.159  16.878  1.00  0.00
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ATOM   3103  HE1 HIP   194      -0.160 -20.234  18.070  1.00  0.00
ATOM   3104  NE2 HIP   194      -1.819 -20.396  19.443  1.00  0.00
ATOM   3105  HE2 HIP   194      -1.489 -19.155  20.468  1.00  0.00
ATOM   3106  CD2 HIP   194      -2.883 -21.286  19.422  1.00  0.00
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END
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REMARK oEQ4

ATOM	1	C1	PYA	1	-0.300	-17.423	20.915	1.00 0.00
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ATOM	3	C2	PYA	1	0.383	-16.033	20.735	1.00 0.00
ATOM	4	O2	PYA	1	-0.340	-15.027	20.949	1.00 0.00
ATOM	5	O3	PYA	1	1.619	-15.954	20.465	1.00 0.00
ATOM	6	C3	PYA	1	-0.486	-17.686	22.407	1.00 0.00
ATOM	7	H1	PYA	1	0.483	-17.646	22.906	1.00 0.00
ATOM	8	H2	PYA	1	-1.144	-16.928	22.837	1.00 0.00
ATOM	9	H3	PYA	1	-0.930	-18.677	22.568	1.00 0.00
ATOM	10	C1	NAD	2	-3.091	-15.311	19.661	1.00 0.00
ATOM	11	H1	NAD	2	-2.317	-15.326	18.904	1.00 0.00
ATOM	12	H2	NAD	2	-1.277	-17.400	20.412	1.00 0.00
ATOM	13	C2	NAD	2	-4.109	-16.276	19.678	1.00 0.00
ATOM	14	C3	NAD	2	-4.324	-17.312	18.580	1.00 0.00
ATOM	15	O1	NAD	2	-4.838	-16.976	17.521	1.00 0.00
ATOM	16	N1	NAD	2	-3.922	-18.562	18.892	1.00 0.00
ATOM	17	H3	NAD	2	-3.563	-18.808	19.813	1.00 0.00
ATOM	18	H4	NAD	2	-3.997	-19.335	18.246	1.00 0.00
ATOM	19	C4	NAD	2	-3.048	-14.344	20.670	1.00 0.00
ATOM	20	H5	NAD	2	-2.219	-13.653	20.718	1.00 0.00
ATOM	21	C5	NAD	2	-5.041	-16.220	20.693	1.00 0.00
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ATOM	24	H7	NAD	2	-4.094	-13.592	22.433	1.00 0.00
ATOM	25	N2	NAD	2	-5.032	-15.243	21.624	1.00 0.00
ATOM	26	C7	NAD	2	-6.160	-15.163	22.552	1.00 0.00
ATOM	2713	CD	ARG	170	3.528	-18.963	15.685	1.00 0.00
ATOM	2716	NE	ARG	170	3.812	-18.211	16.928	1.00 0.00
ATOM	2717	HE	ARG	170	4.778	-18.278	17.235	1.00 0.00
ATOM	2718	CZ	ARG	170	2.918	-17.922	17.924	1.00 0.00
ATOM	2719	NH1	ARG	170	3.326	-17.290	19.006	1.00 0.00
ATOM	2720	HH11	ARG	170	4.326	-17.201	19.119	1.00 0.00
ATOM	2721	HH12	ARG	170	2.618	-16.980	19.740	1.00 0.00
ATOM	2722	NH2	ARG	170	1.599	-18.205	17.757	1.00 0.00
ATOM	2723	HH21	ARG	170	1.551	-19.091	17.233	1.00 0.00
ATOM	2724	HH22	ARG	170	1.093	-18.306	18.653	1.00 0.00
ATOM	3096	CB	HIP	194	-3.608	-23.130	17.959	1.00 0.00

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ATOM   3099  CG  HIP   194      -2.709 -22.025  18.418  1.00  0.00
ATOM   3100  ND1 HIP   194      -1.652 -21.576  17.673  1.00  0.00
ATOM   3101  HD1 HIP   194      -1.317 -21.997  16.800  1.00  0.00
ATOM   3102  CE1 HIP   194      -0.945 -20.716  18.447  1.00  0.00
ATOM   3103  HE1 HIP   194      -0.044 -20.254  18.081  1.00  0.00
ATOM   3104  NE2 HIP   194      -1.493 -20.562  19.637  1.00  0.00
ATOM   3105  HE2 HIP   194      -0.025 -19.286  20.401  1.00  0.00
ATOM   3106  CD2 HIP   194      -2.600 -21.396  19.632  1.00  0.00
ATOM   3107  HD2 HIP   194      -3.236 -21.515  20.492  1.00  0.00
END
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REMARK cEQ1

ATOM	1	C1	PYA	1	-0.351	-17.563	21.422	1.00	0.00
ATOM	2	O1	PYA	1	-1.105	-18.524	21.433	1.00	0.00
ATOM	3	C2	PYA	1	0.639	-17.409	20.230	1.00	0.00
ATOM	4	O2	PYA	1	1.261	-16.322	20.124	1.00	0.00
ATOM	5	O3	PYA	1	0.745	-18.450	19.516	1.00	0.00
ATOM	6	C3	PYA	1	-0.288	-16.570	22.544	1.00	0.00
ATOM	7	H1	PYA	1	0.724	-16.535	22.959	1.00	0.00
ATOM	8	H2	PYA	1	-0.523	-15.565	22.185	1.00	0.00
ATOM	9	H3	PYA	1	-1.007	-16.858	23.310	1.00	0.00
ATOM	10	C1	NAD	2	-2.711	-15.642	20.003	1.00	0.00
ATOM	11	H1	NAD	2	-2.620	-15.225	19.001	1.00	0.00
ATOM	12	H2	NAD	2	-1.730	-16.095	20.182	1.00	0.00
ATOM	13	C2	NAD	2	-3.799	-16.694	20.040	1.00	0.00
ATOM	14	C3	NAD	2	-3.836	-17.659	18.932	1.00	0.00
ATOM	15	O1	NAD	2	-2.889	-17.752	18.136	1.00	0.00
ATOM	16	N1	NAD	2	-4.949	-18.476	18.777	1.00	0.00
ATOM	17	H3	NAD	2	-5.809	-18.241	19.269	1.00	0.00
ATOM	18	H4	NAD	2	-5.104	-18.876	17.857	1.00	0.00
ATOM	19	C4	NAD	2	-2.997	-14.567	21.021	1.00	0.00
ATOM	20	H5	NAD	2	-2.354	-13.697	21.039	1.00	0.00
ATOM	21	C5	NAD	2	-4.723	-16.699	21.028	1.00	0.00
ATOM	22	H6	NAD	2	-5.408	-17.528	21.133	1.00	0.00
ATOM	23	C6	NAD	2	-3.994	-14.635	21.909	1.00	0.00
ATOM	24	H7	NAD	2	-4.196	-13.861	22.635	1.00	0.00
ATOM	25	N2	NAD	2	-4.867	-15.733	21.982	1.00	0.00
ATOM	26	C7	NAD	2	-6.101	-15.683	22.746	1.00	0.00
ATOM	2713	CD	ARG	170	5.018	-18.743	15.879	1.00	0.00
ATOM	2716	NE	ARG	170	4.673	-17.689	16.850	1.00	0.00
ATOM	2717	HE	ARG	170	5.388	-16.994	17.026	1.00	0.00
ATOM	2718	CZ	ARG	170	3.530	-17.579	17.579	1.00	0.00
ATOM	2719	NH1	ARG	170	3.340	-16.459	18.292	1.00	0.00
ATOM	2720	HH11	ARG	170	4.214	-15.970	18.487	1.00	0.00
ATOM	2721	HH12	ARG	170	2.577	-16.430	19.000	1.00	0.00
ATOM	2722	NH2	ARG	170	2.581	-18.513	17.524	1.00	0.00
ATOM	2723	HH21	ARG	170	2.926	-19.426	17.200	1.00	0.00
ATOM	2724	HH22	ARG	170	1.827	-18.516	18.242	1.00	0.00
ATOM	3096	CB	HIP	194	-2.891	-23.783	17.759	1.00	0.00

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ATOM   3099  CG  HIP   194      -2.686 -22.380  18.275  1.00  0.00
ATOM   3100  ND1 HIP   194      -1.613 -21.556  17.982  1.00  0.00
ATOM   3101  HD1 HIP   194      -0.934 -21.709  17.229  1.00  0.00
ATOM   3102  CE1 HIP   194      -1.660 -20.446  18.740  1.00  0.00
ATOM   3103  HE1 HIP   194      -0.945 -19.633  18.732  1.00  0.00
ATOM   3104  NE2 HIP   194      -2.737 -20.561  19.516  1.00  0.00
ATOM   3105  HE2 HIP   194      -3.088 -19.883  20.191  1.00  0.00
ATOM   3106  CD2 HIP   194      -3.397 -21.738  19.241  1.00  0.00
ATOM   3107  HD2 HIP   194      -4.278 -22.018  19.784  1.00  0.00
END
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REMARK mSSTS1

ATOM	1	C1	PYA	1	-0.485	-17.652	21.507	1.00	0.00
ATOM	2	O1	PYA	1	-1.316	-18.552	21.441	1.00	0.00
ATOM	3	C2	PYA	1	0.671	-17.570	20.466	1.00	0.00
ATOM	4	O2	PYA	1	1.361	-16.518	20.471	1.00	0.00
ATOM	5	O3	PYA	1	0.798	-18.597	19.743	1.00	0.00
ATOM	6	C3	PYA	1	-0.504	-16.611	22.578	1.00	0.00
ATOM	7	H1	PYA	1	0.466	-16.608	23.084	1.00	0.00
ATOM	8	H2	PYA	1	-0.628	-15.629	22.114	1.00	0.00
ATOM	9	H3	PYA	1	-1.323	-16.798	23.273	1.00	0.00
ATOM	10	C1	NAD	2	-2.876	-15.688	19.889	1.00	0.00
ATOM	11	H1	NAD	2	-2.824	-15.287	18.875	1.00	0.00
ATOM	12	H2	NAD	2	-1.919	-16.214	20.006	1.00	0.00
ATOM	13	C2	NAD	2	-4.024	-16.670	20.004	1.00	0.00
ATOM	14	C3	NAD	2	-4.071	-17.740	18.996	1.00	0.00
ATOM	15	O1	NAD	2	-3.107	-17.926	18.237	1.00	0.00
ATOM	16	N1	NAD	2	-5.227	-18.484	18.831	1.00	0.00
ATOM	17	H3	NAD	2	-5.950	-18.432	19.547	1.00	0.00
ATOM	18	H4	NAD	2	-5.088	-19.411	18.455	1.00	0.00
ATOM	19	C4	NAD	2	-3.025	-14.595	20.916	1.00	0.00
ATOM	20	H5	NAD	2	-2.301	-13.792	20.927	1.00	0.00
ATOM	21	C5	NAD	2	-4.934	-16.567	21.000	1.00	0.00
ATOM	22	H6	NAD	2	-5.677	-17.336	21.152	1.00	0.00
ATOM	23	C6	NAD	2	-4.001	-14.564	21.830	1.00	0.00
ATOM	24	H7	NAD	2	-4.102	-13.784	22.568	1.00	0.00
ATOM	25	N2	NAD	2	-4.983	-15.559	21.923	1.00	0.00
ATOM	26	C7	NAD	2	-6.149	-15.403	22.775	1.00	0.00
ATOM	2713	CD	ARG	170	4.621	-18.665	15.677	1.00	0.00
ATOM	2716	NE	ARG	170	4.468	-17.663	16.752	1.00	0.00
ATOM	2717	HE	ARG	170	5.288	-17.099	16.928	1.00	0.00
ATOM	2718	CZ	ARG	170	3.445	-17.580	17.644	1.00	0.00
ATOM	2719	NH1	ARG	170	3.463	-16.609	18.565	1.00	0.00
ATOM	2720	HH11	ARG	170	4.377	-16.216	18.754	1.00	0.00
ATOM	2721	HH12	ARG	170	2.753	-16.645	19.321	1.00	0.00
ATOM	2722	NH2	ARG	170	2.376	-18.378	17.555	1.00	0.00
ATOM	2723	HH21	ARG	170	2.595	-19.258	17.066	1.00	0.00
ATOM	2724	HH22	ARG	170	1.774	-18.499	18.404	1.00	0.00
ATOM	3096	CB	HIP	194	-3.474	-23.314	17.866	1.00	0.00

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ATOM   3099  CG  HIP   194      -2.736 -22.060  18.252  1.00  0.00
ATOM   3100  ND1 HIP   194      -1.580 -21.651  17.631  1.00  0.00
ATOM   3101  HD1 HIP   194      -1.148 -22.047  16.791  1.00  0.00
ATOM   3102  CE1 HIP   194      -1.041 -20.624  18.300  1.00  0.00
ATOM   3103  HE1 HIP   194      -0.129 -20.131  18.015  1.00  0.00
ATOM   3104  NE2 HIP   194      -1.820 -20.364  19.339  1.00  0.00
ATOM   3105  HE2 HIP   194      -1.621 -19.616  20.030  1.00  0.00
ATOM   3106  CD2 HIP   194      -2.888 -21.240  19.336  1.00  0.00
ATOM   3107  HD2 HIP   194      -3.648 -21.228  20.098  1.00  0.00
END
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REMARK m(c)EQ2

ATOM	1	C1	PYA	1	-0.511	-17.657	21.589	1.00	0.00
ATOM	2	O1	PYA	1	-1.354	-18.547	21.506	1.00	0.00
ATOM	3	C2	PYA	1	0.711	-17.665	20.629	1.00	0.00
ATOM	4	O2	PYA	1	1.259	-16.551	20.407	1.00	0.00
ATOM	5	O3	PYA	1	1.044	-18.812	20.217	1.00	0.00
ATOM	6	C3	PYA	1	-0.582	-16.571	22.613	1.00	0.00
ATOM	7	H1	PYA	1	0.356	-16.535	23.174	1.00	0.00
ATOM	8	H2	PYA	1	-0.678	-15.602	22.114	1.00	0.00
ATOM	9	H3	PYA	1	-1.440	-16.725	23.267	1.00	0.00
ATOM	10	C1	NAD	2	-2.725	-15.736	19.875	1.00	0.00
ATOM	11	H1	NAD	2	-2.644	-15.354	18.857	1.00	0.00
ATOM	12	H2	NAD	2	-1.762	-16.238	20.033	1.00	0.00
ATOM	13	C2	NAD	2	-3.860	-16.733	19.967	1.00	0.00
ATOM	14	C3	NAD	2	-3.929	-17.771	18.929	1.00	0.00
ATOM	15	O1	NAD	2	-2.976	-17.955	18.153	1.00	0.00
ATOM	16	N1	NAD	2	-5.095	-18.484	18.768	1.00	0.00
ATOM	17	H3	NAD	2	-5.869	-18.380	19.419	1.00	0.00
ATOM	18	H4	NAD	2	-5.064	-19.346	18.247	1.00	0.00
ATOM	19	C4	NAD	2	-2.925	-14.630	20.882	1.00	0.00
ATOM	20	H5	NAD	2	-2.219	-13.807	20.898	1.00	0.00
ATOM	21	C5	NAD	2	-4.767	-16.664	20.967	1.00	0.00
ATOM	22	H6	NAD	2	-5.484	-17.458	21.115	1.00	0.00
ATOM	23	C6	NAD	2	-3.915	-14.622	21.783	1.00	0.00
ATOM	24	H7	NAD	2	-4.051	-13.833	22.507	1.00	0.00
ATOM	25	N2	NAD	2	-4.852	-15.660	21.889	1.00	0.00
ATOM	26	C7	NAD	2	-6.055	-15.529	22.692	1.00	0.00
ATOM	2713	CD	ARG	170	4.555	-18.685	15.706	1.00	0.00
ATOM	2716	NE	ARG	170	4.267	-17.617	16.685	1.00	0.00
ATOM	2717	HE	ARG	170	4.953	-16.876	16.733	1.00	0.00
ATOM	2718	CZ	ARG	170	3.300	-17.604	17.637	1.00	0.00
ATOM	2719	NH1	ARG	170	3.237	-16.554	18.467	1.00	0.00
ATOM	2720	HH11	ARG	170	4.153	-16.132	18.630	1.00	0.00
ATOM	2721	HH12	ARG	170	2.550	-16.597	19.251	1.00	0.00
ATOM	2722	NH2	ARG	170	2.338	-18.545	17.687	1.00	0.00
ATOM	2723	HH21	ARG	170	2.626	-19.408	17.204	1.00	0.00
ATOM	2724	HH22	ARG	170	1.938	-18.733	18.622	1.00	0.00
ATOM	3096	CB	HIP	194	-3.387	-23.318	17.909	1.00	0.00

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ATOM   3099  CG  HIP   194      -2.743 -22.000  18.259  1.00  0.00
ATOM   3100  ND1 HIP   194      -1.631 -21.497  17.622  1.00  0.00
ATOM   3101  HD1 HIP   194      -1.246 -21.767  16.714  1.00  0.00
ATOM   3102  CE1 HIP   194      -1.145 -20.455  18.309  1.00  0.00
ATOM   3103  HE1 HIP   194      -0.295 -19.876  17.989  1.00  0.00
ATOM   3104  NE2 HIP   194      -1.904 -20.287  19.381  1.00  0.00
ATOM   3105  HE2 HIP   194      -1.745 -19.564  20.108  1.00  0.00
ATOM   3106  CD2 HIP   194      -2.916 -21.223  19.370  1.00  0.00
ATOM   3107  HD2 HIP   194      -3.658 -21.273  20.148  1.00  0.00
END
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REMARK c(m)TS2

ATOM	1	C1	PYA	1	-0.878	-17.414	21.242	1.00	0.00
ATOM	2	O1	PYA	1	-1.631	-18.491	21.321	1.00	0.00
ATOM	3	C2	PYA	1	0.437	-17.473	20.413	1.00	0.00
ATOM	4	O2	PYA	1	0.970	-16.366	20.127	1.00	0.00
ATOM	5	O3	PYA	1	0.875	-18.638	20.236	1.00	0.00
ATOM	6	C3	PYA	1	-0.763	-16.628	22.523	1.00	0.00
ATOM	7	H1	PYA	1	0.159	-16.921	23.033	1.00	0.00
ATOM	8	H2	PYA	1	-0.695	-15.556	22.324	1.00	0.00
ATOM	9	H3	PYA	1	-1.623	-16.822	23.166	1.00	0.00
ATOM	10	C1	NAD	2	-2.585	-15.810	20.043	1.00	0.00
ATOM	11	H1	NAD	2	-2.106	-15.606	19.087	1.00	0.00
ATOM	12	H2	NAD	2	-1.618	-16.500	20.496	1.00	0.00
ATOM	13	C2	NAD	2	-3.727	-16.728	19.985	1.00	0.00
ATOM	14	C3	NAD	2	-3.768	-17.723	18.875	1.00	0.00
ATOM	15	O1	NAD	2	-2.949	-17.641	17.960	1.00	0.00
ATOM	16	N1	NAD	2	-4.773	-18.657	18.875	1.00	0.00
ATOM	17	H3	NAD	2	-5.186	-18.915	19.771	1.00	0.00
ATOM	18	H4	NAD	2	-4.632	-19.459	18.275	1.00	0.00
ATOM	19	C4	NAD	2	-2.793	-14.680	20.950	1.00	0.00
ATOM	20	H5	NAD	2	-2.076	-13.869	20.976	1.00	0.00
ATOM	21	C5	NAD	2	-4.724	-16.621	20.902	1.00	0.00
ATOM	22	H6	NAD	2	-5.529	-17.334	20.932	1.00	0.00
ATOM	23	C6	NAD	2	-3.856	-14.629	21.789	1.00	0.00
ATOM	24	H7	NAD	2	-4.034	-13.810	22.469	1.00	0.00
ATOM	25	N2	NAD	2	-4.823	-15.614	21.813	1.00	0.00
ATOM	26	C7	NAD	2	-6.045	-15.474	22.599	1.00	0.00
ATOM	2713	CD	ARG	170	4.508	-18.736	15.745	1.00	0.00
ATOM	2716	NE	ARG	170	4.228	-17.670	16.727	1.00	0.00
ATOM	2717	HE	ARG	170	4.911	-16.925	16.768	1.00	0.00
ATOM	2718	CZ	ARG	170	3.225	-17.617	17.639	1.00	0.00
ATOM	2719	NH1	ARG	170	3.156	-16.548	18.443	1.00	0.00
ATOM	2720	HH11	ARG	170	4.072	-16.142	18.640	1.00	0.00
ATOM	2721	HH12	ARG	170	2.407	-16.530	19.166	1.00	0.00
ATOM	2722	NH2	ARG	170	2.241	-18.534	17.673	1.00	0.00
ATOM	2723	HH21	ARG	170	2.513	-19.413	17.208	1.00	0.00
ATOM	2724	HH22	ARG	170	1.817	-18.702	18.595	1.00	0.00
ATOM	3096	CB	HIP	194	-3.469	-23.281	17.936	1.00	0.00

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ATOM   3099  CG  HIP   194      -2.787 -21.977  18.265  1.00  0.00
ATOM   3100  ND1 HIP   194      -1.668 -21.515  17.618  1.00  0.00
ATOM   3101  HD1 HIP   194      -1.298 -21.787  16.705  1.00  0.00
ATOM   3102  CE1 HIP   194      -1.176 -20.460  18.306  1.00  0.00
ATOM   3103  HE1 HIP   194      -0.312 -19.927  17.940  1.00  0.00
ATOM   3104  NE2 HIP   194      -1.904 -20.221  19.381  1.00  0.00
ATOM   3105  HE2 HIP   194      -1.656 -19.125  20.483  1.00  0.00
ATOM   3106  CD2 HIP   194      -2.916 -21.165  19.365  1.00  0.00
ATOM   3107  HD2 HIP   194      -3.662 -21.214  20.142  1.00  0.00
END
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REMARK c(m)EQ3

ATOM	1	C1	PYA	1	-0.775	-17.292	21.115	1.00	0.00
ATOM	2	O1	PYA	1	-1.522	-18.443	21.402	1.00	0.00
ATOM	3	C2	PYA	1	0.646	-17.536	20.532	1.00	0.00
ATOM	4	O2	PYA	1	1.277	-16.462	20.253	1.00	0.00
ATOM	5	O3	PYA	1	1.050	-18.716	20.406	1.00	0.00
ATOM	6	C3	PYA	1	-0.690	-16.434	22.375	1.00	0.00
ATOM	7	H1	PYA	1	0.117	-16.780	23.023	1.00	0.00
ATOM	8	H2	PYA	1	-0.490	-15.391	22.122	1.00	0.00
ATOM	9	H3	PYA	1	-1.633	-16.492	22.929	1.00	0.00
ATOM	10	C1	NAD	2	-2.988	-15.543	19.887	1.00	0.00
ATOM	11	H1	NAD	2	-2.310	-15.498	19.045	1.00	0.00
ATOM	12	H2	NAD	2	-1.275	-16.705	20.318	1.00	0.00
ATOM	13	C2	NAD	2	-3.894	-16.615	19.969	1.00	0.00
ATOM	14	C3	NAD	2	-3.886	-17.667	18.882	1.00	0.00
ATOM	15	O1	NAD	2	-3.232	-17.456	17.869	1.00	0.00
ATOM	16	N1	NAD	2	-4.689	-18.751	19.059	1.00	0.00
ATOM	17	H3	NAD	2	-4.892	-19.049	20.015	1.00	0.00
ATOM	18	H4	NAD	2	-4.500	-19.549	18.464	1.00	0.00
ATOM	19	C4	NAD	2	-3.022	-14.549	20.874	1.00	0.00
ATOM	20	H5	NAD	2	-2.293	-13.750	20.896	1.00	0.00
ATOM	21	C5	NAD	2	-4.796	-16.624	21.005	1.00	0.00
ATOM	22	H6	NAD	2	-5.482	-17.439	21.161	1.00	0.00
ATOM	23	C6	NAD	2	-4.004	-14.581	21.839	1.00	0.00
ATOM	24	H7	NAD	2	-4.126	-13.822	22.597	1.00	0.00
ATOM	25	N2	NAD	2	-4.899	-15.601	21.884	1.00	0.00
ATOM	26	C7	NAD	2	-6.084	-15.531	22.734	1.00	0.00
ATOM	2713	CD	ARG	170	4.525	-18.799	15.734	1.00	0.00
ATOM	2716	NE	ARG	170	4.242	-17.732	16.713	1.00	0.00
ATOM	2717	HE	ARG	170	4.948	-17.013	16.782	1.00	0.00
ATOM	2718	CZ	ARG	170	3.274	-17.695	17.670	1.00	0.00
ATOM	2719	NH1	ARG	170	3.233	-16.640	18.486	1.00	0.00
ATOM	2720	HH11	ARG	170	4.158	-16.232	18.627	1.00	0.00
ATOM	2721	HH12	ARG	170	2.514	-16.634	19.272	1.00	0.00
ATOM	2722	NH2	ARG	170	2.290	-18.617	17.728	1.00	0.00
ATOM	2723	HH21	ARG	170	2.557	-19.491	17.251	1.00	0.00
ATOM	2724	HH22	ARG	170	1.918	-18.802	18.669	1.00	0.00
ATOM	3096	CB	HIP	194	-3.407	-23.382	17.860	1.00	0.00

ATOM 3099 CG HIP 194 -2.756 -22.059 18.171 1.00 0.00
ATOM 3100 ND1 HIP 194 -1.669 -21.564 17.499 1.00 0.00
ATOM 3101 HD1 HIP 194 -1.290 -21.839 16.592 1.00 0.00
ATOM 3102 CE1 HIP 194 -1.207 -20.479 18.173 1.00 0.00
ATOM 3103 HE1 HIP 194 -0.359 -19.930 17.791 1.00 0.00
ATOM 3104 NE2 HIP 194 -1.924 -20.250 19.255 1.00 0.00
ATOM 3105 HE2 HIP 194 -1.571 -19.046 20.615 1.00 0.00
ATOM 3106 CD2 HIP 194 -2.892 -21.238 19.265 1.00 0.00
ATOM 3107 HD2 HIP 194 -3.607 -21.320 20.069 1.00 0.00
END

REMARK mSSTS3

ATOM	1	C1	PYA	1	-0.810	-17.475	21.021	1.00	0.00
ATOM	2	O1	PYA	1	-1.449	-18.674	21.394	1.00	0.00
ATOM	3	C2	PYA	1	0.681	-17.633	20.609	1.00	0.00
ATOM	4	O2	PYA	1	1.271	-16.527	20.353	1.00	0.00
ATOM	5	O3	PYA	1	1.175	-18.784	20.557	1.00	0.00
ATOM	6	C3	PYA	1	-0.921	-16.498	22.188	1.00	0.00
ATOM	7	H1	PYA	1	-0.255	-16.801	22.994	1.00	0.00
ATOM	8	H2	PYA	1	-0.637	-15.490	21.882	1.00	0.00
ATOM	9	H3	PYA	1	-1.946	-16.484	22.578	1.00	0.00
ATOM	10	C1	NAD	2	-3.021	-15.229	19.990	1.00	0.00
ATOM	11	H1	NAD	2	-2.271	-15.134	19.216	1.00	0.00
ATOM	12	H2	NAD	2	-1.289	-17.049	20.121	1.00	0.00
ATOM	13	C2	NAD	2	-3.828	-16.374	20.021	1.00	0.00
ATOM	14	C3	NAD	2	-3.706	-17.408	18.920	1.00	0.00
ATOM	15	O1	NAD	2	-3.201	-17.079	17.855	1.00	0.00
ATOM	16	N1	NAD	2	-4.252	-18.621	19.175	1.00	0.00
ATOM	17	H3	NAD	2	-4.310	-18.944	20.141	1.00	0.00
ATOM	18	H4	NAD	2	-4.022	-19.384	18.550	1.00	0.00
ATOM	19	C4	NAD	2	-3.172	-14.265	20.989	1.00	0.00
ATOM	20	H5	NAD	2	-2.521	-13.405	21.047	1.00	0.00
ATOM	21	C5	NAD	2	-4.758	-16.493	21.029	1.00	0.00
ATOM	22	H6	NAD	2	-5.362	-17.378	21.146	1.00	0.00
ATOM	23	C6	NAD	2	-4.174	-14.407	21.927	1.00	0.00
ATOM	24	H7	NAD	2	-4.370	-13.695	22.714	1.00	0.00
ATOM	25	N2	NAD	2	-4.969	-15.503	21.926	1.00	0.00
ATOM	26	C7	NAD	2	-6.147	-15.562	22.785	1.00	0.00
ATOM	2713	CD	ARG	170	4.336	-18.742	15.678	1.00	0.00
ATOM	2716	NE	ARG	170	4.087	-17.697	16.692	1.00	0.00
ATOM	2717	HE	ARG	170	4.806	-16.990	16.760	1.00	0.00
ATOM	2718	CZ	ARG	170	3.179	-17.697	17.707	1.00	0.00
ATOM	2719	NH1	ARG	170	3.201	-16.688	18.578	1.00	0.00
ATOM	2720	HH11	ARG	170	4.141	-16.309	18.701	1.00	0.00
ATOM	2721	HH12	ARG	170	2.498	-16.689	19.385	1.00	0.00
ATOM	2722	NH2	ARG	170	2.180	-18.606	17.776	1.00	0.00
ATOM	2723	HH21	ARG	170	2.401	-19.455	17.236	1.00	0.00
ATOM	2724	HH22	ARG	170	1.891	-18.846	18.733	1.00	0.00
ATOM	3096	CB	HIP	194	-3.495	-23.488	17.780	1.00	0.00

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ATOM   3099  CG  HIP   194      -2.802 -22.188  18.087  1.00  0.00
ATOM   3100  ND1 HIP   194      -1.704 -21.740  17.404  1.00  0.00
ATOM   3101  HD1 HIP   194      -1.371 -21.986  16.472  1.00  0.00
ATOM   3102  CE1 HIP   194      -1.165 -20.699  18.090  1.00  0.00
ATOM   3103  HE1 HIP   194      -0.297 -20.191  17.693  1.00  0.00
ATOM   3104  NE2 HIP   194      -1.842 -20.456  19.194  1.00  0.00
ATOM   3105  HE2 HIP   194      -1.491 -19.289  20.622  1.00  0.00
ATOM   3106  CD2 HIP   194      -2.866 -21.388  19.204  1.00  0.00
ATOM   3107  HD2 HIP   194      -3.562 -21.451  20.027  1.00  0.00
END
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REMARK cTS1

ATOM	1	C1	PYA	1	-0.530	-17.574	21.519	1.00	0.00
ATOM	2	O1	PYA	1	-1.344	-18.490	21.501	1.00	0.00
ATOM	3	C2	PYA	1	0.619	-17.548	20.466	1.00	0.00
ATOM	4	O2	PYA	1	1.201	-16.445	20.290	1.00	0.00
ATOM	5	O3	PYA	1	0.908	-18.682	19.969	1.00	0.00
ATOM	6	C3	PYA	1	-0.545	-16.494	22.556	1.00	0.00
ATOM	7	H1	PYA	1	0.391	-16.516	23.125	1.00	0.00
ATOM	8	H2	PYA	1	-0.604	-15.519	22.069	1.00	0.00
ATOM	9	H3	PYA	1	-1.410	-16.630	23.205	1.00	0.00
ATOM	10	C1	NAD	2	-2.721	-15.674	19.877	1.00	0.00
ATOM	11	H1	NAD	2	-2.644	-15.286	18.863	1.00	0.00
ATOM	12	H2	NAD	2	-1.744	-16.148	20.042	1.00	0.00
ATOM	13	C2	NAD	2	-3.820	-16.711	19.964	1.00	0.00
ATOM	14	C3	NAD	2	-3.901	-17.691	18.870	1.00	0.00
ATOM	15	O1	NAD	2	-2.972	-17.799	18.052	1.00	0.00
ATOM	16	N1	NAD	2	-5.037	-18.467	18.736	1.00	0.00
ATOM	17	H3	NAD	2	-5.884	-18.200	19.237	1.00	0.00
ATOM	18	H4	NAD	2	-5.195	-18.909	17.841	1.00	0.00
ATOM	19	C4	NAD	2	-2.950	-14.587	20.897	1.00	0.00
ATOM	20	H5	NAD	2	-2.287	-13.730	20.895	1.00	0.00
ATOM	21	C5	NAD	2	-4.733	-16.677	20.962	1.00	0.00
ATOM	22	H6	NAD	2	-5.420	-17.500	21.106	1.00	0.00
ATOM	23	C6	NAD	2	-3.949	-14.609	21.787	1.00	0.00
ATOM	24	H7	NAD	2	-4.113	-13.823	22.511	1.00	0.00
ATOM	25	N2	NAD	2	-4.837	-15.689	21.900	1.00	0.00
ATOM	26	C7	NAD	2	-6.055	-15.586	22.684	1.00	0.00
ATOM	2713	CD	ARG	170	4.673	-18.691	15.733	1.00	0.00
ATOM	2716	NE	ARG	170	4.387	-17.630	16.720	1.00	0.00
ATOM	2717	HE	ARG	170	5.079	-16.900	16.809	1.00	0.00
ATOM	2718	CZ	ARG	170	3.345	-17.587	17.587	1.00	0.00
ATOM	2719	NH1	ARG	170	3.227	-16.512	18.381	1.00	0.00
ATOM	2720	HH11	ARG	170	4.115	-16.045	18.545	1.00	0.00
ATOM	2721	HH12	ARG	170	2.510	-16.531	19.134	1.00	0.00
ATOM	2722	NH2	ARG	170	2.395	-18.534	17.603	1.00	0.00
ATOM	2723	HH21	ARG	170	2.713	-19.412	17.185	1.00	0.00
ATOM	2724	HH22	ARG	170	1.868	-18.653	18.489	1.00	0.00
ATOM	3096	CB	HIP	194	-3.250	-23.497	17.867	1.00	0.00

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ATOM   3099  CG  HIP   194      -2.755 -22.125  18.256  1.00  0.00
ATOM   3100  ND1 HIP   194      -1.615 -21.530  17.746  1.00  0.00
ATOM   3101  HD1 HIP   194      -1.104 -21.777  16.894  1.00  0.00
ATOM   3102  CE1 HIP   194      -1.335 -20.430  18.458  1.00  0.00
ATOM   3103  HE1 HIP   194      -0.516 -19.764  18.278  1.00  0.00
ATOM   3104  NE2 HIP   194      -2.256 -20.323  19.408  1.00  0.00
ATOM   3105  HE2 HIP   194      -2.259 -19.596  20.131  1.00  0.00
ATOM   3106  CD2 HIP   194      -3.158 -21.358  19.308  1.00  0.00
ATOM   3107  HD2 HIP   194      -3.994 -21.464  19.977  1.00  0.00
END
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REMARK cTS3

ATOM	1	C1	PYA	1	-0.828	-17.535	21.050	1.00	0.00
ATOM	2	O1	PYA	1	-1.455	-18.740	21.423	1.00	0.00
ATOM	3	C2	PYA	1	0.677	-17.652	20.678	1.00	0.00
ATOM	4	O2	PYA	1	1.239	-16.528	20.430	1.00	0.00
ATOM	5	O3	PYA	1	1.214	-18.784	20.661	1.00	0.00
ATOM	6	C3	PYA	1	-0.980	-16.556	22.211	1.00	0.00
ATOM	7	H1	PYA	1	-0.338	-16.862	23.038	1.00	0.00
ATOM	8	H2	PYA	1	-0.689	-15.548	21.917	1.00	0.00
ATOM	9	H3	PYA	1	-2.018	-16.546	22.566	1.00	0.00
ATOM	10	C1	NAD	2	-2.977	-15.135	19.954	1.00	0.00
ATOM	11	H1	NAD	2	-2.217	-14.999	19.195	1.00	0.00
ATOM	12	H2	NAD	2	-1.299	-17.124	20.137	1.00	0.00
ATOM	13	C2	NAD	2	-3.778	-16.285	19.934	1.00	0.00
ATOM	14	C3	NAD	2	-3.653	-17.304	18.815	1.00	0.00
ATOM	15	O1	NAD	2	-3.371	-16.934	17.685	1.00	0.00
ATOM	16	N1	NAD	2	-3.942	-18.572	19.178	1.00	0.00
ATOM	17	H3	NAD	2	-3.803	-18.864	20.147	1.00	0.00
ATOM	18	H4	NAD	2	-3.751	-19.327	18.531	1.00	0.00
ATOM	19	C4	NAD	2	-3.137	-14.216	20.993	1.00	0.00
ATOM	20	H5	NAD	2	-2.481	-13.364	21.090	1.00	0.00
ATOM	21	C5	NAD	2	-4.718	-16.444	20.923	1.00	0.00
ATOM	22	H6	NAD	2	-5.332	-17.332	20.982	1.00	0.00
ATOM	23	C6	NAD	2	-4.144	-14.399	21.920	1.00	0.00
ATOM	24	H7	NAD	2	-4.348	-13.717	22.735	1.00	0.00
ATOM	25	N2	NAD	2	-4.940	-15.494	21.864	1.00	0.00
ATOM	26	C7	NAD	2	-6.141	-15.592	22.681	1.00	0.00
ATOM	2713	CD	ARG	170	4.259	-18.683	15.672	1.00	0.00
ATOM	2716	NE	ARG	170	3.973	-17.622	16.663	1.00	0.00
ATOM	2717	HE	ARG	170	4.704	-16.927	16.759	1.00	0.00
ATOM	2718	CZ	ARG	170	3.081	-17.650	17.691	1.00	0.00
ATOM	2719	NH1	ARG	170	3.116	-16.672	18.594	1.00	0.00
ATOM	2720	HH11	ARG	170	4.078	-16.360	18.755	1.00	0.00
ATOM	2721	HH12	ARG	170	2.428	-16.701	19.416	1.00	0.00
ATOM	2722	NH2	ARG	170	2.063	-18.552	17.737	1.00	0.00
ATOM	2723	HH21	ARG	170	2.285	-19.380	17.162	1.00	0.00
ATOM	2724	HH22	ARG	170	1.842	-18.854	18.690	1.00	0.00
ATOM	3096	CB	HIP	194	-3.565	-23.503	17.778	1.00	0.00

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ATOM   3099  CG  HIP   194      -2.840 -22.238  18.126  1.00  0.00
ATOM   3100  ND1 HIP   194      -1.770 -21.766  17.421  1.00  0.00
ATOM   3101  HD1 HIP   194      -1.469 -21.968  16.469  1.00  0.00
ATOM   3102  CE1 HIP   194      -1.189 -20.773  18.143  1.00  0.00
ATOM   3103  HE1 HIP   194      -0.317 -20.271  17.748  1.00  0.00
ATOM   3104  NE2 HIP   194      -1.817 -20.585  19.286  1.00  0.00
ATOM   3105  HE2 HIP   194      -1.436 -19.390  20.679  1.00  0.00
ATOM   3106  CD2 HIP   194      -2.853 -21.505  19.287  1.00  0.00
ATOM   3107  HD2 HIP   194      -3.506 -21.638  20.135  1.00  0.00
END
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REMARK cEQ4

ATOM	1	C1	PYA	1	-0.659	-17.256	21.256	1.00	0.00
ATOM	2	O1	PYA	1	-1.425	-18.404	21.514	1.00	0.00
ATOM	3	C2	PYA	1	0.806	-17.503	20.802	1.00	0.00
ATOM	4	O2	PYA	1	1.475	-16.429	20.615	1.00	0.00
ATOM	5	O3	PYA	1	1.207	-18.684	20.676	1.00	0.00
ATOM	6	C3	PYA	1	-0.651	-16.391	22.509	1.00	0.00
ATOM	7	H1	PYA	1	-0.014	-16.843	23.270	1.00	0.00
ATOM	8	H2	PYA	1	-0.250	-15.404	22.282	1.00	0.00
ATOM	9	H3	PYA	1	-1.664	-16.295	22.918	1.00	0.00
ATOM	10	C1	NAD	2	-2.916	-15.694	19.645	1.00	0.00
ATOM	11	H1	NAD	2	-2.244	-15.662	18.797	1.00	0.00
ATOM	12	H2	NAD	2	-1.100	-16.684	20.414	1.00	0.00
ATOM	13	C2	NAD	2	-3.856	-16.733	19.728	1.00	0.00
ATOM	14	C3	NAD	2	-3.971	-17.718	18.579	1.00	0.00
ATOM	15	O1	NAD	2	-3.519	-17.404	17.482	1.00	0.00
ATOM	16	N1	NAD	2	-4.667	-18.859	18.825	1.00	0.00
ATOM	17	H3	NAD	2	-4.687	-19.213	19.782	1.00	0.00
ATOM	18	H4	NAD	2	-4.550	-19.617	18.159	1.00	0.00
ATOM	19	C4	NAD	2	-2.882	-14.726	20.653	1.00	0.00
ATOM	20	H5	NAD	2	-2.117	-13.964	20.669	1.00	0.00
ATOM	21	C5	NAD	2	-4.697	-16.759	20.820	1.00	0.00
ATOM	22	H6	NAD	2	-5.388	-17.570	20.983	1.00	0.00
ATOM	23	C6	NAD	2	-3.815	-14.760	21.666	1.00	0.00
ATOM	24	H7	NAD	2	-3.877	-14.018	22.448	1.00	0.00
ATOM	25	N2	NAD	2	-4.721	-15.767	21.741	1.00	0.00
ATOM	26	C7	NAD	2	-5.829	-15.702	22.699	1.00	0.00
ATOM	2713	CD	ARG	170	4.100	-18.615	15.687	1.00	0.00
ATOM	2716	NE	ARG	170	3.996	-17.574	16.730	1.00	0.00
ATOM	2717	HE	ARG	170	4.860	-17.057	16.870	1.00	0.00
ATOM	2718	CZ	ARG	170	3.108	-17.515	17.759	1.00	0.00
ATOM	2719	NH1	ARG	170	3.247	-16.566	18.682	1.00	0.00
ATOM	2720	HH11	ARG	170	4.229	-16.310	18.811	1.00	0.00
ATOM	2721	HH12	ARG	170	2.605	-16.595	19.536	1.00	0.00
ATOM	2722	NH2	ARG	170	2.000	-18.302	17.794	1.00	0.00
ATOM	2723	HH21	ARG	170	2.144	-19.144	17.214	1.00	0.00
ATOM	2724	HH22	ARG	170	1.777	-18.608	18.752	1.00	0.00
ATOM	3096	CB	HIP	194	-3.709	-23.209	17.830	1.00	0.00

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ATOM   3099  CG  HIP   194      -2.961 -21.970  18.245  1.00  0.00
ATOM   3100  ND1 HIP   194      -1.965 -21.391  17.510  1.00  0.00
ATOM   3101  HD1 HIP   194      -1.681 -21.573  16.548  1.00  0.00
ATOM   3102  CE1 HIP   194      -1.399 -20.407  18.255  1.00  0.00
ATOM   3103  HE1 HIP   194      -0.583 -19.827  17.847  1.00  0.00
ATOM   3104  NE2 HIP   194      -1.971 -20.315  19.439  1.00  0.00
ATOM   3105  HE2 HIP   194      -1.442 -19.030  20.751  1.00  0.00
ATOM   3106  CD2 HIP   194      -2.944 -21.300  19.445  1.00  0.00
ATOM   3107  HD2 HIP   194      -3.543 -21.525  20.313  1.00  0.00
END
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Full reference of the Gaussian 09 program:

Gaussian 09, Revision E01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci,B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2013.