

HEADER CSD ENTRY hp1r4									
CRYST1	10.8640	11.5360	16.3200	95.13	108.38	112.18			P-1
SCALE1	0.092047	0.037519	0.040630			0.000000			
SCALE2	0.000000	0.093610	0.022846			0.000000			
SCALE3	0.000000	0.000000	0.066462			0.000000			
HETATM	1	O1A	UNK	0	1	3.586	-0.251	6.344	1.00 0.00
HETATM	2	C1A	UNK	0	1	5.736	1.261	4.302	1.00 0.00
HETATM	3	C2A	UNK	0	1	5.466	0.651	5.271	1.00 0.00
HETATM	4	C3A	UNK	0	1	5.010	-0.105	6.434	1.00 0.00
HETATM	5	C4A	UNK	0	1	5.600	-1.503	6.393	1.00 0.00
HETATM	6	C5A	UNK	0	1	4.805	-2.594	6.610	1.00 0.00
HETATM	7	H5A	UNK	0	1	3.893	-2.486	6.756	1.00 0.00
HETATM	8	C6A	UNK	0	1	5.372	-3.874	6.608	1.00 0.00
HETATM	9	H6A	UNK	0	1	4.838	-4.615	6.781	1.00 0.00
HETATM	10	C7A	UNK	0	1	6.689	-4.044	6.357	1.00 0.00
HETATM	11	H7A	UNK	0	1	7.050	-4.901	6.330	1.00 0.00
HETATM	12	C8A	UNK	0	1	7.492	-2.964	6.145	1.00 0.00
HETATM	13	H8A	UNK	0	1	8.401	-3.078	5.981	1.00 0.00
HETATM	14	C9A	UNK	0	1	6.941	-1.697	6.173	1.00 0.00
HETATM	15	H9A	UNK	0	1	7.491	-0.959	6.043	1.00 0.00
HETATM	16	C10A	UNK	0	1	5.391	0.569	7.731	1.00 0.00
HETATM	17	C11A	UNK	0	1	4.863	0.084	8.907	1.00 0.00
HETATM	18	H11A	UNK	0	1	4.263	-0.626	8.895	1.00 0.00
HETATM	19	C12A	UNK	0	1	5.232	0.669	10.117	1.00 0.00
HETATM	20	H12A	UNK	0	1	4.873	0.353	10.915	1.00 0.00
HETATM	21	C13A	UNK	0	1	6.120	1.703	10.137	1.00 0.00
HETATM	22	H13A	UNK	0	1	6.374	2.074	10.951	1.00 0.00
HETATM	23	C14A	UNK	0	1	6.637	2.199	8.992	1.00 0.00
HETATM	24	H14A	UNK	0	1	7.230	2.915	9.013	1.00 0.00
HETATM	25	C15A	UNK	0	1	6.265	1.617	7.776	1.00 0.00
HETATM	26	H15A	UNK	0	1	6.618	1.950	6.983	1.00 0.00
HETATM	27	O1B	UNK	0	1	7.939	3.289	0.587	1.00 0.00
HETATM	28	C1B	UNK	0	1	6.028	1.957	3.131	1.00 0.00
HETATM	29	C2B	UNK	0	1	6.252	2.525	2.117	1.00 0.00
HETATM	30	C3B	UNK	0	1	6.534	3.276	0.867	1.00 0.00
HETATM	31	C4B	UNK	0	1	6.119	4.728	1.049	1.00 0.00
HETATM	32	C5B	UNK	0	1	7.021	5.761	1.046	1.00 0.00
HETATM	33	H5B	UNK	0	1	7.923	5.585	0.909	1.00 0.00
HETATM	34	C6B	UNK	0	1	6.596	7.067	1.246	1.00 0.00
HETATM	35	H6B	UNK	0	1	7.220	7.756	1.223	1.00 0.00
HETATM	36	C7B	UNK	0	1	5.286	7.361	1.473	1.00 0.00
HETATM	37	H7B	UNK	0	1	5.019	8.240	1.619	1.00 0.00
HETATM	38	C8B	UNK	0	1	4.372	6.345	1.482	1.00 0.00
HETATM	39	H8B	UNK	0	1	3.474	6.531	1.634	1.00 0.00
HETATM	40	C9B	UNK	0	1	4.780	5.041	1.265	1.00 0.00
HETATM	41	H9B	UNK	0	1	4.146	4.360	1.264	1.00 0.00
HETATM	42	C10B	UNK	0	1	5.793	2.687	-0.355	1.00 0.00
HETATM	43	C11B	UNK	0	1	6.030	3.197	-1.611	1.00 0.00
HETATM	44	H11B	UNK	0	1	6.652	3.880	-1.717	1.00 0.00
HETATM	45	C12B	UNK	0	1	5.347	2.707	-2.732	1.00 0.00
HETATM	46	H12B	UNK	0	1	5.512	3.059	-3.576	1.00 0.00
HETATM	47	C13B	UNK	0	1	4.436	1.701	-2.564	1.00 0.00
HETATM	48	H13B	UNK	0	1	3.977	1.375	-3.304	1.00 0.00
HETATM	49	C14B	UNK	0	1	4.186	1.170	-1.341	1.00 0.00
HETATM	50	H14B	UNK	0	1	3.564	0.485	-1.247	1.00 0.00
HETATM	51	C15B	UNK	0	1	4.872	1.661	-0.214	1.00 0.00
HETATM	52	H15B	UNK	0	1	4.707	1.297	0.626	1.00 0.00
HETATM	53	H10A	UNK	0	1	3.321	0.452	6.334	1.00 0.00
HETATM	54	H10B	UNK	0	1	8.254	2.512	0.737	1.00 0.00
HETATM	55	C16A	UNK	0	1	-0.651	0.909	1.830	1.00 0.00
HETATM	56	C17A	UNK	0	1	-1.063	1.514	3.163	1.00 0.00
HETATM	57	H17A	UNK	0	1	-2.030	1.666	3.143	1.00 0.00
HETATM	58	C18A	UNK	0	1	-0.763	0.530	4.257	1.00 0.00
HETATM	59	H18A	UNK	0	1	-1.380	0.361	4.932	1.00 0.00
HETATM	60	C19A	UNK	0	1	0.380	-0.077	4.233	1.00 0.00

HETATM	61	H19A	UNK	0	1	0.615	-0.678	4.902	1.00	0.00
HETATM	62	C20A	UNK	0	1	1.320	0.210	3.101	1.00	0.00
HETATM	63	C21A	UNK	0	1	2.405	-0.866	2.916	1.00	0.00
HETATM	64	H21A	UNK	0	1	2.969	-0.628	2.177	1.00	0.00
HETATM	65	H21B	UNK	0	1	1.989	-1.713	2.741	1.00	0.00
HETATM	66	H21C	UNK	0	1	2.934	-0.928	3.715	1.00	0.00
HETATM	67	O2A	UNK	0	1	-1.347	0.972	0.803	1.00	0.00
HETATM	68	N1A	UNK	0	1	0.514	0.251	1.870	1.00	0.00
HETATM	69	H1NA	UNK	0	1	0.796	-0.155	1.166	1.00	0.00
HETATM	70	O2B	UNK	0	1	2.315	2.119	5.687	1.00	0.00
HETATM	71	N1B	UNK	0	1	0.474	2.899	4.630	1.00	0.00
HETATM	72	H1NB	UNK	0	1	0.205	3.321	5.329	1.00	0.00
HETATM	73	C16B	UNK	0	1	1.619	2.229	4.673	1.00	0.00
HETATM	74	C17B	UNK	0	1	2.058	1.624	3.351	1.00	0.00
HETATM	75	H17B	UNK	0	1	3.027	1.475	3.378	1.00	0.00
HETATM	76	C18B	UNK	0	1	1.752	2.596	2.266	1.00	0.00
HETATM	77	H18B	UNK	0	1	2.365	2.762	1.587	1.00	0.00
HETATM	78	C19B	UNK	0	1	0.590	3.216	2.292	1.00	0.00
HETATM	79	H19B	UNK	0	1	0.356	3.817	1.622	1.00	0.00
HETATM	80	C20B	UNK	0	1	-0.336	2.929	3.419	1.00	0.00
HETATM	81	C21B	UNK	0	1	-1.382	4.033	3.604	1.00	0.00
HETATM	82	H21D	UNK	0	1	-1.955	3.811	4.341	1.00	0.00
HETATM	83	H21E	UNK	0	1	-1.908	4.114	2.805	1.00	0.00
HETATM	84	H21F	UNK	0	1	-0.941	4.867	3.783	1.00	0.00
HETATM	85	O1W	UNK	0	1	-1.279	3.755	6.882	1.00	0.00
HETATM	86	H1WA	UNK	0	1	-0.572	3.149	7.102	1.00	0.00
HETATM	87	H1WB	UNK	0	1	-1.089	4.322	7.854	1.00	0.00

CONNECT	1	4	53
CONNECT	2	3	28
CONNECT	3	4	
CONNECT	4	5	16
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CONNECT	27	30	54
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CONNECT	31	32	40
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CONNECT	33		
CONNECT	34	35	36
CONNECT	35		
CONNECT	36	37	38
CONNECT	37		
CONNECT	38	39	40

HEADER		CSD ENTRY hplrest1								
CRYST1	6.8620	10.2280	12.5800	97.06	92.72	102.46			P-1	
SCALE1	0.145730	0.032188	0.011432			0.000000				
SCALE2	0.000000	0.100127	0.013798			0.000000				
SCALE3	0.000000	0.000000	0.080333			0.000000				
HETATM	1	O1	UNK	0	1	1.550	7.246	3.941	1.00	0.00
HETATM	2	H1	UNK	0	1	1.802	6.696	4.531	1.00	0.00
HETATM	3	C1	UNK	0	1	3.952	8.951	5.688	1.00	0.00
HETATM	4	C2	UNK	0	1	3.279	8.674	4.719	1.00	0.00
HETATM	5	C3	UNK	0	1	2.461	8.304	3.593	1.00	0.00
HETATM	6	C4	UNK	0	1	3.423	7.744	2.439	1.00	0.00
HETATM	7	C5	UNK	0	1	2.979	6.747	1.555	1.00	0.00
HETATM	8	H5	UNK	0	1	2.089	6.384	1.556	1.00	0.00
HETATM	9	C6	UNK	0	1	3.851	6.359	0.537	1.00	0.00
HETATM	10	H6	UNK	0	1	3.651	5.641	-0.068	1.00	0.00
HETATM	11	C7	UNK	0	1	5.049	6.916	0.400	1.00	0.00
HETATM	12	H7	UNK	0	1	5.572	6.714	-0.378	1.00	0.00
HETATM	13	C8	UNK	0	1	5.473	7.854	1.277	1.00	0.00
HETATM	14	H8	UNK	0	1	6.401	8.107	1.236	1.00	0.00
HETATM	15	C9	UNK	0	1	4.638	8.295	2.277	1.00	0.00
HETATM	16	H9	UNK	0	1	4.945	9.019	2.827	1.00	0.00
HETATM	17	C10	UNK	0	1	1.644	9.479	3.181	1.00	0.00
HETATM	18	C11	UNK	0	1	0.600	9.981	3.957	1.00	0.00
HETATM	19	H11	UNK	0	1	0.627	9.335	4.662	1.00	0.00
HETATM	20	C12	UNK	0	1	-0.142	11.081	3.585	1.00	0.00
HETATM	21	H12	UNK	0	1	-0.786	11.376	4.227	1.00	0.00
HETATM	22	C13	UNK	0	1	0.103	11.738	2.373	1.00	0.00
HETATM	23	H13	UNK	0	1	-0.477	12.497	2.337	1.00	0.00
HETATM	24	C14	UNK	0	1	1.115	11.255	1.598	1.00	0.00
HETATM	25	H14	UNK	0	1	1.101	11.669	0.733	1.00	0.00
HETATM	26	C15	UNK	0	1	1.884	10.144	1.981	1.00	0.00
HETATM	27	H15	UNK	0	1	2.590	9.993	1.346	1.00	0.00
HETATM	28	O1	UNK	0	1	7.165	11.013	8.507	1.00	0.00
HETATM	29	H1	UNK	0	1	6.912	11.563	7.917	1.00	0.00
HETATM	30	C1	UNK	0	1	4.763	9.308	6.761	1.00	0.00
HETATM	31	C2	UNK	0	1	5.435	9.585	7.729	1.00	0.00
HETATM	32	C3	UNK	0	1	6.253	9.955	8.856	1.00	0.00
HETATM	33	C4	UNK	0	1	5.291	10.515	10.010	1.00	0.00
HETATM	34	C5	UNK	0	1	5.736	11.512	10.893	1.00	0.00
HETATM	35	H5	UNK	0	1	6.626	11.875	10.892	1.00	0.00
HETATM	36	C6	UNK	0	1	4.864	11.900	11.912	1.00	0.00
HETATM	37	H6	UNK	0	1	5.064	12.618	12.517	1.00	0.00
HETATM	38	C7	UNK	0	1	3.665	11.343	12.049	1.00	0.00
HETATM	39	H7	UNK	0	1	3.142	11.545	12.827	1.00	0.00
HETATM	40	C8	UNK	0	1	3.241	10.405	11.171	1.00	0.00
HETATM	41	H8	UNK	0	1	2.314	10.152	11.212	1.00	0.00
HETATM	42	C9	UNK	0	1	4.076	9.964	10.171	1.00	0.00
HETATM	43	H9	UNK	0	1	3.769	9.240	9.621	1.00	0.00
HETATM	44	C10	UNK	0	1	7.071	8.780	9.268	1.00	0.00
HETATM	45	C11	UNK	0	1	8.114	8.278	8.491	1.00	0.00
HETATM	46	H11	UNK	0	1	8.088	8.924	7.786	1.00	0.00
HETATM	47	C12	UNK	0	1	8.856	7.178	8.863	1.00	0.00
HETATM	48	H12	UNK	0	1	9.500	6.883	8.221	1.00	0.00
HETATM	49	C13	UNK	0	1	8.611	6.521	10.076	1.00	0.00
HETATM	50	H13	UNK	0	1	9.192	5.762	10.112	1.00	0.00
HETATM	51	C14	UNK	0	1	7.600	7.004	10.850	1.00	0.00
HETATM	52	H14	UNK	0	1	7.614	6.590	11.715	1.00	0.00
HETATM	53	C15	UNK	0	1	6.831	8.115	10.468	1.00	0.00
HETATM	54	H15	UNK	0	1	6.124	8.267	11.103	1.00	0.00
HETATM	55	O2	UNK	0	1	1.220	3.154	7.420	1.00	0.00
HETATM	56	N1	UNK	0	1	0.329	3.831	5.461	1.00	0.00
HETATM	57	H1N1	UNK	0	1	1.216	4.055	5.172	1.00	0.00
HETATM	58	C16	UNK	0	1	0.249	3.308	6.640	1.00	0.00
HETATM	59	C17	UNK	0	1	-1.148	2.847	7.155	1.00	0.00
HETATM	60	H17	UNK	0	1	-1.095	2.193	7.856	1.00	0.00

HETATM	61	C18	UNK	0	1	-1.847	2.270	6.004	1.00	0.00
HETATM	62	H18	UNK	0	1	-2.388	1.492	6.157	1.00	0.00
HETATM	63	C19	UNK	0	1	-1.791	2.815	4.821	1.00	0.00
HETATM	64	H19	UNK	0	1	-2.255	2.403	4.089	1.00	0.00
HETATM	65	C20	UNK	0	1	-0.926	4.091	4.714	1.00	0.00
HETATM	66	C21	UNK	0	1	-0.536	4.413	3.258	1.00	0.00
HETATM	67	H21A	UNK	0	1	-1.326	4.565	2.734	1.00	0.00
HETATM	68	H21B	UNK	0	1	-0.055	3.663	2.902	1.00	0.00
HETATM	69	H21C	UNK	0	1	0.021	5.194	3.229	1.00	0.00
HETATM	70	O2	UNK	0	1	-4.024	5.118	5.028	1.00	0.00
HETATM	71	N1	UNK	0	1	-3.133	4.441	6.987	1.00	0.00
HETATM	72	H1N1	UNK	0	1	-4.020	4.217	7.276	1.00	0.00
HETATM	73	C16	UNK	0	1	-3.052	4.964	5.808	1.00	0.00
HETATM	74	C17	UNK	0	1	-1.655	5.425	5.293	1.00	0.00
HETATM	75	H17	UNK	0	1	-1.709	6.079	4.592	1.00	0.00
HETATM	76	C18	UNK	0	1	-0.956	6.002	6.444	1.00	0.00
HETATM	77	H18	UNK	0	1	-0.416	6.780	6.291	1.00	0.00
HETATM	78	C19	UNK	0	1	-1.012	5.457	7.627	1.00	0.00
HETATM	79	H19	UNK	0	1	-0.548	5.869	8.359	1.00	0.00
HETATM	80	C20	UNK	0	1	-1.878	4.181	7.734	1.00	0.00
HETATM	81	C21	UNK	0	1	-2.267	3.859	9.190	1.00	0.00
HETATM	82	H21A	UNK	0	1	-1.477	3.707	9.715	1.00	0.00
HETATM	83	H21B	UNK	0	1	-2.748	4.609	9.546	1.00	0.00
HETATM	84	H21C	UNK	0	1	-2.825	3.078	9.219	1.00	0.00
CONNECT	1	2			5					
CONNECT	2									
CONNECT	3	4			30					
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CONNECT	5	6			17					
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CONNECT	17	18			26					
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CONNECT	35									
CONNECT	36	37			38					
CONNECT	37									
CONNECT	38	39			40					
CONNECT	39									
CONNECT	40	41			42					
CONNECT	41									

HEADER CSD ENTRY pyr102r12									
CRYST1	7.7433	7.7868	13.5188	88.12	76.67	86.03			P-1
SCALE1	0.129144	-0.008963	-0.030436			0.000000			
SCALE2	0.000000	0.128731	-0.002246			0.000000			
SCALE3	0.000000	0.000000	0.076029			0.000000			
HETATM	1	O1	UNK	0	1	7.234	1.123	3.125	1.00 0.00
HETATM	2	H1O1	UNK	0	1	7.872	1.021	3.762	1.00 0.00
HETATM	3	C1	UNK	0	1	5.542	0.145	5.899	1.00 0.00
HETATM	4	C2	UNK	0	1	5.735	0.200	4.718	1.00 0.00
HETATM	5	C3	UNK	0	1	6.112	0.261	3.288	1.00 0.00
HETATM	6	C4	UNK	0	1	6.438	-1.161	2.809	1.00 0.00
HETATM	7	C5	UNK	0	1	7.608	-1.440	2.118	1.00 0.00
HETATM	8	H5	UNK	0	1	8.232	-0.767	1.969	1.00 0.00
HETATM	9	C6	UNK	0	1	7.849	-2.732	1.645	1.00 0.00
HETATM	10	H6	UNK	0	1	8.633	-2.916	1.182	1.00 0.00
HETATM	11	C7	UNK	0	1	6.945	-3.719	1.856	1.00 0.00
HETATM	12	H7	UNK	0	1	7.114	-4.577	1.540	1.00 0.00
HETATM	13	C8	UNK	0	1	5.771	-3.454	2.537	1.00 0.00
HETATM	14	H8	UNK	0	1	5.149	-4.133	2.675	1.00 0.00
HETATM	15	C9	UNK	0	1	5.526	-2.182	3.013	1.00 0.00
HETATM	16	H9	UNK	0	1	4.738	-2.009	3.475	1.00 0.00
HETATM	17	C10	UNK	0	1	4.999	0.830	2.427	1.00 0.00
HETATM	18	C11	UNK	0	1	5.282	1.135	1.088	1.00 0.00
HETATM	19	H11	UNK	0	1	6.126	0.959	0.739	1.00 0.00
HETATM	20	C12	UNK	0	1	4.316	1.695	0.287	1.00 0.00
HETATM	21	H12	UNK	0	1	4.519	1.916	-0.593	1.00 0.00
HETATM	22	C13	UNK	0	1	3.064	1.927	0.768	1.00 0.00
HETATM	23	H13	UNK	0	1	2.417	2.305	0.218	1.00 0.00
HETATM	24	C14	UNK	0	1	2.761	1.607	2.061	1.00 0.00
HETATM	25	H14	UNK	0	1	1.903	1.761	2.386	1.00 0.00
HETATM	26	C15	UNK	0	1	3.712	1.059	2.884	1.00 0.00
HETATM	27	H15	UNK	0	1	3.490	0.838	3.760	1.00 0.00
HETATM	28	O1	UNK	0	1	3.625	-0.894	10.028	1.00 0.00
HETATM	29	H1O1	UNK	0	1	2.987	-0.792	9.391	1.00 0.00
HETATM	30	C1	UNK	0	1	5.317	0.085	7.254	1.00 0.00
HETATM	31	C2	UNK	0	1	5.124	0.030	8.435	1.00 0.00
HETATM	32	C3	UNK	0	1	4.747	-0.031	9.865	1.00 0.00
HETATM	33	C4	UNK	0	1	4.421	1.391	10.343	1.00 0.00
HETATM	34	C5	UNK	0	1	3.251	1.669	11.035	1.00 0.00
HETATM	35	H5	UNK	0	1	2.627	0.996	11.184	1.00 0.00
HETATM	36	C6	UNK	0	1	3.010	2.962	11.507	1.00 0.00
HETATM	37	H6	UNK	0	1	2.226	3.146	11.970	1.00 0.00
HETATM	38	C7	UNK	0	1	3.914	3.948	11.297	1.00 0.00
HETATM	39	H7	UNK	0	1	3.745	4.807	11.613	1.00 0.00
HETATM	40	C8	UNK	0	1	5.088	3.684	10.616	1.00 0.00
HETATM	41	H8	UNK	0	1	5.710	4.362	10.478	1.00 0.00
HETATM	42	C9	UNK	0	1	5.333	2.412	10.140	1.00 0.00
HETATM	43	H9	UNK	0	1	6.121	2.238	9.678	1.00 0.00
HETATM	44	C10	UNK	0	1	5.860	-0.601	10.726	1.00 0.00
HETATM	45	C11	UNK	0	1	5.577	-0.906	12.065	1.00 0.00
HETATM	46	H11	UNK	0	1	4.733	-0.730	12.414	1.00 0.00
HETATM	47	C12	UNK	0	1	6.543	-1.465	12.866	1.00 0.00
HETATM	48	H12	UNK	0	1	6.340	-1.687	13.746	1.00 0.00
HETATM	49	C13	UNK	0	1	7.795	-1.698	12.385	1.00 0.00
HETATM	50	H13	UNK	0	1	8.442	-2.075	12.935	1.00 0.00
HETATM	51	C14	UNK	0	1	8.098	-1.377	11.092	1.00 0.00
HETATM	52	H14	UNK	0	1	8.956	-1.531	10.767	1.00 0.00
HETATM	53	C15	UNK	0	1	7.147	-0.829	10.268	1.00 0.00
HETATM	54	H15	UNK	0	1	7.369	-0.608	9.392	1.00 0.00
HETATM	55	O2	UNK	0	1	2.490	6.773	7.921	1.00 0.00
HETATM	56	N1	UNK	0	1	1.995	5.803	5.957	1.00 0.00
HETATM	57	H1N1	UNK	0	1	0.993	6.485	5.721	1.00 0.00
HETATM	58	C16	UNK	0	1	2.453	5.761	7.205	1.00 0.00
HETATM	59	C17	UNK	0	1	2.919	4.410	7.688	1.00 0.00
HETATM	60	H17	UNK	0	1	3.453	4.517	8.503	1.00 0.00

HETATM	61	C18	UNK	0	1	3.758	3.809	6.615	1.00	0.00
HETATM	62	H18	UNK	0	1	4.563	3.393	6.822	1.00	0.00
HETATM	63	C19	UNK	0	1	3.346	3.877	5.369	1.00	0.00
HETATM	64	H19	UNK	0	1	3.837	3.520	4.665	1.00	0.00
HETATM	65	C20	UNK	0	1	2.033	4.564	5.155	1.00	0.00
HETATM	66	H20	UNK	0	1	1.987	4.823	4.210	1.00	0.00
HETATM	67	O2	UNK	0	1	1.165	1.225	5.232	1.00	0.00
HETATM	68	N1	UNK	0	1	1.660	2.195	7.196	1.00	0.00
HETATM	69	H1N1	UNK	0	1	2.662	1.512	7.431	1.00	0.00
HETATM	70	C16	UNK	0	1	1.202	2.237	5.948	1.00	0.00
HETATM	71	C17	UNK	0	1	0.736	3.588	5.465	1.00	0.00
HETATM	72	H17	UNK	0	1	0.202	3.480	4.650	1.00	0.00
HETATM	73	C18	UNK	0	1	-0.103	4.188	6.538	1.00	0.00
HETATM	74	H18	UNK	0	1	-0.908	4.605	6.330	1.00	0.00
HETATM	75	C19	UNK	0	1	0.309	4.121	7.784	1.00	0.00
HETATM	76	H19	UNK	0	1	-0.182	4.477	8.488	1.00	0.00
HETATM	77	C20	UNK	0	1	1.622	3.434	7.998	1.00	0.00
HETATM	78	H20	UNK	0	1	1.667	3.175	8.943	1.00	0.00
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HEADER	CSD ENTRY pyr102rest1									
CRYST1	6.1510	9.1140	13.1100	95.93	93.28	100.18		P-1		
SCALE1	0.162575	0.029193	0.012772			0.000000				
SCALE2	0.000000	0.111476	0.012954			0.000000				
SCALE3	0.000000	0.000000	0.076917			0.000000				
HETATM	1	O1	UNK	0	1	1.458	3.606	9.397	1.00	0.00
HETATM	2	H1O1	UNK	0	1	1.650	2.811	9.471	1.00	0.00
HETATM	3	C1	UNK	0	1	-0.898	3.731	7.127	1.00	0.00
HETATM	4	C2	UNK	0	1	-0.466	3.724	8.218	1.00	0.00
HETATM	5	C3	UNK	0	1	0.092	3.765	9.540	1.00	0.00
HETATM	6	C4	UNK	0	1	-0.487	2.828	10.467	1.00	0.00
HETATM	7	C5	UNK	0	1	0.162	2.531	11.642	1.00	0.00
HETATM	8	H5	UNK	0	1	0.997	2.899	11.824	1.00	0.00
HETATM	9	C6	UNK	0	1	-0.422	1.701	12.529	1.00	0.00
HETATM	10	H6	UNK	0	1	-0.005	1.535	13.342	1.00	0.00
HETATM	11	C7	UNK	0	1	-1.594	1.113	12.265	1.00	0.00
HETATM	12	H7	UNK	0	1	-1.971	0.546	12.900	1.00	0.00
HETATM	13	C8	UNK	0	1	-2.241	1.323	11.099	1.00	0.00
HETATM	14	H8	UNK	0	1	-3.053	0.916	10.903	1.00	0.00
HETATM	15	C9	UNK	0	1	-1.624	2.170	10.232	1.00	0.00
HETATM	16	H9	UNK	0	1	-2.031	2.302	9.405	1.00	0.00
HETATM	17	C10	UNK	0	1	-0.145	5.147	10.090	1.00	0.00
HETATM	18	C11	UNK	0	1	-1.373	5.672	10.069	1.00	0.00
HETATM	19	H11	UNK	0	1	-2.070	5.188	9.687	1.00	0.00
HETATM	20	C12	UNK	0	1	-1.640	6.952	10.619	1.00	0.00
HETATM	21	H12	UNK	0	1	-2.487	7.332	10.563	1.00	0.00
HETATM	22	C13	UNK	0	1	-0.660	7.578	11.203	1.00	0.00
HETATM	23	H13	UNK	0	1	-0.834	8.390	11.623	1.00	0.00
HETATM	24	C14	UNK	0	1	0.601	7.090	11.224	1.00	0.00
HETATM	25	H14	UNK	0	1	1.291	7.594	11.587	1.00	0.00
HETATM	26	C15	UNK	0	1	0.853	5.816	10.692	1.00	0.00
HETATM	27	H15	UNK	0	1	1.699	5.440	10.757	1.00	0.00
HETATM	28	O1	UNK	0	1	-3.819	3.854	3.604	1.00	0.00
HETATM	29	H1O1	UNK	0	1	-4.011	4.648	3.530	1.00	0.00
HETATM	30	C1	UNK	0	1	-1.463	3.729	5.874	1.00	0.00
HETATM	31	C2	UNK	0	1	-1.895	3.736	4.783	1.00	0.00
HETATM	32	C3	UNK	0	1	-2.453	3.695	3.461	1.00	0.00
HETATM	33	C4	UNK	0	1	-1.874	4.632	2.534	1.00	0.00
HETATM	34	C5	UNK	0	1	-2.523	4.928	1.359	1.00	0.00
HETATM	35	H5	UNK	0	1	-3.358	4.560	1.177	1.00	0.00
HETATM	36	C6	UNK	0	1	-1.938	5.759	0.472	1.00	0.00
HETATM	37	H6	UNK	0	1	-2.356	5.925	-0.341	1.00	0.00
HETATM	38	C7	UNK	0	1	-0.767	6.346	0.736	1.00	0.00
HETATM	39	H7	UNK	0	1	-0.389	6.913	0.101	1.00	0.00
HETATM	40	C8	UNK	0	1	-0.120	6.136	1.902	1.00	0.00
HETATM	41	H8	UNK	0	1	0.692	6.543	2.098	1.00	0.00
HETATM	42	C9	UNK	0	1	-0.737	5.290	2.769	1.00	0.00
HETATM	43	H9	UNK	0	1	-0.330	5.158	3.596	1.00	0.00
HETATM	44	C10	UNK	0	1	-2.216	2.313	2.911	1.00	0.00
HETATM	45	C11	UNK	0	1	-0.988	1.788	2.932	1.00	0.00
HETATM	46	H11	UNK	0	1	-0.291	2.272	3.314	1.00	0.00
HETATM	47	C12	UNK	0	1	-0.721	0.507	2.382	1.00	0.00
HETATM	48	H12	UNK	0	1	0.126	0.128	2.438	1.00	0.00
HETATM	49	C13	UNK	0	1	-1.701	-0.118	1.798	1.00	0.00
HETATM	50	H13	UNK	0	1	-1.527	-0.930	1.378	1.00	0.00
HETATM	51	C14	UNK	0	1	-2.962	0.369	1.777	1.00	0.00
HETATM	52	H14	UNK	0	1	-3.652	-0.135	1.415	1.00	0.00
HETATM	53	C15	UNK	0	1	-3.214	1.643	2.309	1.00	0.00
HETATM	54	H15	UNK	0	1	-4.060	2.020	2.244	1.00	0.00
HETATM	55	O2	UNK	0	1	0.120	10.010	8.733	1.00	0.00
HETATM	56	N1	UNK	0	1	-0.198	8.091	7.793	1.00	0.00
HETATM	57	H1	UNK	0	1	-0.522	7.771	8.522	1.00	0.00
HETATM	58	C16	UNK	0	1	0.197	9.333	7.746	1.00	0.00
HETATM	59	C17	UNK	0	1	0.775	9.741	6.471	1.00	0.00
HETATM	60	H17	UNK	0	1	0.814	10.720	6.439	1.00	0.00

HETATM	61	C18	UNK	0	1	-0.056	9.282	5.412	1.00	0.00
HETATM	62	H18	UNK	0	1	-0.314	9.840	4.715	1.00	0.00
HETATM	63	C19	UNK	0	1	-0.434	8.087	5.444	1.00	0.00
HETATM	64	H19	UNK	0	1	-0.922	7.723	4.736	1.00	0.00
HETATM	65	C20	UNK	0	1	-0.085	7.286	6.585	1.00	0.00
HETATM	66	H20	UNK	0	1	-0.716	6.540	6.654	1.00	0.00
HETATM	67	O2	UNK	0	1	2.060	6.420	4.268	1.00	0.00
HETATM	68	N1	UNK	0	1	2.377	8.339	5.208	1.00	0.00
HETATM	69	H1	UNK	0	1	2.701	8.659	4.479	1.00	0.00
HETATM	70	C16	UNK	0	1	1.982	7.097	5.255	1.00	0.00
HETATM	71	C17	UNK	0	1	1.404	6.689	6.530	1.00	0.00
HETATM	72	H17	UNK	0	1	1.365	5.711	6.562	1.00	0.00
HETATM	73	C18	UNK	0	1	2.235	7.149	7.589	1.00	0.00
HETATM	74	H18	UNK	0	1	2.493	6.590	8.286	1.00	0.00
HETATM	75	C19	UNK	0	1	2.614	8.343	7.558	1.00	0.00
HETATM	76	H19	UNK	0	1	3.101	8.707	8.265	1.00	0.00
HETATM	77	C20	UNK	0	1	2.264	9.144	6.416	1.00	0.00
HETATM	78	H20	UNK	0	1	2.895	9.890	6.347	1.00	0.00

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HEADER CSD ENTRY pyr102r13									
CRYST1	10.4770	13.4500	16.9960	81.25	81.08	81.88			P-1
SCALE1	0.095447	-0.013618	-0.013292			0.000000			
SCALE2	0.000000	0.075102	-0.010095			0.000000			
SCALE3	0.000000	0.000000	0.060094			0.000000			
HETATM	1	O1A	UNK	0	1	6.025	4.117	5.764	1.00 0.00
HETATM	2	H10A	UNK	0	1	5.338	3.696	5.616	1.00 0.00
HETATM	3	C1A	UNK	0	1	6.506	1.774	8.117	1.00 0.00
HETATM	4	C2A	UNK	0	1	6.377	2.896	7.718	1.00 0.00
HETATM	5	C3A	UNK	0	1	6.204	4.244	7.137	1.00 0.00
HETATM	6	C4A	UNK	0	1	4.893	4.795	7.798	1.00 0.00
HETATM	7	C5A	UNK	0	1	3.871	5.349	7.057	1.00 0.00
HETATM	8	H5A	UNK	0	1	3.905	5.300	6.129	1.00 0.00
HETATM	9	C6A	UNK	0	1	2.812	5.966	7.651	1.00 0.00
HETATM	10	H6A	UNK	0	1	2.148	6.336	7.117	1.00 0.00
HETATM	11	C7A	UNK	0	1	2.700	6.056	9.006	1.00 0.00
HETATM	12	H7A	UNK	0	1	1.957	6.432	9.420	1.00 0.00
HETATM	13	C8A	UNK	0	1	3.758	5.554	9.713	1.00 0.00
HETATM	14	H8A	UNK	0	1	3.766	5.701	10.632	1.00 0.00
HETATM	15	C9A	UNK	0	1	4.759	4.883	9.199	1.00 0.00
HETATM	16	H9A	UNK	0	1	5.379	4.468	9.756	1.00 0.00
HETATM	17	C10A	UNK	0	1	7.350	5.165	7.397	1.00 0.00
HETATM	18	C11A	UNK	0	1	7.326	6.379	6.743	1.00 0.00
HETATM	19	H11A	UNK	0	1	6.598	6.606	6.210	1.00 0.00
HETATM	20	C12A	UNK	0	1	8.376	7.249	6.879	1.00 0.00
HETATM	21	H12A	UNK	0	1	8.360	8.071	6.443	1.00 0.00
HETATM	22	C13A	UNK	0	1	9.446	6.909	7.658	1.00 0.00
HETATM	23	H13A	UNK	0	1	10.193	7.463	7.708	1.00 0.00
HETATM	24	C14A	UNK	0	1	9.396	5.719	8.374	1.00 0.00
HETATM	25	H14A	UNK	0	1	10.083	5.508	8.963	1.00 0.00
HETATM	26	C15A	UNK	0	1	8.356	4.867	8.224	1.00 0.00
HETATM	27	H15A	UNK	0	1	8.342	4.068	8.701	1.00 0.00
HETATM	28	O1A	UNK	0	1	7.088	-1.880	10.876	1.00 0.00
HETATM	29	H10A	UNK	0	1	7.776	-1.460	11.024	1.00 0.00
HETATM	30	C1A	UNK	0	1	6.608	0.463	8.523	1.00 0.00
HETATM	31	C2A	UNK	0	1	6.737	-0.659	8.923	1.00 0.00
HETATM	32	C3A	UNK	0	1	6.909	-2.007	9.503	1.00 0.00
HETATM	33	C4A	UNK	0	1	8.220	-2.558	8.843	1.00 0.00
HETATM	34	C5A	UNK	0	1	9.243	-3.113	9.583	1.00 0.00
HETATM	35	H5A	UNK	0	1	9.208	-3.064	10.512	1.00 0.00
HETATM	36	C6A	UNK	0	1	10.301	-3.729	8.989	1.00 0.00
HETATM	37	H6A	UNK	0	1	10.966	-4.099	9.523	1.00 0.00
HETATM	38	C7A	UNK	0	1	10.414	-3.819	7.635	1.00 0.00
HETATM	39	H7A	UNK	0	1	11.156	-4.196	7.220	1.00 0.00
HETATM	40	C8A	UNK	0	1	9.356	-3.318	6.927	1.00 0.00
HETATM	41	H8A	UNK	0	1	9.348	-3.464	6.009	1.00 0.00
HETATM	42	C9A	UNK	0	1	8.354	-2.647	7.442	1.00 0.00
HETATM	43	H9A	UNK	0	1	7.734	-2.232	6.884	1.00 0.00
HETATM	44	C10A	UNK	0	1	5.763	-2.928	9.244	1.00 0.00
HETATM	45	C11A	UNK	0	1	5.787	-4.142	9.898	1.00 0.00
HETATM	46	H11A	UNK	0	1	6.515	-4.369	10.430	1.00 0.00
HETATM	47	C12A	UNK	0	1	4.738	-5.013	9.761	1.00 0.00
HETATM	48	H12A	UNK	0	1	4.753	-5.834	10.197	1.00 0.00
HETATM	49	C13A	UNK	0	1	3.668	-4.673	8.983	1.00 0.00
HETATM	50	H13A	UNK	0	1	2.921	-5.227	8.933	1.00 0.00
HETATM	51	C14A	UNK	0	1	3.718	-3.483	8.267	1.00 0.00
HETATM	52	H14A	UNK	0	1	3.030	-3.271	7.678	1.00 0.00
HETATM	53	C15A	UNK	0	1	4.757	-2.630	8.417	1.00 0.00
HETATM	54	H15A	UNK	0	1	4.771	-1.832	7.939	1.00 0.00
HETATM	55	O2A	UNK	0	1	10.299	2.957	10.324	1.00 0.00
HETATM	56	N1A	UNK	0	1	10.774	0.858	9.871	1.00 0.00
HETATM	57	H1NA	UNK	0	1	9.933	0.186	10.500	1.00 0.00
HETATM	58	C16A	UNK	0	1	11.023	2.142	9.773	1.00 0.00
HETATM	59	C17A	UNK	0	1	12.286	2.459	8.964	1.00 0.00
HETATM	60	H17A	UNK	0	1	12.596	3.360	9.189	1.00 0.00

HETATM	61	C18A	UNK	0	1	13.295	1.465	9.397	1.00	0.00
HETATM	62	H18A	UNK	0	1	14.140	1.772	9.637	1.00	0.00
HETATM	63	C19A	UNK	0	1	13.066	0.210	9.457	1.00	0.00
HETATM	64	H19A	UNK	0	1	13.728	-0.413	9.657	1.00	0.00
HETATM	65	C20A	UNK	0	1	11.681	-0.167	9.187	1.00	0.00
HETATM	66	H20A	UNK	0	1	11.513	-1.049	9.583	1.00	0.00
HETATM	67	O2A	UNK	0	1	13.292	-0.721	6.317	1.00	0.00
HETATM	68	N1A	UNK	0	1	12.816	1.379	6.769	1.00	0.00
HETATM	69	H1NA	UNK	0	1	13.657	2.050	6.140	1.00	0.00
HETATM	70	C16A	UNK	0	1	12.568	0.095	6.868	1.00	0.00
HETATM	71	C17A	UNK	0	1	11.305	-0.223	7.676	1.00	0.00
HETATM	72	H17A	UNK	0	1	10.994	-1.124	7.452	1.00	0.00
HETATM	73	C18A	UNK	0	1	10.296	0.771	7.244	1.00	0.00
HETATM	74	H18A	UNK	0	1	9.451	0.465	7.004	1.00	0.00
HETATM	75	C19A	UNK	0	1	10.524	2.027	7.184	1.00	0.00
HETATM	76	H19A	UNK	0	1	9.862	2.650	6.984	1.00	0.00
HETATM	77	C20A	UNK	0	1	11.909	2.404	7.453	1.00	0.00
HETATM	78	H20A	UNK	0	1	12.077	3.285	7.057	1.00	0.00
HETATM	79	O1B	UNK	0	1	2.535	16.138	0.256	1.00	0.00
HETATM	80	H10B	UNK	0	1	3.157	16.419	-0.198	1.00	0.00
HETATM	81	C1B	UNK	0	1	3.206	14.003	2.674	1.00	0.00
HETATM	82	C2B	UNK	0	1	3.087	15.087	2.236	1.00	0.00
HETATM	83	C3B	UNK	0	1	2.822	16.335	1.627	1.00	0.00
HETATM	84	C4B	UNK	0	1	1.603	17.027	2.266	1.00	0.00
HETATM	85	C5B	UNK	0	1	0.700	17.647	1.473	1.00	0.00
HETATM	86	H5B	UNK	0	1	0.809	17.681	0.551	1.00	0.00
HETATM	87	C6B	UNK	0	1	-0.427	18.250	2.108	1.00	0.00
HETATM	88	H6B	UNK	0	1	-1.100	18.620	1.584	1.00	0.00
HETATM	89	C7B	UNK	0	1	-0.536	18.291	3.410	1.00	0.00
HETATM	90	H7B	UNK	0	1	-1.271	18.708	3.797	1.00	0.00
HETATM	91	C8B	UNK	0	1	0.424	17.726	4.208	1.00	0.00
HETATM	92	H8B	UNK	0	1	0.371	17.809	5.134	1.00	0.00
HETATM	93	C9B	UNK	0	1	1.476	17.026	3.628	1.00	0.00
HETATM	94	H9B	UNK	0	1	2.086	16.566	4.158	1.00	0.00
HETATM	95	C10B	UNK	0	1	4.006	17.338	1.759	1.00	0.00
HETATM	96	C11B	UNK	0	1	4.071	18.395	0.909	1.00	0.00
HETATM	97	H11B	UNK	0	1	3.437	18.510	0.235	1.00	0.00
HETATM	98	C12B	UNK	0	1	5.103	19.291	1.078	1.00	0.00
HETATM	99	H12B	UNK	0	1	5.126	20.056	0.551	1.00	0.00
HETATM	100	C13B	UNK	0	1	6.129	19.097	2.014	1.00	0.00
HETATM	101	H13B	UNK	0	1	6.870	19.653	2.097	1.00	0.00
HETATM	102	C14B	UNK	0	1	5.906	17.969	2.807	1.00	0.00
HETATM	103	H14B	UNK	0	1	6.511	17.816	3.498	1.00	0.00
HETATM	104	C15B	UNK	0	1	4.921	17.099	2.676	1.00	0.00
HETATM	105	H15B	UNK	0	1	4.876	16.342	3.213	1.00	0.00
HETATM	106	O1C	UNK	0	1	3.946	10.202	5.362	1.00	0.00
HETATM	107	H10C	UNK	0	1	3.705	10.921	5.674	1.00	0.00
HETATM	108	C1C	UNK	0	1	3.329	12.708	3.132	1.00	0.00
HETATM	109	C2C	UNK	0	1	3.485	11.588	3.468	1.00	0.00
HETATM	110	C3C	UNK	0	1	3.721	10.198	3.959	1.00	0.00
HETATM	111	C4C	UNK	0	1	4.963	9.599	3.212	1.00	0.00
HETATM	112	C5C	UNK	0	1	5.980	9.038	3.929	1.00	0.00
HETATM	113	H5C	UNK	0	1	5.938	9.024	4.859	1.00	0.00
HETATM	114	C6C	UNK	0	1	7.029	8.509	3.310	1.00	0.00
HETATM	115	H6C	UNK	0	1	7.693	8.099	3.817	1.00	0.00
HETATM	116	C7C	UNK	0	1	7.166	8.550	1.925	1.00	0.00
HETATM	117	H7C	UNK	0	1	7.910	8.187	1.503	1.00	0.00
HETATM	118	C8C	UNK	0	1	6.146	9.153	1.203	1.00	0.00
HETATM	119	H8C	UNK	0	1	6.231	9.245	0.281	1.00	0.00
HETATM	120	C9C	UNK	0	1	4.987	9.634	1.865	1.00	0.00
HETATM	121	H9C	UNK	0	1	4.259	9.961	1.383	1.00	0.00
HETATM	122	C10C	UNK	0	1	2.538	9.295	3.711	1.00	0.00
HETATM	123	C11C	UNK	0	1	2.535	8.049	4.242	1.00	0.00
HETATM	124	H11C	UNK	0	1	3.287	7.762	4.709	1.00	0.00
HETATM	125	C12C	UNK	0	1	1.489	7.205	4.120	1.00	0.00

HETATM	126	H12C	UNK	0	1	1.490	6.381	4.553	1.00	0.00
HETATM	127	C13C	UNK	0	1	0.426	7.584	3.345	1.00	0.00
HETATM	128	H13C	UNK	0	1	-0.285	6.999	3.205	1.00	0.00
HETATM	129	C14C	UNK	0	1	0.414	8.789	2.794	1.00	0.00
HETATM	130	H14C	UNK	0	1	-0.306	9.023	2.253	1.00	0.00
HETATM	131	C15C	UNK	0	1	1.401	9.693	2.980	1.00	0.00
HETATM	132	H15C	UNK	0	1	1.331	10.555	2.636	1.00	0.00
HETATM	133	O2B	UNK	0	1	8.388	0.326	11.602	1.00	0.00
HETATM	134	N1B	UNK	0	1	7.947	2.400	12.178	1.00	0.00
HETATM	135	H1NB	UNK	0	1	8.336	2.979	11.665	1.00	0.00
HETATM	136	C16B	UNK	0	1	7.630	1.131	12.178	1.00	0.00
HETATM	137	C17B	UNK	0	1	6.243	0.877	12.862	1.00	0.00
HETATM	138	H17B	UNK	0	1	5.906	-0.001	12.582	1.00	0.00
HETATM	139	C18B	UNK	0	1	5.350	1.824	12.477	1.00	0.00
HETATM	140	H18B	UNK	0	1	4.471	1.571	12.304	1.00	0.00
HETATM	141	C19B	UNK	0	1	5.668	3.083	12.339	1.00	0.00
HETATM	142	H19B	UNK	0	1	5.094	3.704	11.956	1.00	0.00
HETATM	143	C20B	UNK	0	1	6.933	3.408	12.812	1.00	0.00
HETATM	144	H20B	UNK	0	1	7.153	4.303	12.477	1.00	0.00
HETATM	145	O2C	UNK	0	1	5.235	3.947	15.577	1.00	0.00
HETATM	146	N1C	UNK	0	1	5.562	1.794	15.018	1.00	0.00
HETATM	147	H1NC	UNK	0	1	4.753	1.761	15.775	1.00	0.00
HETATM	148	C16C	UNK	0	1	5.958	3.052	15.051	1.00	0.00
HETATM	149	C17C	UNK	0	1	7.272	3.377	14.377	1.00	0.00
HETATM	150	H17C	UNK	0	1	7.605	4.248	14.675	1.00	0.00
HETATM	151	C18C	UNK	0	1	8.222	2.313	14.735	1.00	0.00
HETATM	152	H18C	UNK	0	1	9.116	2.508	14.897	1.00	0.00
HETATM	153	C19C	UNK	0	1	7.789	1.057	14.827	1.00	0.00
HETATM	154	H19C	UNK	0	1	8.323	0.366	15.146	1.00	0.00
HETATM	155	C20C	UNK	0	1	6.487	0.852	14.414	1.00	0.00
HETATM	156	H20C	UNK	0	1	6.229	-0.039	14.729	1.00	0.00
HETATM	157	O1W	UNK	0	1	3.613	1.289	16.725	0.34	0.00

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