

ATOM	1	C1	BEN	1	14.181	12.567	3.568	1.00	0.00	BENZ C
ATOM	2	H1	BEN	1	13.631	11.615	3.568	1.00	0.00	BENZ H
ATOM	3	C2	BEN	1	15.576	12.567	3.568	1.00	0.00	BENZ C
ATOM	4	H2	BEN	1	16.125	11.615	3.568	1.00	0.00	BENZ H
ATOM	5	C3	BEN	1	16.273	13.775	3.568	1.00	0.00	BENZ C
ATOM	6	H3	BEN	1	17.372	13.775	3.568	1.00	0.00	BENZ H
ATOM	7	C4	BEN	1	15.576	14.983	3.568	1.00	0.00	BENZ C
ATOM	8	H4	BEN	1	16.125	15.936	3.568	1.00	0.00	BENZ H
ATOM	9	C5	BEN	1	14.181	14.983	3.568	1.00	0.00	BENZ C
ATOM	10	H5	BEN	1	13.631	15.936	3.568	1.00	0.00	BENZ H
ATOM	11	C6	BEN	1	13.484	13.775	3.568	1.00	0.00	BENZ C
ATOM	12	H6	BEN	1	12.385	13.775	3.568	1.00	0.00	BENZ H
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ATOM	193	CR01	TSB	1	38.939	127.873	3.507	1.00	0.00	TSBA C
ATOM	194	CR02	TSB	1	40.076	128.737	3.497	1.00	0.00	TSBA C
ATOM	195	CR03	TSB	1	41.384	128.195	3.582	1.00	0.00	TSBA C
ATOM	196	CR04	TSB	1	41.544	126.786	3.716	1.00	0.00	TSBA C
ATOM	197	CR05	TSB	1	40.447	125.906	3.674	1.00	0.00	TSBA C
ATOM	198	CR06	TSB	1	39.140	126.468	3.595	1.00	0.00	TSBA C
ATOM	199	HR02	TSB	1	39.954	129.807	3.398	1.00	0.00	TSBA H
ATOM	200	HR04	TSB	1	42.536	126.368	3.814	1.00	0.00	TSBA H
ATOM	201	HR06	TSB	1	38.285	125.808	3.574	1.00	0.00	TSBA H
ATOM	202	CR11	TSB	1	35.773	130.226	3.626	1.00	0.00	TSBA C
ATOM	203	CR12	TSB	1	34.601	129.442	3.486	1.00	0.00	TSBA C
ATOM	204	CR13	TSB	1	33.298	129.996	3.533	1.00	0.00	TSBA C
ATOM	205	CR14	TSB	1	33.198	131.403	3.542	1.00	0.00	TSBA C
ATOM	206	CR15	TSB	1	34.365	132.238	3.497	1.00	0.00	TSBA C
ATOM	207	CR16	TSB	1	35.647	131.651	3.638	1.00	0.00	TSBA C
ATOM	208	HR12	TSB	1	34.700	128.370	3.390	1.00	0.00	TSBA H
ATOM	209	HR14	TSB	1	32.229	131.877	3.476	1.00	0.00	TSBA H
ATOM	210	HR16	TSB	1	36.531	132.272	3.641	1.00	0.00	TSBA H
ATOM	211	CR21	TSB	1	40.107	121.975	3.488	1.00	0.00	TSBA C
ATOM	212	CR22	TSB	1	41.424	121.449	3.460	1.00	0.00	TSBA C
ATOM	213	CR23	TSB	1	41.701	120.095	3.487	1.00	0.00	TSBA C
ATOM	214	CR24	TSB	1	40.586	119.259	3.541	1.00	0.00	TSBA C
ATOM	215	CR25	TSB	1	39.249	119.698	3.574	1.00	0.00	TSBA C
ATOM	216	CR26	TSB	1	39.018	121.070	3.516	1.00	0.00	TSBA C
ATOM	217	HR22	TSB	1	42.290	122.096	3.445	1.00	0.00	TSBA H
ATOM	218	HR24	TSB	1	40.717	118.187	3.587	1.00	0.00	TSBA H
ATOM	219	HR26	TSB	1	38.003	121.442	3.485	1.00	0.00	TSBA H
ATOM	220	CR31	TSB	1	45.054	129.719	3.460	1.00	0.00	TSBA C
ATOM	221	CR32	TSB	1	45.013	131.138	3.497	1.00	0.00	TSBA C
ATOM	222	CR33	TSB	1	46.120	131.948	3.503	1.00	0.00	TSBA C
ATOM	223	CR34	TSB	1	47.341	131.340	3.493	1.00	0.00	TSBA C
ATOM	224	CR35	TSB	1	47.507	129.944	3.468	1.00	0.00	TSBA C
ATOM	225	CR36	TSB	1	46.353	129.165	3.432	1.00	0.00	TSBA C
ATOM	226	HR32	TSB	1	44.047	131.624	3.470	1.00	0.00	TSBA H
ATOM	227	HR34	TSB	1	48.223	131.963	3.544	1.00	0.00	TSBA H
ATOM	228	HR36	TSB	1	46.487	128.094	3.365	1.00	0.00	TSBA H
ATOM	229	CL11	TSB	1	37.557	128.392	3.354	1.00	0.00	TSBA C

ATOM	230	CL12	TSB	1	37.127	129.629	3.725	1.00	0.00	TSBA	C
ATOM	231	HL11	TSB	1	36.835	127.708	2.920	1.00	0.00	TSBA	H
ATOM	232	HL12	TSB	1	37.858	130.294	4.174	1.00	0.00	TSBA	H
ATOM	233	CL21	TSB	1	40.686	124.441	3.753	1.00	0.00	TSBA	C
ATOM	234	CL22	TSB	1	39.844	123.427	3.374	1.00	0.00	TSBA	C
ATOM	235	HL21	TSB	1	41.614	124.156	4.237	1.00	0.00	TSBA	H
ATOM	236	HL22	TSB	1	38.918	123.703	2.880	1.00	0.00	TSBA	H
ATOM	237	CL31	TSB	1	42.583	129.074	3.661	1.00	0.00	TSBA	C
ATOM	238	CL32	TSB	1	43.884	128.803	3.343	1.00	0.00	TSBA	C
ATOM	239	HL31	TSB	1	42.353	130.091	3.962	1.00	0.00	TSBA	H
ATOM	240	HL32	TSB	1	44.112	127.794	3.017	1.00	0.00	TSBA	H
ATOM	241	013	TSB	1	32.219	129.100	3.594	1.00	0.00	TSBA	O
ATOM	242	CA1	TSB	1	30.880	129.572	3.546	1.00	0.00	TSBA	C
ATOM	243	HA1	TSB	1	30.725	130.253	4.387	1.00	0.00	TSBA	H
ATOM	244	HA21	TSB	1	30.685	130.131	2.627	1.00	0.00	TSBA	H
ATOM	245	CA2	TSB	1	29.906	128.459	3.681	1.00	0.00	TSBA	C
ATOM	246	HA2	TSB	1	30.114	127.900	4.597	1.00	0.00	TSBA	H
ATOM	247	HA22	TSB	1	30.066	127.786	2.835	1.00	0.00	TSBA	H
ATOM	248	CA3	TSB	1	28.467	128.890	3.679	1.00	0.00	TSBA	C
ATOM	249	HA3	TSB	1	28.324	129.514	2.793	1.00	0.00	TSBA	H
ATOM	250	HA23	TSB	1	28.326	129.529	4.554	1.00	0.00	TSBA	H
ATOM	251	CA4	TSB	1	27.394	127.846	3.700	1.00	0.00	TSBA	C
ATOM	252	HA4	TSB	1	27.541	127.228	4.589	1.00	0.00	TSBA	H
ATOM	253	HA24	TSB	1	27.527	127.195	2.831	1.00	0.00	TSBA	H
ATOM	254	CA5	TSB	1	25.974	128.303	3.695	1.00	0.00	TSBA	C
ATOM	255	HA5	TSB	1	25.839	128.951	2.826	1.00	0.00	TSBA	H
ATOM	256	HA25	TSB	1	25.828	128.916	4.589	1.00	0.00	TSBA	H
ATOM	257	CA6	TSB	1	24.939	127.206	3.672	1.00	0.00	TSBA	C
ATOM	258	HA6	TSB	1	25.100	126.570	2.803	1.00	0.00	TSBA	H
ATOM	259	HA26	TSB	1	23.904	127.545	3.638	1.00	0.00	TSBA	H
ATOM	260	HA27	TSB	1	25.094	126.564	4.538	1.00	0.00	TSBA	H
ATOM	261	015	TSB	1	34.117	133.602	3.453	1.00	0.00	TSBA	O
ATOM	262	CB1	TSB	1	35.107	134.588	3.631	1.00	0.00	TSBA	C
ATOM	263	HB1	TSB	1	35.709	134.420	4.528	1.00	0.00	TSBA	H
ATOM	264	HB21	TSB	1	35.742	134.549	2.743	1.00	0.00	TSBA	H
ATOM	265	CB2	TSB	1	34.431	135.922	3.656	1.00	0.00	TSBA	C
ATOM	266	HB2	TSB	1	33.814	135.924	4.559	1.00	0.00	TSBA	H
ATOM	267	HB22	TSB	1	33.744	135.975	2.807	1.00	0.00	TSBA	H
ATOM	268	CB3	TSB	1	35.271	137.164	3.680	1.00	0.00	TSBA	C
ATOM	269	HB3	TSB	1	35.900	137.140	2.787	1.00	0.00	TSBA	H
ATOM	270	HB23	TSB	1	35.925	137.105	4.554	1.00	0.00	TSBA	H
ATOM	271	CB4	TSB	1	34.556	138.465	3.686	1.00	0.00	TSBA	C
ATOM	272	HB4	TSB	1	33.888	138.487	4.551	1.00	0.00	TSBA	H
ATOM	273	HB24	TSB	1	33.927	138.485	2.792	1.00	0.00	TSBA	H
ATOM	274	CB5	TSB	1	35.361	139.689	3.701	1.00	0.00	TSBA	C
ATOM	275	HB5	TSB	1	35.978	139.722	4.602	1.00	0.00	TSBA	H
ATOM	276	HB25	TSB	1	36.045	139.622	2.851	1.00	0.00	TSBA	H
ATOM	277	CB6	TSB	1	34.575	140.965	3.663	1.00	0.00	TSBA	C
ATOM	278	HB6	TSB	1	33.969	141.043	4.564	1.00	0.00	TSBA	H
ATOM	279	HB26	TSB	1	33.897	140.918	2.813	1.00	0.00	TSBA	H
ATOM	280	HB27	TSB	1	35.127	141.899	3.572	1.00	0.00	TSBA	H

ATOM	281	023	TSB	1	43.050	119.701	3.594	1.00	0.00	TSBA 0
ATOM	282	CC1	TSB	1	43.425	118.319	3.621	1.00	0.00	TSBA C
ATOM	283	HC1	TSB	1	43.092	117.843	4.547	1.00	0.00	TSBA H
ATOM	284	HC21	TSB	1	43.069	117.758	2.754	1.00	0.00	TSBA H
ATOM	285	CC2	TSB	1	44.917	118.213	3.649	1.00	0.00	TSBA C
ATOM	286	HC2	TSB	1	45.274	118.716	2.747	1.00	0.00	TSBA H
ATOM	287	HC22	TSB	1	45.253	118.789	4.516	1.00	0.00	TSBA H
ATOM	288	CC3	TSB	1	45.460	116.819	3.702	1.00	0.00	TSBA C
ATOM	289	HC3	TSB	1	45.047	116.344	2.808	1.00	0.00	TSBA H
ATOM	290	HC23	TSB	1	45.054	116.295	4.571	1.00	0.00	TSBA H
ATOM	291	CC4	TSB	1	46.954	116.613	3.666	1.00	0.00	TSBA C
ATOM	292	HC4	TSB	1	47.314	117.029	4.610	1.00	0.00	TSBA H
ATOM	293	HC24	TSB	1	47.417	117.203	2.872	1.00	0.00	TSBA H
ATOM	294	CC5	TSB	1	47.474	115.214	3.681	1.00	0.00	TSBA C
ATOM	295	HC5	TSB	1	47.102	114.787	2.746	1.00	0.00	TSBA H
ATOM	296	HC25	TSB	1	47.033	114.672	4.522	1.00	0.00	TSBA H
ATOM	297	CC6	TSB	1	48.973	115.050	3.640	1.00	0.00	TSBA C
ATOM	298	HC6	TSB	1	49.313	114.016	3.638	1.00	0.00	TSBA H
ATOM	299	HC26	TSB	1	49.335	115.578	2.759	1.00	0.00	TSBA H
ATOM	300	HC27	TSB	1	49.461	115.573	4.461	1.00	0.00	TSBA H
ATOM	301	025	TSB	1	38.243	118.733	3.558	1.00	0.00	TSBA 0
ATOM	302	CD1	TSB	1	36.879	119.099	3.640	1.00	0.00	TSBA C
ATOM	303	HD1	TSB	1	36.709	119.689	4.544	1.00	0.00	TSBA H
ATOM	304	HD21	TSB	1	36.597	119.716	2.782	1.00	0.00	TSBA H
ATOM	305	CD2	TSB	1	36.035	117.825	3.657	1.00	0.00	TSBA C
ATOM	306	HD2	TSB	1	36.329	117.201	4.506	1.00	0.00	TSBA H
ATOM	307	HD22	TSB	1	36.241	117.230	2.764	1.00	0.00	TSBA H
ATOM	308	CD3	TSB	1	34.523	118.150	3.735	1.00	0.00	TSBA C
ATOM	309	HD3	TSB	1	34.305	118.712	4.647	1.00	0.00	TSBA H
ATOM	310	HD23	TSB	1	34.249	118.806	2.904	1.00	0.00	TSBA H
ATOM	311	CD4	TSB	1	33.643	116.882	3.656	1.00	0.00	TSBA C
ATOM	312	HD4	TSB	1	33.851	116.228	4.507	1.00	0.00	TSBA H
ATOM	313	HD24	TSB	1	33.918	116.293	2.777	1.00	0.00	TSBA H
ATOM	314	CD5	TSB	1	32.156	117.233	3.585	1.00	0.00	TSBA C
ATOM	315	HD5	TSB	1	31.594	116.318	3.384	1.00	0.00	TSBA H
ATOM	316	HD25	TSB	1	31.923	117.900	2.751	1.00	0.00	TSBA H
ATOM	317	CD6	TSB	1	31.574	117.825	4.849	1.00	0.00	TSBA C
ATOM	318	HD6	TSB	1	32.063	118.778	5.044	1.00	0.00	TSBA H
ATOM	319	HD26	TSB	1	31.733	117.191	5.720	1.00	0.00	TSBA H
ATOM	320	HD27	TSB	1	30.508	118.030	4.760	1.00	0.00	TSBA H
ATOM	321	033	TSB	1	45.881	133.269	3.409	1.00	0.00	TSBA 0
ATOM	322	CE1	TSB	1	46.854	134.261	3.669	1.00	0.00	TSBA C
ATOM	323	HE1	TSB	1	47.396	133.997	4.581	1.00	0.00	TSBA H
ATOM	324	HE21	TSB	1	47.583	134.262	2.855	1.00	0.00	TSBA H
ATOM	325	CE2	TSB	1	46.316	135.649	3.863	1.00	0.00	TSBA C
ATOM	326	HE2	TSB	1	45.828	135.983	2.943	1.00	0.00	TSBA H
ATOM	327	HE22	TSB	1	45.547	135.594	4.638	1.00	0.00	TSBA H
ATOM	328	CE3	TSB	1	47.371	136.651	4.329	1.00	0.00	TSBA C
ATOM	329	HE3	TSB	1	48.149	136.725	3.565	1.00	0.00	TSBA H
ATOM	330	HE23	TSB	1	47.864	136.280	5.231	1.00	0.00	TSBA H
ATOM	331	CE4	TSB	1	46.884	138.061	4.650	1.00	0.00	TSBA C

ATOM	332	HE4	TSB	1	47.718	138.614	5.090	1.00	0.00	TSBA	H
ATOM	333	HE24	TSB	1	46.105	138.020	5.414	1.00	0.00	TSBA	H
ATOM	334	CE5	TSB	1	46.378	138.813	3.443	1.00	0.00	TSBA	C
ATOM	335	HE5	TSB	1	47.188	138.803	2.709	1.00	0.00	TSBA	H
ATOM	336	HE25	TSB	1	45.534	138.297	2.978	1.00	0.00	TSBA	H
ATOM	337	CE6	TSB	1	46.023	140.267	3.718	1.00	0.00	TSBA	C
ATOM	338	HE6	TSB	1	45.767	140.835	2.825	1.00	0.00	TSBA	H
ATOM	339	HE26	TSB	1	45.161	140.322	4.381	1.00	0.00	TSBA	H
ATOM	340	HE27	TSB	1	46.833	140.791	4.224	1.00	0.00	TSBA	H
ATOM	341	O35	TSB	1	48.824	129.438	3.621	1.00	0.00	TSBA	O
ATOM	342	CF1	TSB	1	49.167	128.104	3.634	1.00	0.00	TSBA	C
ATOM	343	HF1	TSB	1	48.685	127.665	4.512	1.00	0.00	TSBA	H
ATOM	344	HF21	TSB	1	48.755	127.649	2.729	1.00	0.00	TSBA	H
ATOM	345	CF2	TSB	1	50.639	127.974	3.661	1.00	0.00	TSBA	C
ATOM	346	HF2	TSB	1	51.054	128.479	2.784	1.00	0.00	TSBA	H
ATOM	347	HF22	TSB	1	51.007	128.516	4.536	1.00	0.00	TSBA	H
ATOM	348	CF3	TSB	1	51.204	126.576	3.693	1.00	0.00	TSBA	C
ATOM	349	HF3	TSB	1	50.843	126.012	2.829	1.00	0.00	TSBA	H
ATOM	350	HF23	TSB	1	50.818	126.080	4.587	1.00	0.00	TSBA	H
ATOM	351	CF4	TSB	1	52.690	126.487	3.705	1.00	0.00	TSBA	C
ATOM	352	HF4	TSB	1	53.097	127.016	2.839	1.00	0.00	TSBA	H
ATOM	353	HF24	TSB	1	53.073	127.004	4.588	1.00	0.00	TSBA	H
ATOM	354	CF5	TSB	1	53.223	125.053	3.670	1.00	0.00	TSBA	C
ATOM	355	HF5	TSB	1	52.798	124.540	2.804	1.00	0.00	TSBA	H
ATOM	356	HF25	TSB	1	52.845	124.526	4.550	1.00	0.00	TSBA	H
ATOM	357	CF6	TSB	1	54.734	124.958	3.605	1.00	0.00	TSBA	C
ATOM	358	HF6	TSB	1	55.216	125.367	4.492	1.00	0.00	TSBA	H
ATOM	359	HF26	TSB	1	55.138	125.502	2.754	1.00	0.00	TSBA	H
ATOM	360	HF27	TSB	1	55.028	123.914	3.514	1.00	0.00	TSBA	H
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ATOM	2881	CR01	TSB	17	25.110	114.289	3.673	1.00	0.00	TSBB	C
ATOM	2882	CR02	TSB	17	24.928	115.689	3.540	1.00	0.00	TSBB	C
ATOM	2883	CR03	TSB	17	26.044	116.565	3.485	1.00	0.00	TSBB	C
ATOM	2884	CR04	TSB	17	27.354	116.016	3.531	1.00	0.00	TSBB	C
ATOM	2885	CR05	TSB	17	27.564	114.631	3.634	1.00	0.00	TSBB	C
ATOM	2886	CR06	TSB	17	26.425	113.765	3.733	1.00	0.00	TSBB	C
ATOM	2887	HR02	TSB	17	23.928	116.095	3.494	1.00	0.00	TSBB	H
ATOM	2888	HR04	TSB	17	28.209	116.672	3.445	1.00	0.00	TSBB	H
ATOM	2889	HR06	TSB	17	26.564	112.696	3.821	1.00	0.00	TSBB	H
ATOM	2890	CR11	TSB	17	21.523	112.626	3.474	1.00	0.00	TSBB	C
ATOM	2891	CR12	TSB	17	21.693	111.219	3.456	1.00	0.00	TSBB	C
ATOM	2892	CR13	TSB	17	20.575	110.337	3.501	1.00	0.00	TSBB	C
ATOM	2893	CR14	TSB	17	19.270	110.897	3.545	1.00	0.00	TSBB	C
ATOM	2894	CR15	TSB	17	19.063	112.299	3.531	1.00	0.00	TSBB	C
ATOM	2895	CR16	TSB	17	20.196	113.151	3.501	1.00	0.00	TSBB	C
ATOM	2896	HR12	TSB	17	22.690	110.801	3.422	1.00	0.00	TSBB	H
ATOM	2897	HR14	TSB	17	18.396	110.262	3.576	1.00	0.00	TSBB	H
ATOM	2898	HR16	TSB	17	20.049	114.221	3.506	1.00	0.00	TSBB	H
ATOM	2899	CR21	TSB	17	30.701	112.234	3.449	1.00	0.00	TSBB	C
ATOM	2900	CR22	TSB	17	31.897	113.028	3.435	1.00	0.00	TSBB	C
ATOM	2901	CR23	TSB	17	33.171	112.476	3.489	1.00	0.00	TSBB	C

ATOM	2902	CR24	TSB	17	33.246	111.084	3.536	1.00	0.00	TSBB	C
ATOM	2903	CR25	TSB	17	32.127	110.237	3.574	1.00	0.00	TSBB	C
ATOM	2904	CR26	TSB	17	30.875	110.838	3.539	1.00	0.00	TSBB	C
ATOM	2905	HR22	TSB	17	31.862	114.106	3.354	1.00	0.00	TSBB	H
ATOM	2906	HR24	TSB	17	34.217	110.612	3.588	1.00	0.00	TSBB	H
ATOM	2907	HR26	TSB	17	30.006	110.196	3.548	1.00	0.00	TSBB	H
ATOM	2908	CR31	TSB	17	26.316	120.500	3.613	1.00	0.00	TSBB	C
ATOM	2909	CR32	TSB	17	25.005	121.048	3.600	1.00	0.00	TSBB	C
ATOM	2910	CR33	TSB	17	24.729	122.412	3.478	1.00	0.00	TSBB	C
ATOM	2911	CR34	TSB	17	25.826	123.258	3.481	1.00	0.00	TSBB	C
ATOM	2912	CR35	TSB	17	27.162	122.806	3.526	1.00	0.00	TSBB	C
ATOM	2913	CR36	TSB	17	27.388	121.426	3.529	1.00	0.00	TSBB	C
ATOM	2914	HR32	TSB	17	24.165	120.374	3.697	1.00	0.00	TSBB	H
ATOM	2915	HR34	TSB	17	25.648	124.324	3.448	1.00	0.00	TSBB	H
ATOM	2916	HR36	TSB	17	28.417	121.096	3.550	1.00	0.00	TSBB	H
ATOM	2917	CL11	TSB	17	23.953	113.364	3.742	1.00	0.00	TSBB	C
ATOM	2918	CL12	TSB	17	22.658	113.583	3.374	1.00	0.00	TSBB	C
ATOM	2919	HL11	TSB	17	24.176	112.401	4.189	1.00	0.00	TSBB	H
ATOM	2920	HL12	TSB	17	22.410	114.538	2.921	1.00	0.00	TSBB	H
ATOM	2921	CL21	TSB	17	28.932	114.075	3.683	1.00	0.00	TSBB	C
ATOM	2922	CL22	TSB	17	29.326	112.799	3.385	1.00	0.00	TSBB	C
ATOM	2923	HL21	TSB	17	29.682	114.767	4.051	1.00	0.00	TSBB	H
ATOM	2924	HL22	TSB	17	28.570	112.118	3.008	1.00	0.00	TSBB	H
ATOM	2925	CL31	TSB	17	25.800	118.022	3.365	1.00	0.00	TSBB	C
ATOM	2926	CL32	TSB	17	26.627	119.047	3.718	1.00	0.00	TSBB	C
ATOM	2927	HL31	TSB	17	24.800	118.272	3.024	1.00	0.00	TSBB	H
ATOM	2928	HL32	TSB	17	27.625	118.783	4.054	1.00	0.00	TSBB	H
ATOM	2929	013	TSB	17	20.869	108.967	3.549	1.00	0.00	TSBB	O
ATOM	2930	CA1	TSB	17	19.868	107.988	3.648	1.00	0.00	TSBB	C
ATOM	2931	HA1	TSB	17	19.260	108.118	4.547	1.00	0.00	TSBB	H
ATOM	2932	HA21	TSB	17	19.217	108.075	2.774	1.00	0.00	TSBB	H
ATOM	2933	CA2	TSB	17	20.497	106.630	3.633	1.00	0.00	TSBB	C
ATOM	2934	HA2	TSB	17	21.163	106.539	4.495	1.00	0.00	TSBB	H
ATOM	2935	HA22	TSB	17	21.126	106.584	2.740	1.00	0.00	TSBB	H
ATOM	2936	CA3	TSB	17	19.525	105.490	3.711	1.00	0.00	TSBB	C
ATOM	2937	HA3	TSB	17	18.839	105.603	2.867	1.00	0.00	TSBB	H
ATOM	2938	HA23	TSB	17	18.940	105.614	4.626	1.00	0.00	TSBB	H
ATOM	2939	CA4	TSB	17	20.065	104.089	3.738	1.00	0.00	TSBB	C
ATOM	2940	HA4	TSB	17	20.724	103.922	4.594	1.00	0.00	TSBB	H
ATOM	2941	HA24	TSB	17	20.688	104.034	2.842	1.00	0.00	TSBB	H
ATOM	2942	CA5	TSB	17	19.073	102.970	3.672	1.00	0.00	TSBB	C
ATOM	2943	HA5	TSB	17	18.400	103.116	2.823	1.00	0.00	TSBB	H
ATOM	2944	HA25	TSB	17	18.466	103.042	4.578	1.00	0.00	TSBB	H
ATOM	2945	CA6	TSB	17	19.665	101.587	3.656	1.00	0.00	TSBB	C
ATOM	2946	HA6	TSB	17	20.398	101.531	4.459	1.00	0.00	TSBB	H
ATOM	2947	HA26	TSB	17	20.193	101.391	2.724	1.00	0.00	TSBB	H
ATOM	2948	HA27	TSB	17	18.971	100.766	3.830	1.00	0.00	TSBB	H
ATOM	2949	015	TSB	17	17.724	112.743	3.568	1.00	0.00	TSBB	O
ATOM	2950	CB1	TSB	17	17.396	114.115	3.632	1.00	0.00	TSBB	C
ATOM	2951	HB1	TSB	17	17.788	114.555	4.553	1.00	0.00	TSBB	H
ATOM	2952	HB21	TSB	17	17.826	114.646	2.778	1.00	0.00	TSBB	H

ATOM	2953	CB2	TSB	17	15.902	114.219	3.663	1.00	0.00	TSBB	C
ATOM	2954	HB2	TSB	17	15.490	113.707	4.536	1.00	0.00	TSBB	H
ATOM	2955	HB22	TSB	17	15.569	113.670	2.779	1.00	0.00	TSBB	H
ATOM	2956	CB3	TSB	17	15.377	115.628	3.709	1.00	0.00	TSBB	C
ATOM	2957	HB3	TSB	17	15.811	116.113	2.831	1.00	0.00	TSBB	H
ATOM	2958	HB23	TSB	17	15.761	116.149	4.589	1.00	0.00	TSBB	H
ATOM	2959	CB4	TSB	17	13.888	115.818	3.722	1.00	0.00	TSBB	C
ATOM	2960	HB4	TSB	17	13.427	115.411	4.626	1.00	0.00	TSBB	H
ATOM	2961	HB24	TSB	17	13.513	115.223	2.885	1.00	0.00	TSBB	H
ATOM	2962	CB5	TSB	17	13.418	117.238	3.656	1.00	0.00	TSBB	C
ATOM	2963	HB5	TSB	17	13.810	117.776	4.523	1.00	0.00	TSBB	H
ATOM	2964	HB25	TSB	17	13.865	117.671	2.758	1.00	0.00	TSBB	H
ATOM	2965	CB6	TSB	17	11.922	117.425	3.631	1.00	0.00	TSBB	C
ATOM	2966	HB6	TSB	17	11.591	118.461	3.691	1.00	0.00	TSBB	H
ATOM	2967	HB26	TSB	17	11.474	116.881	4.461	1.00	0.00	TSBB	H
ATOM	2968	HB27	TSB	17	11.500	117.005	2.719	1.00	0.00	TSBB	H
ATOM	2969	023	TSB	17	34.240	113.358	3.604	1.00	0.00	TSBB	O
ATOM	2970	CC1	TSB	17	35.581	112.886	3.596	1.00	0.00	TSBB	C
ATOM	2971	HC1	TSB	17	35.779	112.252	4.463	1.00	0.00	TSBB	H
ATOM	2972	HC21	TSB	17	35.756	112.320	2.678	1.00	0.00	TSBB	H
ATOM	2973	CC2	TSB	17	36.548	114.014	3.628	1.00	0.00	TSBB	C
ATOM	2974	HC2	TSB	17	36.251	114.629	2.775	1.00	0.00	TSBB	H
ATOM	2975	HC22	TSB	17	36.405	114.604	4.537	1.00	0.00	TSBB	H
ATOM	2976	CC3	TSB	17	38.000	113.615	3.668	1.00	0.00	TSBB	C
ATOM	2977	HC3	TSB	17	38.150	112.987	2.787	1.00	0.00	TSBB	H
ATOM	2978	HC23	TSB	17	38.170	112.987	4.547	1.00	0.00	TSBB	H
ATOM	2979	CC4	TSB	17	39.053	114.679	3.707	1.00	0.00	TSBB	C
ATOM	2980	HC4	TSB	17	38.992	115.313	4.595	1.00	0.00	TSBB	H
ATOM	2981	HC24	TSB	17	38.848	115.314	2.841	1.00	0.00	TSBB	H
ATOM	2982	CC5	TSB	17	40.459	114.195	3.651	1.00	0.00	TSBB	C
ATOM	2983	HC5	TSB	17	40.541	113.548	2.774	1.00	0.00	TSBB	H
ATOM	2984	HC25	TSB	17	40.587	113.574	4.541	1.00	0.00	TSBB	H
ATOM	2985	CC6	TSB	17	41.548	115.248	3.655	1.00	0.00	TSBB	C
ATOM	2986	HC6	TSB	17	41.526	115.833	2.736	1.00	0.00	TSBB	H
ATOM	2987	HC26	TSB	17	42.551	114.856	3.814	1.00	0.00	TSBB	H
ATOM	2988	HC27	TSB	17	41.346	115.966	4.448	1.00	0.00	TSBB	H
ATOM	2989	025	TSB	17	32.361	108.856	3.548	1.00	0.00	TSBB	O
ATOM	2990	CD1	TSB	17	31.361	107.899	3.637	1.00	0.00	TSBB	C
ATOM	2991	HD1	TSB	17	30.794	108.079	4.554	1.00	0.00	TSBB	H
ATOM	2992	HD21	TSB	17	30.682	108.011	2.788	1.00	0.00	TSBB	H
ATOM	2993	CD2	TSB	17	31.973	106.539	3.654	1.00	0.00	TSBB	C
ATOM	2994	HD2	TSB	17	32.643	106.483	4.516	1.00	0.00	TSBB	H
ATOM	2995	HD22	TSB	17	32.597	106.436	2.763	1.00	0.00	TSBB	H
ATOM	2996	CD3	TSB	17	30.995	105.387	3.694	1.00	0.00	TSBB	C
ATOM	2997	HD3	TSB	17	30.372	105.496	4.586	1.00	0.00	TSBB	H
ATOM	2998	HD23	TSB	17	30.336	105.472	2.827	1.00	0.00	TSBB	H
ATOM	2999	CD4	TSB	17	31.582	104.001	3.695	1.00	0.00	TSBB	C
ATOM	3000	HD4	TSB	17	32.221	103.903	4.577	1.00	0.00	TSBB	H
ATOM	3001	HD24	TSB	17	32.233	103.894	2.824	1.00	0.00	TSBB	H
ATOM	3002	CD5	TSB	17	30.595	102.865	3.700	1.00	0.00	TSBB	C
ATOM	3003	HD5	TSB	17	29.951	102.979	2.824	1.00	0.00	TSBB	H

ATOM	3004	HD25	TSB	17	29.955	102.953	4.582	1.00	0.00	TSBB	H
ATOM	3005	CD6	TSB	17	31.231	101.491	3.664	1.00	0.00	TSBB	C
ATOM	3006	HD6	TSB	17	31.799	101.300	4.573	1.00	0.00	TSBB	H
ATOM	3007	HD26	TSB	17	31.925	101.418	2.828	1.00	0.00	TSBB	H
ATOM	3008	HD27	TSB	17	30.520	100.678	3.522	1.00	0.00	TSBB	H
ATOM	3009	033	TSB	17	23.400	122.780	3.540	1.00	0.00	TSBB	O
ATOM	3010	CE1	TSB	17	22.999	124.131	3.636	1.00	0.00	TSBB	C
ATOM	3011	HE1	TSB	17	23.440	124.634	4.500	1.00	0.00	TSBB	H
ATOM	3012	HE21	TSB	17	23.357	124.627	2.729	1.00	0.00	TSBB	H
ATOM	3013	CE2	TSB	17	21.519	124.264	3.644	1.00	0.00	TSBB	C
ATOM	3014	HE2	TSB	17	21.195	123.688	2.774	1.00	0.00	TSBB	H
ATOM	3015	HE22	TSB	17	21.096	123.798	4.538	1.00	0.00	TSBB	H
ATOM	3016	CE3	TSB	17	20.990	125.668	3.683	1.00	0.00	TSBB	C
ATOM	3017	HE3	TSB	17	21.425	126.175	2.818	1.00	0.00	TSBB	H
ATOM	3018	HE23	TSB	17	21.388	126.150	4.579	1.00	0.00	TSBB	H
ATOM	3019	CE4	TSB	17	19.512	125.881	3.719	1.00	0.00	TSBB	C
ATOM	3020	HE4	TSB	17	19.028	125.432	4.589	1.00	0.00	TSBB	H
ATOM	3021	HE24	TSB	17	19.158	125.355	2.829	1.00	0.00	TSBB	H
ATOM	3022	CE5	TSB	17	19.047	127.297	3.629	1.00	0.00	TSBB	C
ATOM	3023	HE5	TSB	17	19.416	127.792	4.531	1.00	0.00	TSBB	H
ATOM	3024	HE25	TSB	17	19.515	127.772	2.763	1.00	0.00	TSBB	H
ATOM	3025	CE6	TSB	17	17.557	127.519	3.636	1.00	0.00	TSBB	C
ATOM	3026	HE6	TSB	17	17.069	127.092	2.762	1.00	0.00	TSBB	H
ATOM	3027	HE26	TSB	17	17.157	127.044	4.531	1.00	0.00	TSBB	H
ATOM	3028	HE27	TSB	17	17.230	128.558	3.656	1.00	0.00	TSBB	H
ATOM	3029	035	TSB	17	28.174	123.767	3.389	1.00	0.00	TSBB	O
ATOM	3030	CF1	TSB	17	29.517	123.512	3.679	1.00	0.00	TSBB	C
ATOM	3031	HF1	TSB	17	29.578	122.966	4.623	1.00	0.00	TSBB	H
ATOM	3032	HF21	TSB	17	29.943	122.887	2.890	1.00	0.00	TSBB	H
ATOM	3033	CF2	TSB	17	30.228	124.824	3.787	1.00	0.00	TSBB	C
ATOM	3034	HF2	TSB	17	30.272	125.294	2.801	1.00	0.00	TSBB	H
ATOM	3035	HF22	TSB	17	29.623	125.493	4.403	1.00	0.00	TSBB	H
ATOM	3036	CF3	TSB	17	31.631	124.783	4.435	1.00	0.00	TSBB	C
ATOM	3037	HF3	TSB	17	31.550	124.338	5.430	1.00	0.00	TSBB	H
ATOM	3038	HF23	TSB	17	31.953	125.816	4.592	1.00	0.00	TSBB	H
ATOM	3039	CF4	TSB	17	32.679	124.005	3.653	1.00	0.00	TSBB	C
ATOM	3040	HF4	TSB	17	32.295	123.010	3.415	1.00	0.00	TSBB	H
ATOM	3041	HF24	TSB	17	32.857	124.515	2.703	1.00	0.00	TSBB	H
ATOM	3042	CF5	TSB	17	34.000	123.878	4.391	1.00	0.00	TSBB	C
ATOM	3043	HF5	TSB	17	33.807	123.401	5.355	1.00	0.00	TSBB	H
ATOM	3044	HF25	TSB	17	34.357	124.887	4.610	1.00	0.00	TSBB	H
ATOM	3045	CF6	TSB	17	35.073	123.099	3.634	1.00	0.00	TSBB	C
ATOM	3046	HF6	TSB	17	35.344	123.644	2.731	1.00	0.00	TSBB	H
ATOM	3047	HF26	TSB	17	34.720	122.117	3.323	1.00	0.00	TSBB	H
ATOM	3048	HF27	TSB	17	35.983	122.966	4.217	1.00	0.00	TSBB	H

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