

Supplementary Material

The SAMPL5 Host-Guest Challenge:

Computing Binding Free Energies and Enthalpies from Explicit Solvent Simulations by the Attach-Pull-Release (APR) Method

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A tutorial for the APR method will be available soon on the webpage of AMBER tutorials. Please check <http://ambermd.org/tutorials>

To compute the flip percentage in each OAH and OAMe systems, we first abstracted 7500 frames evenly from 750 ns MD simulations, and then analyzed the motions of all four benzoic acid flaps by recording the values of four torsion angles (Figure S1 a). Only if one of the torsion angles was smaller than 140 degrees (Figure S1 c, d), that structure was counted as a flipped conformation. Usually a flipped conformation contains one flipped flap, but structures with two flipped flaps were also observed (Figure S1 b), although very rarely. The total number of the flipped conformations was then divided by the number of frames, 7500, to obtain the flip percentage (Table S1). The torsion angles were most frequently observed at ~ 270 degrees (Figure S1 f) and the flap with a 180-degree torsion angle is a “transition state” between the “up” and “down” conformation (Figure S1 e).

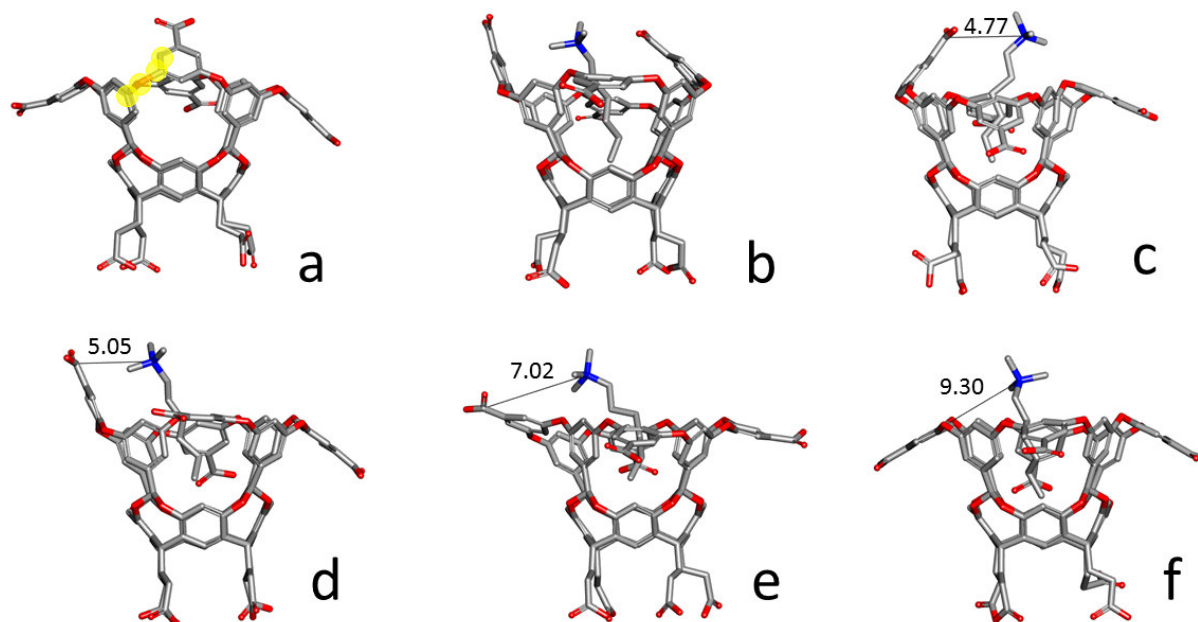


Fig S1. (a) One of the C-O-C-C torsion angles selected to monitor the motions of benzoic acid moiety highlighted in yellow; (b) A double flip-over conformation observed in the trajectories of OAH-G3. Two flaps are “up” simultaneously; Different conformations observed in the 750 ns trajectories of OAH-G3: The value of the C-O-C-C torsion angle on the left flap is (c) 60, (d) 140, (e) 180 and (f) 270 degrees. The distance (Å) between the carbon atom in the carboxyl group on the left flap and nitrogen atom in the amine group is labeled in conformation c-f.

Table S1. The flip-over percentage of bound and unbound hosts.

	OAH (%)	OAMe (%)
free host	0.28	0.00
G1	1.17	0.00
G2	0.89	0.00
G3	10.15	0.00
G4	0.00	0.00
G5	10.15	0.00
G6	3.01	0.00

Representative binding poses obtained via clustering over 750 ns of MD simulations using TIP3P water model (in PDB format)

OAH-G1

ATOM	1	C1	OCT	X	4	20.493	22.799	29.719	1.00	0.00	C
ATOM	2	C2	OCT	X	4	22.647	21.613	30.976	1.00	0.00	C
ATOM	3	C3	OCT	X	4	21.191	21.706	29.113	1.00	0.00	C
ATOM	4	C4	OCT	X	4	20.996	23.260	30.899	1.00	0.00	C
ATOM	5	C5	OCT	X	4	22.075	22.746	31.515	1.00	0.00	C
ATOM	6	C6	OCT	X	4	22.242	21.082	29.753	1.00	0.00	C
ATOM	7	O1	OCT	X	4	23.563	20.964	31.840	1.00	0.00	O
ATOM	8	C7	OCT	X	4	22.937	19.837	29.225	1.00	0.00	C
ATOM	9	C8	OCT	X	4	23.150	19.695	32.463	1.00	0.00	C
ATOM	10	O2	OCT	X	4	23.638	18.604	31.709	1.00	0.00	O
ATOM	11	C9	OCT	X	4	22.738	17.939	30.933	1.00	0.00	C
ATOM	12	C10	OCT	X	4	22.274	18.480	29.699	1.00	0.00	C
ATOM	13	C11	OCT	X	4	21.270	17.822	28.888	1.00	0.00	C
ATOM	14	C12	OCT	X	4	22.209	16.720	31.305	1.00	0.00	C
ATOM	15	C13	OCT	X	4	20.674	16.697	29.422	1.00	0.00	C
ATOM	16	C14	OCT	X	4	21.155	16.176	30.652	1.00	0.00	C
ATOM	17	O3	OCT	X	4	20.459	15.137	31.268	1.00	0.00	O
ATOM	18	C15	OCT	X	4	19.388	16.170	28.722	1.00	0.00	C
ATOM	19	C16	OCT	X	4	18.073	16.669	29.302	1.00	0.00	C
ATOM	20	C17	OCT	X	4	17.543	16.070	30.408	1.00	0.00	C
ATOM	21	C18	OCT	X	4	19.212	15.334	31.965	1.00	0.00	C
ATOM	22	O4	OCT	X	4	18.175	14.994	31.017	1.00	0.00	O
ATOM	23	O5	OCT	X	4	20.259	24.272	31.600	1.00	0.00	O
ATOM	24	C19	OCT	X	4	19.164	23.353	29.071	1.00	0.00	C
ATOM	25	C20	OCT	X	4	17.948	22.647	29.625	1.00	0.00	C
ATOM	26	O6	OCT	X	4	17.831	24.079	31.589	1.00	0.00	O
ATOM	27	C21	OCT	X	4	17.366	23.114	30.810	1.00	0.00	C
ATOM	28	C22	OCT	X	4	16.413	16.577	31.058	1.00	0.00	C
ATOM	29	C23	OCT	X	4	15.807	17.650	30.499	1.00	0.00	C
ATOM	30	C24	OCT	X	4	16.274	22.443	31.399	1.00	0.00	C
ATOM	31	C25	OCT	X	4	15.759	21.279	30.772	1.00	0.00	C
ATOM	32	O7	OCT	X	4	14.803	18.115	31.254	1.00	0.00	O
ATOM	33	O8	OCT	X	4	14.731	20.509	31.450	1.00	0.00	O
ATOM	34	C26	OCT	X	4	15.037	19.267	32.148	1.00	0.00	C
ATOM	35	C27	OCT	X	4	17.428	21.473	29.040	1.00	0.00	C
ATOM	36	C28	OCT	X	4	16.346	20.778	29.584	1.00	0.00	C
ATOM	37	C29	OCT	X	4	17.378	17.719	28.760	1.00	0.00	C
ATOM	38	C30	OCT	X	4	15.707	19.598	28.854	1.00	0.00	C
ATOM	39	C31	OCT	X	4	16.265	18.279	29.294	1.00	0.00	C
ATOM	40	C32	OCT	X	4	19.016	23.834	32.396	1.00	0.00	C
ATOM	41	C33	OCT	X	4	19.414	16.284	27.166	1.00	0.00	C
ATOM	42	C34	OCT	X	4	20.318	15.177	26.642	1.00	0.00	C
ATOM	43	C35	OCT	X	4	20.703	15.359	25.156	1.00	0.00	C
ATOM	44	O9	OCT	X	4	21.849	15.440	24.817	1.00	0.00	O
ATOM	45	C36	OCT	X	4	23.226	19.815	27.656	1.00	0.00	C
ATOM	46	C37	OCT	X	4	24.439	18.907	27.405	1.00	0.00	C
ATOM	47	C38	OCT	X	4	24.975	19.158	26.065	1.00	0.00	C
ATOM	48	O10	OCT	X	4	25.903	19.918	25.938	1.00	0.00	O
ATOM	49	C39	OCT	X	4	19.199	23.393	27.549	1.00	0.00	C
ATOM	50	C40	OCT	X	4	19.915	24.633	27.058	1.00	0.00	C
ATOM	51	C41	OCT	X	4	19.673	24.631	25.558	1.00	0.00	C
ATOM	52	O11	OCT	X	4	20.334	23.950	24.817	1.00	0.00	O
ATOM	53	C42	OCT	X	4	15.738	19.791	27.351	1.00	0.00	C
ATOM	54	C43	OCT	X	4	14.759	18.832	26.712	1.00	0.00	C
ATOM	55	C44	OCT	X	4	14.552	19.174	25.230	1.00	0.00	C

ATOM	56	O12	OCT	X	4	13.641	18.614	24.579	1.00	0.00	O
ATOM	57	C45	OCT	X	4	23.560	19.530	33.885	1.00	0.00	C
ATOM	58	C46	OCT	X	4	24.309	19.267	36.617	1.00	0.00	C
ATOM	59	C47	OCT	X	4	23.755	18.253	34.517	1.00	0.00	C
ATOM	60	C48	OCT	X	4	23.606	20.636	34.745	1.00	0.00	C
ATOM	61	C49	OCT	X	4	23.894	20.506	36.089	1.00	0.00	C
ATOM	62	C50	OCT	X	4	24.194	18.125	35.807	1.00	0.00	C
ATOM	63	C51	OCT	X	4	18.952	24.286	33.911	1.00	0.00	C
ATOM	64	C52	OCT	X	4	18.848	24.757	36.703	1.00	0.00	C
ATOM	65	C53	OCT	X	4	17.773	24.216	34.636	1.00	0.00	C
ATOM	66	C54	OCT	X	4	20.102	24.561	34.577	1.00	0.00	C
ATOM	67	C55	OCT	X	4	20.058	24.875	35.987	1.00	0.00	C
ATOM	68	C56	OCT	X	4	17.669	24.491	36.057	1.00	0.00	C
ATOM	69	C57	OCT	X	4	14.268	19.233	33.501	1.00	0.00	C
ATOM	70	C58	OCT	X	4	12.997	18.993	36.004	1.00	0.00	C
ATOM	71	C59	OCT	X	4	14.190	18.001	34.141	1.00	0.00	C
ATOM	72	C60	OCT	X	4	13.827	20.400	34.132	1.00	0.00	C
ATOM	73	C61	OCT	X	4	13.201	20.289	35.382	1.00	0.00	C
ATOM	74	C62	OCT	X	4	13.495	17.884	35.369	1.00	0.00	C
ATOM	75	C63	OCT	X	4	19.154	14.461	33.220	1.00	0.00	C
ATOM	76	C64	OCT	X	4	19.025	13.036	35.663	1.00	0.00	C
ATOM	77	C65	OCT	X	4	17.909	14.263	33.836	1.00	0.00	C
ATOM	78	C66	OCT	X	4	20.312	14.167	33.959	1.00	0.00	C
ATOM	79	C67	OCT	X	4	20.234	13.531	35.210	1.00	0.00	C
ATOM	80	C68	OCT	X	4	17.814	13.406	35.052	1.00	0.00	C
ATOM	81	O13	OCT	X	4	21.100	25.411	36.697	1.00	0.00	O
ATOM	82	O14	OCT	X	4	12.805	21.478	36.009	1.00	0.00	O
ATOM	83	O15	OCT	X	4	13.359	16.618	36.006	1.00	0.00	O
ATOM	84	O16	OCT	X	4	23.929	21.596	36.987	1.00	0.00	O
ATOM	85	O17	OCT	X	4	24.368	16.966	36.441	1.00	0.00	O
ATOM	86	O18	OCT	X	4	16.681	13.215	35.747	1.00	0.00	O
ATOM	87	O19	OCT	X	4	21.435	13.333	35.910	1.00	0.00	O
ATOM	88	C69	OCT	X	4	13.430	22.709	35.794	1.00	0.00	C
ATOM	89	C70	OCT	X	4	14.598	25.192	35.331	1.00	0.00	C
ATOM	90	C71	OCT	X	4	14.671	22.985	36.350	1.00	0.00	C
ATOM	91	C72	OCT	X	4	12.827	23.588	34.886	1.00	0.00	C
ATOM	92	C73	OCT	X	4	13.340	24.884	34.738	1.00	0.00	C
ATOM	93	C74	OCT	X	4	15.218	24.188	36.085	1.00	0.00	C
ATOM	94	O20	OCT	X	4	16.469	24.447	36.660	1.00	0.00	O
ATOM	95	C75	OCT	X	4	23.711	22.917	36.570	1.00	0.00	C
ATOM	96	C76	OCT	X	4	23.364	25.582	35.981	1.00	0.00	C
ATOM	97	C77	OCT	X	4	24.713	23.618	35.910	1.00	0.00	C
ATOM	98	C78	OCT	X	4	22.485	23.533	36.880	1.00	0.00	C
ATOM	99	C79	OCT	X	4	22.346	24.873	36.539	1.00	0.00	C
ATOM	100	C80	OCT	X	4	24.599	24.937	35.639	1.00	0.00	C
ATOM	101	C81	OCT	X	4	13.819	15.431	35.504	1.00	0.00	C
ATOM	102	C82	OCT	X	4	14.762	13.059	34.503	1.00	0.00	C
ATOM	103	C83	OCT	X	4	13.070	14.719	34.534	1.00	0.00	C
ATOM	104	C84	OCT	X	4	15.047	15.005	35.906	1.00	0.00	C
ATOM	105	C85	OCT	X	4	15.509	13.756	35.443	1.00	0.00	C
ATOM	106	C86	OCT	X	4	13.513	13.447	34.069	1.00	0.00	C
ATOM	107	C87	OCT	X	4	12.727	12.601	33.155	1.00	0.00	C
ATOM	108	O21	OCT	X	4	11.903	13.071	32.382	1.00	0.00	O
ATOM	109	C88	OCT	X	4	25.999	12.915	34.253	1.00	0.00	C
ATOM	110	O22	OCT	X	4	27.072	13.420	34.046	1.00	0.00	O
ATOM	111	C89	OCT	X	4	25.728	25.693	34.979	1.00	0.00	C
ATOM	112	O23	OCT	X	4	26.853	25.279	34.972	1.00	0.00	O
ATOM	113	O24	OCT	X	4	19.842	15.009	24.338	1.00	0.00	O
ATOM	114	O25	OCT	X	4	15.289	19.944	24.617	1.00	0.00	O
ATOM	115	O26	OCT	X	4	18.663	25.240	25.091	1.00	0.00	O

ATOM	116	C90	OCT	X	4	12.656	25.870	33.822	1.00	0.00	C
ATOM	117	O27	OCT	X	4	13.101	26.977	33.736	1.00	0.00	O
ATOM	118	O28	OCT	X	4	25.750	11.768	34.030	1.00	0.00	O
ATOM	119	O29	OCT	X	4	12.884	11.383	33.180	1.00	0.00	O
ATOM	120	O30	OCT	X	4	11.783	25.538	33.081	1.00	0.00	O
ATOM	121	O31	OCT	X	4	25.505	26.817	34.546	1.00	0.00	O
ATOM	122	O32	OCT	X	4	24.712	18.426	25.076	1.00	0.00	O
ATOM	123	C91	OCT	X	4	24.128	15.729	35.889	1.00	0.00	C
ATOM	124	C92	OCT	X	4	23.645	13.204	34.963	1.00	0.00	C
ATOM	125	C93	OCT	X	4	22.890	15.202	36.038	1.00	0.00	C
ATOM	126	C94	OCT	X	4	25.182	15.068	35.272	1.00	0.00	C
ATOM	127	C95	OCT	X	4	24.992	13.766	34.884	1.00	0.00	C
ATOM	128	C96	OCT	X	4	22.642	13.914	35.580	1.00	0.00	C
ATOM	129	H1	OCT	X	4	20.710	21.203	28.278	1.00	0.00	H
ATOM	130	H2	OCT	X	4	22.346	23.004	32.535	1.00	0.00	H
ATOM	131	H3	OCT	X	4	23.937	19.847	29.664	1.00	0.00	H
ATOM	132	H4	OCT	X	4	22.062	19.617	32.323	1.00	0.00	H
ATOM	133	H5	OCT	X	4	20.806	18.376	28.076	1.00	0.00	H
ATOM	134	H6	OCT	X	4	22.510	16.203	32.212	1.00	0.00	H
ATOM	135	H7	OCT	X	4	19.420	15.083	28.824	1.00	0.00	H
ATOM	136	H8	OCT	X	4	19.194	16.380	32.305	1.00	0.00	H
ATOM	137	H9	OCT	X	4	18.937	24.377	29.375	1.00	0.00	H
ATOM	138	H10	OCT	X	4	15.990	16.092	31.934	1.00	0.00	H
ATOM	139	H11	OCT	X	4	15.717	22.888	32.219	1.00	0.00	H
ATOM	140	H12	OCT	X	4	16.084	19.311	32.485	1.00	0.00	H
ATOM	141	H13	OCT	X	4	17.948	21.093	28.164	1.00	0.00	H
ATOM	142	H14	OCT	X	4	17.751	18.099	27.812	1.00	0.00	H
ATOM	143	H15	OCT	X	4	14.635	19.649	29.054	1.00	0.00	H
ATOM	144	H16	OCT	X	4	19.166	22.749	32.500	1.00	0.00	H
ATOM	145	H17	OCT	X	4	18.455	16.115	26.672	1.00	0.00	H
ATOM	146	H18	OCT	X	4	19.890	17.186	26.776	1.00	0.00	H
ATOM	147	H19	OCT	X	4	21.237	15.042	27.216	1.00	0.00	H
ATOM	148	H20	OCT	X	4	19.930	14.168	26.798	1.00	0.00	H
ATOM	149	H21	OCT	X	4	23.395	20.866	27.411	1.00	0.00	H
ATOM	150	H22	OCT	X	4	22.372	19.506	27.051	1.00	0.00	H
ATOM	151	H23	OCT	X	4	25.284	19.045	28.083	1.00	0.00	H
ATOM	152	H24	OCT	X	4	24.032	17.909	27.580	1.00	0.00	H
ATOM	153	H25	OCT	X	4	19.355	22.437	27.043	1.00	0.00	H
ATOM	154	H26	OCT	X	4	18.142	23.611	27.382	1.00	0.00	H
ATOM	155	H27	OCT	X	4	19.494	25.599	27.345	1.00	0.00	H
ATOM	156	H28	OCT	X	4	20.973	24.545	27.314	1.00	0.00	H
ATOM	157	H29	OCT	X	4	15.438	20.829	27.195	1.00	0.00	H
ATOM	158	H30	OCT	X	4	16.715	19.661	26.881	1.00	0.00	H
ATOM	159	H31	OCT	X	4	15.039	17.781	26.817	1.00	0.00	H
ATOM	160	H32	OCT	X	4	13.762	19.005	27.123	1.00	0.00	H
ATOM	161	H33	OCT	X	4	24.645	19.137	37.643	1.00	0.00	H
ATOM	162	H34	OCT	X	4	23.632	17.402	33.853	1.00	0.00	H
ATOM	163	H35	OCT	X	4	23.341	21.643	34.433	1.00	0.00	H
ATOM	164	H36	OCT	X	4	18.859	24.773	37.790	1.00	0.00	H
ATOM	165	H37	OCT	X	4	16.867	23.964	34.092	1.00	0.00	H
ATOM	166	H38	OCT	X	4	21.007	24.676	33.987	1.00	0.00	H
ATOM	167	H39	OCT	X	4	12.413	18.888	36.914	1.00	0.00	H
ATOM	168	H40	OCT	X	4	14.591	17.099	33.686	1.00	0.00	H
ATOM	169	H41	OCT	X	4	13.962	21.354	33.628	1.00	0.00	H
ATOM	170	H42	OCT	X	4	18.979	12.388	36.535	1.00	0.00	H
ATOM	171	H43	OCT	X	4	17.011	14.589	33.319	1.00	0.00	H
ATOM	172	H44	OCT	X	4	21.277	14.526	33.609	1.00	0.00	H
ATOM	173	H45	OCT	X	4	15.060	26.175	35.289	1.00	0.00	H
ATOM	174	H46	OCT	X	4	15.252	22.364	37.027	1.00	0.00	H
ATOM	175	H47	OCT	X	4	11.911	23.328	34.360	1.00	0.00	H

ATOM	176	H48	OCT	X	4	23.202	26.643	35.806	1.00	0.00	H
ATOM	177	H49	OCT	X	4	25.615	23.124	35.559	1.00	0.00	H
ATOM	178	H50	OCT	X	4	21.644	23.071	37.391	1.00	0.00	H
ATOM	179	H51	OCT	X	4	15.312	12.167	34.212	1.00	0.00	H
ATOM	180	H52	OCT	X	4	12.083	15.112	34.301	1.00	0.00	H
ATOM	181	H53	OCT	X	4	15.716	15.575	36.545	1.00	0.00	H
ATOM	182	H54	OCT	X	4	23.368	12.210	34.620	1.00	0.00	H
ATOM	183	H55	OCT	X	4	22.094	15.768	36.515	1.00	0.00	H
ATOM	184	H56	OCT	X	4	26.200	15.445	35.323	1.00	0.00	H
ATOM	185	C1	MOL	X	5	19.081	19.148	31.967	1.00	0.00	C
ATOM	186	C2	MOL	X	5	19.251	19.348	33.118	1.00	0.00	C
ATOM	187	C3	MOL	X	5	19.373	19.409	34.553	1.00	0.00	C
ATOM	188	C4	MOL	X	5	19.953	18.119	35.189	1.00	0.00	C
ATOM	189	C5	MOL	X	5	20.313	18.517	36.643	1.00	0.00	C
ATOM	190	C6	MOL	X	5	19.134	18.377	37.573	1.00	0.00	C
ATOM	191	O1	MOL	X	5	18.405	19.396	37.585	1.00	0.00	O
ATOM	192	O2	MOL	X	5	18.890	17.341	38.174	1.00	0.00	O
ATOM	193	H1	MOL	X	5	18.999	18.966	30.920	1.00	0.00	H
ATOM	194	H2	MOL	X	5	20.006	20.297	34.605	1.00	0.00	H
ATOM	195	H3	MOL	X	5	18.444	19.677	35.061	1.00	0.00	H
ATOM	196	H4	MOL	X	5	19.308	17.240	35.257	1.00	0.00	H
ATOM	197	H5	MOL	X	5	20.857	17.855	34.637	1.00	0.00	H
ATOM	198	H6	MOL	X	5	21.041	17.847	37.106	1.00	0.00	H
ATOM	199	H7	MOL	X	5	20.779	19.492	36.796	1.00	0.00	H
END											

OAH-G2

ATOM	1	C1	OCB	X	4	21.513	24.979	29.928	1.00	0.00	C
ATOM	2	C2	OCB	X	4	23.845	24.168	31.247	1.00	0.00	C
ATOM	3	C3	OCB	X	4	22.140	23.850	29.509	1.00	0.00	C
ATOM	4	C4	OCB	X	4	22.023	25.737	30.986	1.00	0.00	C
ATOM	5	C5	OCB	X	4	23.212	25.309	31.622	1.00	0.00	C
ATOM	6	C6	OCB	X	4	23.305	23.395	30.178	1.00	0.00	C
ATOM	7	O1	OCB	X	4	24.874	23.603	31.922	1.00	0.00	O
ATOM	8	C7	OCB	X	4	23.983	22.089	29.692	1.00	0.00	C
ATOM	9	C8	OCB	X	4	24.354	22.516	32.734	1.00	0.00	C
ATOM	10	O2	OCB	X	4	24.804	21.234	32.345	1.00	0.00	O
ATOM	11	C9	OCB	X	4	23.798	20.561	31.732	1.00	0.00	C
ATOM	12	C10	OCB	X	4	23.343	20.916	30.439	1.00	0.00	C
ATOM	13	C11	OCB	X	4	22.217	20.196	29.970	1.00	0.00	C
ATOM	14	C12	OCB	X	4	23.194	19.532	32.401	1.00	0.00	C
ATOM	15	C13	OCB	X	4	21.580	19.205	30.640	1.00	0.00	C
ATOM	16	C14	OCB	X	4	22.064	18.925	31.944	1.00	0.00	C
ATOM	17	O3	OCB	X	4	21.441	17.973	32.751	1.00	0.00	O
ATOM	18	C15	OCB	X	4	20.342	18.469	30.131	1.00	0.00	C
ATOM	19	C16	OCB	X	4	19.028	19.166	30.534	1.00	0.00	C
ATOM	20	C17	OCB	X	4	18.500	18.929	31.781	1.00	0.00	C
ATOM	21	C18	OCB	X	4	20.263	18.500	33.370	1.00	0.00	C
ATOM	22	O4	OCB	X	4	19.148	18.028	32.657	1.00	0.00	O
ATOM	23	O5	OCB	X	4	21.348	26.792	31.492	1.00	0.00	O
ATOM	24	C19	OCB	X	4	20.329	25.523	29.125	1.00	0.00	C
ATOM	25	C20	OCB	X	4	19.033	25.022	29.803	1.00	0.00	C
ATOM	26	O6	OCB	X	4	18.998	26.851	31.511	1.00	0.00	O
ATOM	27	C21	OCB	X	4	18.466	25.748	30.866	1.00	0.00	C
ATOM	28	C22	OCB	X	4	17.320	19.565	32.281	1.00	0.00	C
ATOM	29	C23	OCB	X	4	16.722	20.469	31.444	1.00	0.00	C
ATOM	30	C24	OCB	X	4	17.422	25.197	31.573	1.00	0.00	C
ATOM	31	C25	OCB	X	4	16.847	24.016	31.122	1.00	0.00	C

ATOM	32	O7	OCB	X	4	15.671	21.081	32.055	1.00	0.00	O
ATOM	33	O8	OCB	X	4	15.816	23.443	31.855	1.00	0.00	O
ATOM	34	C26	OCB	X	4	16.101	22.326	32.689	1.00	0.00	C
ATOM	35	C27	OCB	X	4	18.425	23.821	29.342	1.00	0.00	C
ATOM	36	C28	OCB	X	4	17.297	23.367	29.992	1.00	0.00	C
ATOM	37	C29	OCB	X	4	18.448	20.226	29.735	1.00	0.00	C
ATOM	38	C30	OCB	X	4	16.671	22.026	29.497	1.00	0.00	C
ATOM	39	C31	OCB	X	4	17.269	20.836	30.201	1.00	0.00	C
ATOM	40	C32	OCB	X	4	20.162	26.541	32.272	1.00	0.00	C
ATOM	41	C33	OCB	X	4	20.504	18.030	28.671	1.00	0.00	C
ATOM	42	C34	OCB	X	4	19.429	16.943	28.375	1.00	0.00	C
ATOM	43	C35	OCB	X	4	19.457	16.546	26.965	1.00	0.00	C
ATOM	44	O9	OCB	X	4	18.760	17.166	26.205	1.00	0.00	O
ATOM	45	C36	OCB	X	4	24.160	21.984	28.190	1.00	0.00	C
ATOM	46	C37	OCB	X	4	24.892	20.722	27.873	1.00	0.00	C
ATOM	47	C38	OCB	X	4	25.247	20.709	26.386	1.00	0.00	C
ATOM	48	O10	OCB	X	4	26.352	21.014	26.024	1.00	0.00	O
ATOM	49	C39	OCB	X	4	20.348	25.349	27.582	1.00	0.00	C
ATOM	50	C40	OCB	X	4	21.643	25.869	26.956	1.00	0.00	C
ATOM	51	C41	OCB	X	4	21.330	26.116	25.462	1.00	0.00	C
ATOM	52	O11	OCB	X	4	21.275	25.194	24.657	1.00	0.00	O
ATOM	53	C42	OCB	X	4	16.476	21.929	27.906	1.00	0.00	C
ATOM	54	C43	OCB	X	4	15.593	20.727	27.478	1.00	0.00	C
ATOM	55	C44	OCB	X	4	15.202	20.869	25.993	1.00	0.00	C
ATOM	56	O12	OCB	X	4	15.798	20.392	25.121	1.00	0.00	O
ATOM	57	C45	OCB	X	4	24.763	22.773	34.217	1.00	0.00	C
ATOM	58	C46	OCB	X	4	25.797	23.264	36.896	1.00	0.00	C
ATOM	59	C47	OCB	X	4	25.121	21.732	35.095	1.00	0.00	C
ATOM	60	C48	OCB	X	4	25.012	24.030	34.722	1.00	0.00	C
ATOM	61	C49	OCB	X	4	25.446	24.315	36.022	1.00	0.00	C
ATOM	62	C50	OCB	X	4	25.638	21.982	36.414	1.00	0.00	C
ATOM	63	C51	OCB	X	4	20.202	27.434	33.493	1.00	0.00	C
ATOM	64	C52	OCB	X	4	20.230	28.899	35.833	1.00	0.00	C
ATOM	65	C53	OCB	X	4	19.056	27.898	34.069	1.00	0.00	C
ATOM	66	C54	OCB	X	4	21.387	27.823	34.024	1.00	0.00	C
ATOM	67	C55	OCB	X	4	21.366	28.704	35.118	1.00	0.00	C
ATOM	68	C56	OCB	X	4	19.037	28.558	35.252	1.00	0.00	C
ATOM	69	C57	OCB	X	4	15.569	22.583	34.080	1.00	0.00	C
ATOM	70	C58	OCB	X	4	14.590	23.020	36.710	1.00	0.00	C
ATOM	71	C59	OCB	X	4	15.409	21.506	34.955	1.00	0.00	C
ATOM	72	C60	OCB	X	4	15.302	23.884	34.543	1.00	0.00	C
ATOM	73	C61	OCB	X	4	14.785	24.123	35.818	1.00	0.00	C
ATOM	74	C62	OCB	X	4	14.939	21.742	36.304	1.00	0.00	C
ATOM	75	C63	OCB	X	4	20.162	17.990	34.808	1.00	0.00	C
ATOM	76	C64	OCB	X	4	20.187	17.267	37.558	1.00	0.00	C
ATOM	77	C65	OCB	X	4	18.998	17.648	35.460	1.00	0.00	C
ATOM	78	C66	OCB	X	4	21.356	17.969	35.578	1.00	0.00	C
ATOM	79	C67	OCB	X	4	21.381	17.635	36.913	1.00	0.00	C
ATOM	80	C68	OCB	X	4	18.991	17.388	36.855	1.00	0.00	C
ATOM	81	O13	OCB	X	4	22.540	29.192	35.646	1.00	0.00	O
ATOM	82	O14	OCB	X	4	14.504	25.338	36.381	1.00	0.00	O
ATOM	83	O15	OCB	X	4	14.749	20.696	37.183	1.00	0.00	O
ATOM	84	O16	OCB	X	4	25.630	25.549	36.525	1.00	0.00	O
ATOM	85	O17	OCB	X	4	25.880	20.861	37.226	1.00	0.00	O
ATOM	86	O18	OCB	X	4	17.863	17.178	37.570	1.00	0.00	O
ATOM	87	O19	OCB	X	4	22.556	17.497	37.670	1.00	0.00	O
ATOM	88	C69	OCB	X	4	14.946	26.528	35.762	1.00	0.00	C
ATOM	89	C70	OCB	X	4	15.731	28.906	34.724	1.00	0.00	C
ATOM	90	C71	OCB	X	4	16.249	27.006	36.169	1.00	0.00	C
ATOM	91	C72	OCB	X	4	14.142	27.135	34.830	1.00	0.00	C

ATOM	92	C73	OCB	X	4	14.540	28.319	34.249	1.00	0.00	C
ATOM	93	C74	OCB	X	4	16.587	28.272	35.591	1.00	0.00	C
ATOM	94	O20	OCB	X	4	17.832	28.879	35.892	1.00	0.00	O
ATOM	95	C75	OCB	X	4	25.216	26.683	35.880	1.00	0.00	C
ATOM	96	C76	OCB	X	4	24.723	29.155	34.690	1.00	0.00	C
ATOM	97	C77	OCB	X	4	26.207	27.289	35.058	1.00	0.00	C
ATOM	98	C78	OCB	X	4	23.971	27.286	36.125	1.00	0.00	C
ATOM	99	C79	OCB	X	4	23.771	28.485	35.482	1.00	0.00	C
ATOM	100	C80	OCB	X	4	25.946	28.523	34.395	1.00	0.00	C
ATOM	101	C81	OCB	X	4	15.098	19.444	36.958	1.00	0.00	C
ATOM	102	C82	OCB	X	4	15.753	16.751	36.553	1.00	0.00	C
ATOM	103	C83	OCB	X	4	14.132	18.554	36.392	1.00	0.00	C
ATOM	104	C84	OCB	X	4	16.296	18.953	37.389	1.00	0.00	C
ATOM	105	C85	OCB	X	4	16.592	17.628	37.226	1.00	0.00	C
ATOM	106	C86	OCB	X	4	14.491	17.234	36.149	1.00	0.00	C
ATOM	107	C87	OCB	X	4	13.657	16.323	35.236	1.00	0.00	C
ATOM	108	O21	OCB	X	4	14.139	15.447	34.517	1.00	0.00	O
ATOM	109	C88	OCB	X	4	26.635	16.406	35.214	1.00	0.00	C
ATOM	110	O22	OCB	X	4	25.999	15.429	34.880	1.00	0.00	O
ATOM	111	C89	OCB	X	4	27.030	29.204	33.624	1.00	0.00	C
ATOM	112	O23	OCB	X	4	26.797	30.265	33.109	1.00	0.00	O
ATOM	113	O24	OCB	X	4	20.133	15.589	26.647	1.00	0.00	O
ATOM	114	O25	OCB	X	4	14.166	21.453	25.736	1.00	0.00	O
ATOM	115	O26	OCB	X	4	20.832	27.189	25.104	1.00	0.00	O
ATOM	116	C90	OCB	X	4	13.733	28.981	33.189	1.00	0.00	C
ATOM	117	O27	OCB	X	4	12.598	28.493	32.876	1.00	0.00	O
ATOM	118	O28	OCB	X	4	27.661	16.737	34.703	1.00	0.00	O
ATOM	119	O29	OCB	X	4	12.447	16.393	35.149	1.00	0.00	O
ATOM	120	O30	OCB	X	4	14.034	30.027	32.658	1.00	0.00	O
ATOM	121	O31	OCB	X	4	28.189	28.855	33.916	1.00	0.00	O
ATOM	122	O32	OCB	X	4	24.338	20.554	25.563	1.00	0.00	O
ATOM	123	C91	OCB	X	4	25.395	19.616	37.068	1.00	0.00	C
ATOM	124	C92	OCB	X	4	24.566	17.145	36.410	1.00	0.00	C
ATOM	125	C93	OCB	X	4	24.172	19.192	37.537	1.00	0.00	C
ATOM	126	C94	OCB	X	4	26.331	18.765	36.454	1.00	0.00	C
ATOM	127	C95	OCB	X	4	25.901	17.459	36.076	1.00	0.00	C
ATOM	128	C96	OCB	X	4	23.757	17.951	37.210	1.00	0.00	C
ATOM	129	C97	OCB	X	4	23.332	20.159	38.269	1.00	0.00	C
ATOM	130	C98	OCB	X	4	22.946	26.784	37.140	1.00	0.00	C
ATOM	131	C99	OCB	X	4	17.163	26.247	37.142	1.00	0.00	C
ATOM	132	C	OCB	X	4	17.326	19.988	37.849	1.00	0.00	C
ATOM	133	H1	OCB	X	4	21.812	23.138	28.756	1.00	0.00	H
ATOM	134	H2	OCB	X	4	23.702	25.969	32.334	1.00	0.00	H
ATOM	135	H3	OCB	X	4	25.027	22.067	30.012	1.00	0.00	H
ATOM	136	H4	OCB	X	4	23.255	22.555	32.712	1.00	0.00	H
ATOM	137	H5	OCB	X	4	21.863	20.328	28.951	1.00	0.00	H
ATOM	138	H6	OCB	X	4	23.558	19.324	33.404	1.00	0.00	H
ATOM	139	H7	OCB	X	4	20.312	17.434	30.476	1.00	0.00	H
ATOM	140	H8	OCB	X	4	20.243	19.599	33.334	1.00	0.00	H
ATOM	141	H9	OCB	X	4	20.283	26.607	29.252	1.00	0.00	H
ATOM	142	H10	OCB	X	4	16.934	19.364	33.277	1.00	0.00	H
ATOM	143	H11	OCB	X	4	17.062	25.694	32.471	1.00	0.00	H
ATOM	144	H12	OCB	X	4	17.199	22.272	32.703	1.00	0.00	H
ATOM	145	H13	OCB	X	4	18.825	23.256	28.503	1.00	0.00	H
ATOM	146	H14	OCB	X	4	18.914	20.551	28.809	1.00	0.00	H
ATOM	147	H15	OCB	X	4	15.634	22.197	29.793	1.00	0.00	H
ATOM	148	H16	OCB	X	4	20.167	25.471	32.529	1.00	0.00	H
ATOM	149	H17	OCB	X	4	20.490	18.874	27.977	1.00	0.00	H
ATOM	150	H18	OCB	X	4	21.487	17.626	28.421	1.00	0.00	H
ATOM	151	H19	OCB	X	4	19.662	16.024	28.917	1.00	0.00	H

ATOM	152	H20	OCB	X	4	18.444	17.218	28.758	1.00	0.00	H
ATOM	153	H21	OCB	X	4	24.779	22.759	27.734	1.00	0.00	H
ATOM	154	H22	OCB	X	4	23.290	22.092	27.539	1.00	0.00	H
ATOM	155	H23	OCB	X	4	25.854	20.561	28.364	1.00	0.00	H
ATOM	156	H24	OCB	X	4	24.365	19.810	28.160	1.00	0.00	H
ATOM	157	H25	OCB	X	4	20.200	24.377	27.106	1.00	0.00	H
ATOM	158	H26	OCB	X	4	19.506	25.904	27.163	1.00	0.00	H
ATOM	159	H27	OCB	X	4	21.867	26.806	27.472	1.00	0.00	H
ATOM	160	H28	OCB	X	4	22.509	25.218	27.092	1.00	0.00	H
ATOM	161	H29	OCB	X	4	15.892	22.816	27.653	1.00	0.00	H
ATOM	162	H30	OCB	X	4	17.408	21.804	27.351	1.00	0.00	H
ATOM	163	H31	OCB	X	4	16.147	19.806	27.674	1.00	0.00	H
ATOM	164	H32	OCB	X	4	14.703	20.808	28.106	1.00	0.00	H
ATOM	165	H33	OCB	X	4	26.072	23.437	37.933	1.00	0.00	H
ATOM	166	H34	OCB	X	4	25.080	20.738	34.656	1.00	0.00	H
ATOM	167	H35	OCB	X	4	24.943	24.856	34.019	1.00	0.00	H
ATOM	168	H36	OCB	X	4	20.176	29.407	36.792	1.00	0.00	H
ATOM	169	H37	OCB	X	4	18.115	27.591	33.619	1.00	0.00	H
ATOM	170	H38	OCB	X	4	22.370	27.631	33.602	1.00	0.00	H
ATOM	171	H39	OCB	X	4	14.236	23.204	37.721	1.00	0.00	H
ATOM	172	H40	OCB	X	4	15.674	20.513	34.603	1.00	0.00	H
ATOM	173	H41	OCB	X	4	15.519	24.768	33.949	1.00	0.00	H
ATOM	174	H42	OCB	X	4	20.197	17.053	38.624	1.00	0.00	H
ATOM	175	H43	OCB	X	4	18.035	17.646	34.957	1.00	0.00	H
ATOM	176	H44	OCB	X	4	22.310	18.183	35.104	1.00	0.00	H
ATOM	177	H45	OCB	X	4	16.001	29.882	34.329	1.00	0.00	H
ATOM	178	H46	OCB	X	4	13.253	26.612	34.489	1.00	0.00	H
ATOM	179	H47	OCB	X	4	24.521	30.121	34.234	1.00	0.00	H
ATOM	180	H48	OCB	X	4	27.179	26.826	34.906	1.00	0.00	H
ATOM	181	H49	OCB	X	4	15.976	15.695	36.425	1.00	0.00	H
ATOM	182	H50	OCB	X	4	13.181	18.984	36.088	1.00	0.00	H
ATOM	183	H51	OCB	X	4	24.107	16.229	36.049	1.00	0.00	H
ATOM	184	H52	OCB	X	4	27.339	19.077	36.197	1.00	0.00	H
ATOM	185	H53	OCB	X	4	22.853	20.828	37.552	1.00	0.00	H
ATOM	186	H54	OCB	X	4	22.597	19.593	38.846	1.00	0.00	H
ATOM	187	H55	OCB	X	4	23.882	20.798	38.963	1.00	0.00	H
ATOM	188	H56	OCB	X	4	23.468	26.378	38.009	1.00	0.00	H
ATOM	189	H57	OCB	X	4	22.348	27.634	37.475	1.00	0.00	H
ATOM	190	H58	OCB	X	4	22.353	25.996	36.670	1.00	0.00	H
ATOM	191	H59	OCB	X	4	16.673	25.381	37.592	1.00	0.00	H
ATOM	192	H60	OCB	X	4	18.104	25.932	36.686	1.00	0.00	H
ATOM	193	H61	OCB	X	4	17.444	26.893	37.975	1.00	0.00	H
ATOM	194	H62	OCB	X	4	17.608	20.634	37.015	1.00	0.00	H
ATOM	195	H63	OCB	X	4	16.991	20.645	38.655	1.00	0.00	H
ATOM	196	H64	OCB	X	4	18.261	19.534	38.183	1.00	0.00	H
ATOM	197	C1	MOL	X	5	19.085	23.161	37.149	1.00	0.00	C
ATOM	198	C2	MOL	X	5	19.077	23.013	35.799	1.00	0.00	C
ATOM	199	C3	MOL	X	5	20.320	22.883	35.137	1.00	0.00	C
ATOM	200	C4	MOL	X	5	21.494	23.061	35.862	1.00	0.00	C
ATOM	201	C5	MOL	X	5	21.501	23.252	37.227	1.00	0.00	C
ATOM	202	C6	MOL	X	5	20.283	23.390	37.896	1.00	0.00	C
ATOM	203	C7	MOL	X	5	20.213	22.632	33.730	1.00	0.00	C
ATOM	204	N1	MOL	X	5	20.132	22.555	32.610	1.00	0.00	N
ATOM	205	C8	MOL	X	5	20.169	23.552	39.390	1.00	0.00	C
ATOM	206	O1	MOL	X	5	21.179	23.533	40.047	1.00	0.00	O
ATOM	207	O2	MOL	X	5	19.064	23.627	39.896	1.00	0.00	O
ATOM	208	H1	MOL	X	5	18.142	23.140	37.690	1.00	0.00	H
ATOM	209	H2	MOL	X	5	18.164	22.886	35.223	1.00	0.00	H
ATOM	210	H3	MOL	X	5	22.362	22.928	35.221	1.00	0.00	H
ATOM	211	H4	MOL	X	5	22.375	23.548	37.801	1.00	0.00	H

END

OAH-G3

ATOM	1	C1	OCT	X	4	17.696	23.291	29.292	1.00	0.00	C
ATOM	2	C2	OCT	X	4	18.946	25.421	30.648	1.00	0.00	C
ATOM	3	C3	OCT	X	4	18.943	23.777	28.803	1.00	0.00	C
ATOM	4	C4	OCT	X	4	17.126	23.811	30.469	1.00	0.00	C
ATOM	5	C5	OCT	X	4	17.702	24.894	31.105	1.00	0.00	C
ATOM	6	C6	OCT	X	4	19.559	24.879	29.491	1.00	0.00	C
ATOM	7	O1	OCT	X	4	19.630	26.336	31.457	1.00	0.00	O
ATOM	8	C7	OCT	X	4	20.977	25.387	29.128	1.00	0.00	C
ATOM	9	C8	OCT	X	4	20.582	25.832	32.354	1.00	0.00	C
ATOM	10	O2	OCT	X	4	21.902	26.029	31.766	1.00	0.00	O
ATOM	11	C9	OCT	X	4	22.517	24.956	31.131	1.00	0.00	C
ATOM	12	C10	OCT	X	4	22.128	24.601	29.833	1.00	0.00	C
ATOM	13	C11	OCT	X	4	22.668	23.448	29.292	1.00	0.00	C
ATOM	14	C12	OCT	X	4	23.522	24.260	31.833	1.00	0.00	C
ATOM	15	C13	OCT	X	4	23.678	22.737	29.960	1.00	0.00	C
ATOM	16	C14	OCT	X	4	24.037	23.124	31.201	1.00	0.00	C
ATOM	17	O3	OCT	X	4	24.969	22.369	31.846	1.00	0.00	O
ATOM	18	C15	OCT	X	4	24.266	21.413	29.308	1.00	0.00	C
ATOM	19	C16	OCT	X	4	23.407	20.198	29.704	1.00	0.00	C
ATOM	20	C17	OCT	X	4	23.815	19.547	30.920	1.00	0.00	C
ATOM	21	C18	OCT	X	4	24.441	21.219	32.606	1.00	0.00	C
ATOM	22	O4	OCT	X	4	24.787	20.035	31.803	1.00	0.00	O
ATOM	23	O5	OCT	X	4	15.988	23.230	31.094	1.00	0.00	O
ATOM	24	C19	OCT	X	4	17.067	22.089	28.590	1.00	0.00	C
ATOM	25	C20	OCT	X	4	17.496	20.717	29.183	1.00	0.00	C
ATOM	26	O6	OCT	X	4	15.802	20.904	30.908	1.00	0.00	O
ATOM	27	C21	OCT	X	4	16.801	20.210	30.316	1.00	0.00	C
ATOM	28	C22	OCT	X	4	23.102	18.453	31.353	1.00	0.00	C
ATOM	29	C23	OCT	X	4	21.955	18.022	30.726	1.00	0.00	C
ATOM	30	C24	OCT	X	4	17.182	19.024	30.873	1.00	0.00	C
ATOM	31	C25	OCT	X	4	18.293	18.365	30.404	1.00	0.00	C
ATOM	32	O7	OCT	X	4	21.161	17.110	31.423	1.00	0.00	O
ATOM	33	O8	OCT	X	4	18.777	17.295	31.111	1.00	0.00	O
ATOM	34	C26	OCT	X	4	19.917	17.585	32.052	1.00	0.00	C
ATOM	35	C27	OCT	X	4	18.612	20.024	28.682	1.00	0.00	C
ATOM	36	C28	OCT	X	4	19.028	18.859	29.286	1.00	0.00	C
ATOM	37	C29	OCT	X	4	22.228	19.764	29.073	1.00	0.00	C
ATOM	38	C30	OCT	X	4	20.236	18.012	28.719	1.00	0.00	C
ATOM	39	C31	OCT	X	4	21.536	18.548	29.470	1.00	0.00	C
ATOM	40	C32	OCT	X	4	16.177	22.015	31.760	1.00	0.00	C
ATOM	41	C33	OCT	X	4	24.532	21.420	27.735	1.00	0.00	C
ATOM	42	C34	OCT	X	4	25.782	22.041	27.267	1.00	0.00	C
ATOM	43	C35	OCT	X	4	25.900	21.718	25.814	1.00	0.00	C
ATOM	44	O9	OCT	X	4	26.004	20.550	25.506	1.00	0.00	O
ATOM	45	C36	OCT	X	4	21.096	25.437	27.598	1.00	0.00	C
ATOM	46	C37	OCT	X	4	22.090	26.425	27.136	1.00	0.00	C
ATOM	47	C38	OCT	X	4	22.097	26.423	25.641	1.00	0.00	C
ATOM	48	O10	OCT	X	4	21.522	27.271	24.997	1.00	0.00	O
ATOM	49	C39	OCT	X	4	17.156	22.130	27.047	1.00	0.00	C
ATOM	50	C40	OCT	X	4	16.428	20.998	26.341	1.00	0.00	C
ATOM	51	C41	OCT	X	4	16.318	21.331	24.840	1.00	0.00	C
ATOM	52	O11	OCT	X	4	17.285	21.541	24.214	1.00	0.00	O
ATOM	53	C42	OCT	X	4	20.268	17.852	27.199	1.00	0.00	C
ATOM	54	C43	OCT	X	4	19.044	17.236	26.545	1.00	0.00	C
ATOM	55	C44	OCT	X	4	19.076	17.012	25.058	1.00	0.00	C
ATOM	56	O12	OCT	X	4	18.374	17.771	24.401	1.00	0.00	O

ATOM	57	C45	OCT	X	4	20.402	26.445	33.703	1.00	0.00	C
ATOM	58	C46	OCT	X	4	20.084	26.799	36.429	1.00	0.00	C
ATOM	59	C47	OCT	X	4	21.572	26.388	34.587	1.00	0.00	C
ATOM	60	C48	OCT	X	4	19.152	26.771	34.219	1.00	0.00	C
ATOM	61	C49	OCT	X	4	19.022	27.030	35.592	1.00	0.00	C
ATOM	62	C50	OCT	X	4	21.343	26.536	35.974	1.00	0.00	C
ATOM	63	C51	OCT	X	4	15.456	22.084	33.147	1.00	0.00	C
ATOM	64	C52	OCT	X	4	14.194	22.129	35.544	1.00	0.00	C
ATOM	65	C53	OCT	X	4	15.190	20.833	33.764	1.00	0.00	C
ATOM	66	C54	OCT	X	4	15.115	23.309	33.678	1.00	0.00	C
ATOM	67	C55	OCT	X	4	14.399	23.295	34.833	1.00	0.00	C
ATOM	68	C56	OCT	X	4	14.624	20.890	35.055	1.00	0.00	C
ATOM	69	C57	OCT	X	4	19.713	16.909	33.418	1.00	0.00	C
ATOM	70	C58	OCT	X	4	19.449	15.884	35.965	1.00	0.00	C
ATOM	71	C59	OCT	X	4	20.806	16.747	34.253	1.00	0.00	C
ATOM	72	C60	OCT	X	4	18.434	16.780	33.964	1.00	0.00	C
ATOM	73	C61	OCT	X	4	18.343	16.211	35.179	1.00	0.00	C
ATOM	74	C62	OCT	X	4	20.692	16.257	35.559	1.00	0.00	C
ATOM	75	C63	OCT	X	4	25.043	21.207	33.956	1.00	0.00	C
ATOM	76	C64	OCT	X	4	26.123	21.135	36.490	1.00	0.00	C
ATOM	77	C65	OCT	X	4	25.102	19.982	34.652	1.00	0.00	C
ATOM	78	C66	OCT	X	4	25.342	22.460	34.606	1.00	0.00	C
ATOM	79	C67	OCT	X	4	25.881	22.390	35.938	1.00	0.00	C
ATOM	80	C68	OCT	X	4	25.616	19.963	35.947	1.00	0.00	C
ATOM	81	O13	OCT	X	4	13.983	24.491	35.386	1.00	0.00	O
ATOM	82	O14	OCT	X	4	17.094	15.888	35.612	1.00	0.00	O
ATOM	83	O15	OCT	X	4	21.661	16.065	36.506	1.00	0.00	O
ATOM	84	O16	OCT	X	4	17.801	27.287	36.188	1.00	0.00	O
ATOM	85	O17	OCT	X	4	22.401	26.418	36.928	1.00	0.00	O
ATOM	86	O18	OCT	X	4	25.675	18.804	36.650	1.00	0.00	O
ATOM	87	O19	OCT	X	4	26.242	23.594	36.607	1.00	0.00	O
ATOM	88	C69	OCT	X	4	16.003	16.617	35.223	1.00	0.00	C
ATOM	89	C70	OCT	X	4	13.718	17.965	34.421	1.00	0.00	C
ATOM	90	C71	OCT	X	4	15.700	17.822	35.818	1.00	0.00	C
ATOM	91	C72	OCT	X	4	15.135	16.070	34.304	1.00	0.00	C
ATOM	92	C73	OCT	X	4	13.921	16.680	33.990	1.00	0.00	C
ATOM	93	C74	OCT	X	4	14.555	18.517	35.361	1.00	0.00	C
ATOM	94	O20	OCT	X	4	14.264	19.774	35.873	1.00	0.00	O
ATOM	95	C75	OCT	X	4	16.564	27.068	35.547	1.00	0.00	C
ATOM	96	C76	OCT	X	4	13.976	26.771	34.730	1.00	0.00	C
ATOM	97	C77	OCT	X	4	15.941	28.125	34.926	1.00	0.00	C
ATOM	98	C78	OCT	X	4	15.989	25.816	35.642	1.00	0.00	C
ATOM	99	C79	OCT	X	4	14.683	25.673	35.235	1.00	0.00	C
ATOM	100	C80	OCT	X	4	14.653	27.958	34.367	1.00	0.00	C
ATOM	101	C81	OCT	X	4	23.000	16.251	36.316	1.00	0.00	C
ATOM	102	C82	OCT	X	4	25.787	16.593	35.718	1.00	0.00	C
ATOM	103	C83	OCT	X	4	23.729	15.259	35.640	1.00	0.00	C
ATOM	104	C84	OCT	X	4	23.687	17.440	36.549	1.00	0.00	C
ATOM	105	C85	OCT	X	4	25.042	17.592	36.352	1.00	0.00	C
ATOM	106	C86	OCT	X	4	25.115	15.437	35.403	1.00	0.00	C
ATOM	107	C87	OCT	X	4	25.881	14.289	34.687	1.00	0.00	C
ATOM	108	O21	OCT	X	4	27.080	14.210	34.748	1.00	0.00	O
ATOM	109	C88	OCT	X	4	26.835	28.506	36.025	1.00	0.00	C
ATOM	110	O22	OCT	X	4	26.332	29.544	35.573	1.00	0.00	O
ATOM	111	C89	OCT	X	4	13.909	28.982	33.557	1.00	0.00	C
ATOM	112	O23	OCT	X	4	12.846	28.820	33.029	1.00	0.00	O
ATOM	113	O24	OCT	X	4	26.034	22.591	24.947	1.00	0.00	O
ATOM	114	O25	OCT	X	4	20.072	16.510	24.552	1.00	0.00	O
ATOM	115	O26	OCT	X	4	15.218	21.740	24.451	1.00	0.00	O
ATOM	116	C90	OCT	X	4	12.918	15.987	33.103	1.00	0.00	C

ATOM	117	O27	OCT	X	4	12.207	16.657	32.388	1.00	0.00	O
ATOM	118	O28	OCT	X	4	28.045	28.457	36.148	1.00	0.00	O
ATOM	119	O29	OCT	X	4	25.273	13.326	34.227	1.00	0.00	O
ATOM	120	O30	OCT	X	4	12.939	14.740	33.057	1.00	0.00	O
ATOM	121	O31	OCT	X	4	14.391	30.098	33.489	1.00	0.00	O
ATOM	122	O32	OCT	X	4	22.723	25.522	25.058	1.00	0.00	O
ATOM	123	C91	OCT	X	4	23.716	26.354	36.679	1.00	0.00	C
ATOM	124	C92	OCT	X	4	26.475	25.922	36.191	1.00	0.00	C
ATOM	125	C93	OCT	X	4	24.274	25.037	36.760	1.00	0.00	C
ATOM	126	C94	OCT	X	4	24.588	27.374	36.390	1.00	0.00	C
ATOM	127	C95	OCT	X	4	25.953	27.198	36.226	1.00	0.00	C
ATOM	128	C96	OCT	X	4	25.655	24.849	36.471	1.00	0.00	C
ATOM	129	H1	OCT	X	4	19.392	23.312	27.929	1.00	0.00	H
ATOM	130	H2	OCT	X	4	17.238	25.401	31.947	1.00	0.00	H
ATOM	131	H3	OCT	X	4	21.039	26.406	29.515	1.00	0.00	H
ATOM	132	H4	OCT	X	4	20.516	24.735	32.397	1.00	0.00	H
ATOM	133	H5	OCT	X	4	22.342	23.049	28.335	1.00	0.00	H
ATOM	134	H6	OCT	X	4	23.828	24.614	32.814	1.00	0.00	H
ATOM	135	H7	OCT	X	4	25.279	21.313	29.705	1.00	0.00	H
ATOM	136	H8	OCT	X	4	23.342	21.220	32.650	1.00	0.00	H
ATOM	137	H9	OCT	X	4	15.975	22.095	28.618	1.00	0.00	H
ATOM	138	H10	OCT	X	4	23.409	17.947	32.265	1.00	0.00	H
ATOM	139	H11	OCT	X	4	16.576	18.545	31.637	1.00	0.00	H
ATOM	140	H12	OCT	X	4	19.917	18.678	32.173	1.00	0.00	H
ATOM	141	H13	OCT	X	4	19.239	20.469	27.913	1.00	0.00	H
ATOM	142	H14	OCT	X	4	21.963	20.247	28.136	1.00	0.00	H
ATOM	143	H15	OCT	X	4	20.068	16.978	29.027	1.00	0.00	H
ATOM	144	H16	OCT	X	4	17.237	21.769	31.924	1.00	0.00	H
ATOM	145	H17	OCT	X	4	24.463	20.429	27.280	1.00	0.00	H
ATOM	146	H18	OCT	X	4	23.655	21.920	27.318	1.00	0.00	H
ATOM	147	H19	OCT	X	4	25.683	23.114	27.440	1.00	0.00	H
ATOM	148	H20	OCT	X	4	26.551	21.614	27.915	1.00	0.00	H
ATOM	149	H21	OCT	X	4	20.109	25.764	27.263	1.00	0.00	H
ATOM	150	H22	OCT	X	4	21.217	24.456	27.134	1.00	0.00	H
ATOM	151	H23	OCT	X	4	21.981	27.440	27.522	1.00	0.00	H
ATOM	152	H24	OCT	X	4	23.081	26.134	27.491	1.00	0.00	H
ATOM	153	H25	OCT	X	4	16.617	23.028	26.739	1.00	0.00	H
ATOM	154	H26	OCT	X	4	18.181	22.276	26.701	1.00	0.00	H
ATOM	155	H27	OCT	X	4	16.944	20.037	26.389	1.00	0.00	H
ATOM	156	H28	OCT	X	4	15.428	20.761	26.710	1.00	0.00	H
ATOM	157	H29	OCT	X	4	20.792	18.711	26.775	1.00	0.00	H
ATOM	158	H30	OCT	X	4	21.039	17.082	27.125	1.00	0.00	H
ATOM	159	H31	OCT	X	4	18.847	16.277	27.030	1.00	0.00	H
ATOM	160	H32	OCT	X	4	18.149	17.799	26.820	1.00	0.00	H
ATOM	161	H33	OCT	X	4	19.941	26.789	37.506	1.00	0.00	H
ATOM	162	H34	OCT	X	4	22.598	26.355	34.229	1.00	0.00	H
ATOM	163	H35	OCT	X	4	18.275	26.649	33.588	1.00	0.00	H
ATOM	164	H36	OCT	X	4	13.720	22.244	36.516	1.00	0.00	H
ATOM	165	H37	OCT	X	4	15.429	19.954	33.170	1.00	0.00	H
ATOM	166	H38	OCT	X	4	15.425	24.256	33.244	1.00	0.00	H
ATOM	167	H39	OCT	X	4	19.335	15.425	36.944	1.00	0.00	H
ATOM	168	H40	OCT	X	4	21.805	16.978	33.892	1.00	0.00	H
ATOM	169	H41	OCT	X	4	17.564	16.918	33.327	1.00	0.00	H
ATOM	170	H42	OCT	X	4	26.750	20.991	37.366	1.00	0.00	H
ATOM	171	H43	OCT	X	4	24.818	19.066	34.141	1.00	0.00	H
ATOM	172	H44	OCT	X	4	25.154	23.441	34.177	1.00	0.00	H
ATOM	173	H45	OCT	X	4	12.883	18.586	34.108	1.00	0.00	H
ATOM	174	H46	OCT	X	4	16.375	18.230	36.566	1.00	0.00	H
ATOM	175	H47	OCT	X	4	15.492	15.198	33.762	1.00	0.00	H
ATOM	176	H48	OCT	X	4	12.924	26.576	34.541	1.00	0.00	H

ATOM	177	H49	OCT	X	4	16.319	29.143	34.960	1.00	0.00	H
ATOM	178	H50	OCT	X	4	16.610	25.059	36.112	1.00	0.00	H
ATOM	179	H51	OCT	X	4	26.833	16.779	35.484	1.00	0.00	H
ATOM	180	H52	OCT	X	4	23.199	14.374	35.297	1.00	0.00	H
ATOM	181	H53	OCT	X	4	23.191	18.312	36.965	1.00	0.00	H
ATOM	182	H54	OCT	X	4	27.519	25.693	35.995	1.00	0.00	H
ATOM	183	H55	OCT	X	4	23.540	24.272	37.001	1.00	0.00	H
ATOM	184	H56	OCT	X	4	24.218	28.383	36.556	1.00	0.00	H
ATOM	185	C1	MOL	X	5	20.298	21.392	32.058	1.00	0.00	C
ATOM	186	C2	MOL	X	5	19.823	21.601	33.521	1.00	0.00	C
ATOM	187	C3	MOL	X	5	19.329	20.330	34.165	1.00	0.00	C
ATOM	188	C4	MOL	X	5	18.580	20.617	35.480	1.00	0.00	C
ATOM	189	C5	MOL	X	5	19.315	21.396	36.521	1.00	0.00	C
ATOM	190	C6	MOL	X	5	18.632	21.403	37.876	1.00	0.00	C
ATOM	191	N1	MOL	X	5	19.323	22.205	39.027	1.00	0.00	N
ATOM	192	C7	MOL	X	5	19.326	23.686	38.764	1.00	0.00	C
ATOM	193	C8	MOL	X	5	20.706	21.627	39.185	1.00	0.00	C
ATOM	194	C9	MOL	X	5	18.606	21.940	40.340	1.00	0.00	C
ATOM	195	H1	MOL	X	5	20.991	20.570	31.865	1.00	0.00	H
ATOM	196	H2	MOL	X	5	19.423	21.205	31.432	1.00	0.00	H
ATOM	197	H3	MOL	X	5	19.019	22.336	33.594	1.00	0.00	H
ATOM	198	H4	MOL	X	5	20.662	22.053	34.054	1.00	0.00	H
ATOM	199	H5	MOL	X	5	20.191	19.738	34.479	1.00	0.00	H
ATOM	200	H6	MOL	X	5	18.751	19.735	33.454	1.00	0.00	H
ATOM	201	H7	MOL	X	5	18.280	19.642	35.869	1.00	0.00	H
ATOM	202	H8	MOL	X	5	17.631	21.124	35.294	1.00	0.00	H
ATOM	203	H9	MOL	X	5	19.391	22.438	36.203	1.00	0.00	H
ATOM	204	H10	MOL	X	5	20.295	20.922	36.603	1.00	0.00	H
ATOM	205	H11	MOL	X	5	18.595	20.402	38.310	1.00	0.00	H
ATOM	206	H12	MOL	X	5	17.660	21.889	37.782	1.00	0.00	H
ATOM	207	H13	MOL	X	5	20.725	22.324	31.682	1.00	0.00	H
ATOM	208	H14	MOL	X	5	18.340	24.079	38.513	1.00	0.00	H
ATOM	209	H15	MOL	X	5	19.672	24.211	39.655	1.00	0.00	H
ATOM	210	H16	MOL	X	5	19.940	23.976	37.910	1.00	0.00	H
ATOM	211	H17	MOL	X	5	20.637	20.541	39.265	1.00	0.00	H
ATOM	212	H18	MOL	X	5	21.302	21.930	38.324	1.00	0.00	H
ATOM	213	H19	MOL	X	5	21.204	22.069	40.049	1.00	0.00	H
ATOM	214	H20	MOL	X	5	17.619	22.363	40.148	1.00	0.00	H
ATOM	215	H21	MOL	X	5	18.474	20.859	40.402	1.00	0.00	H
ATOM	216	H22	MOL	X	5	19.069	22.560	41.110	1.00	0.00	H

END

OAH-G4

ATOM	1	C1	OCT	X	4	19.992	21.071	25.480	1.00	0.00	C
ATOM	2	C2	OCT	X	4	22.139	19.875	26.898	1.00	0.00	C
ATOM	3	C3	OCT	X	4	20.567	19.928	25.044	1.00	0.00	C
ATOM	4	C4	OCT	X	4	20.507	21.603	26.720	1.00	0.00	C
ATOM	5	C5	OCT	X	4	21.640	21.120	27.303	1.00	0.00	C
ATOM	6	C6	OCT	X	4	21.565	19.230	25.764	1.00	0.00	C
ATOM	7	O1	OCT	X	4	23.149	19.264	27.516	1.00	0.00	O
ATOM	8	C7	OCT	X	4	22.214	17.944	25.210	1.00	0.00	C
ATOM	9	C8	OCT	X	4	22.720	18.236	28.431	1.00	0.00	C
ATOM	10	O2	OCT	X	4	23.061	16.944	27.902	1.00	0.00	O
ATOM	11	C9	OCT	X	4	22.118	16.274	27.142	1.00	0.00	C
ATOM	12	C10	OCT	X	4	21.624	16.703	25.911	1.00	0.00	C
ATOM	13	C11	OCT	X	4	20.439	16.210	25.434	1.00	0.00	C
ATOM	14	C12	OCT	X	4	21.509	15.235	27.769	1.00	0.00	C
ATOM	15	C13	OCT	X	4	19.694	15.161	26.083	1.00	0.00	C

ATOM	16	C14	OCT	X	4	20.314	14.677	27.266	1.00	0.00	C
ATOM	17	O3	OCT	X	4	19.520	13.950	28.183	1.00	0.00	O
ATOM	18	C15	OCT	X	4	18.466	14.601	25.460	1.00	0.00	C
ATOM	19	C16	OCT	X	4	17.268	15.393	26.016	1.00	0.00	C
ATOM	20	C17	OCT	X	4	16.594	14.930	27.166	1.00	0.00	C
ATOM	21	C18	OCT	X	4	18.248	14.393	28.784	1.00	0.00	C
ATOM	22	O4	OCT	X	4	17.162	13.975	27.988	1.00	0.00	O
ATOM	23	O5	OCT	X	4	19.928	22.766	27.235	1.00	0.00	O
ATOM	24	C19	OCT	X	4	18.738	21.688	24.799	1.00	0.00	C
ATOM	25	C20	OCT	X	4	17.399	21.249	25.391	1.00	0.00	C
ATOM	26	O6	OCT	X	4	17.555	22.987	27.105	1.00	0.00	O
ATOM	27	C21	OCT	X	4	16.906	21.979	26.522	1.00	0.00	C
ATOM	28	C22	OCT	X	4	15.464	15.632	27.605	1.00	0.00	C
ATOM	29	C23	OCT	X	4	15.038	16.757	26.995	1.00	0.00	C
ATOM	30	C24	OCT	X	4	15.676	21.556	27.096	1.00	0.00	C
ATOM	31	C25	OCT	X	4	15.014	20.370	26.633	1.00	0.00	C
ATOM	32	O7	OCT	X	4	13.941	17.383	27.601	1.00	0.00	O
ATOM	33	O8	OCT	X	4	13.934	19.839	27.399	1.00	0.00	O
ATOM	34	C26	OCT	X	4	14.138	18.732	28.302	1.00	0.00	C
ATOM	35	C27	OCT	X	4	16.785	20.123	24.939	1.00	0.00	C
ATOM	36	C28	OCT	X	4	15.581	19.653	25.589	1.00	0.00	C
ATOM	37	C29	OCT	X	4	16.695	16.417	25.264	1.00	0.00	C
ATOM	38	C30	OCT	X	4	14.985	18.327	25.008	1.00	0.00	C
ATOM	39	C31	OCT	X	4	15.651	17.199	25.822	1.00	0.00	C
ATOM	40	C32	OCT	X	4	18.733	22.627	27.932	1.00	0.00	C
ATOM	41	C33	OCT	X	4	18.577	14.317	23.957	1.00	0.00	C
ATOM	42	C34	OCT	X	4	17.308	13.601	23.487	1.00	0.00	C
ATOM	43	C35	OCT	X	4	17.450	13.281	22.010	1.00	0.00	C
ATOM	44	O9	OCT	X	4	16.575	13.507	21.212	1.00	0.00	O
ATOM	45	C36	OCT	X	4	22.468	17.962	23.777	1.00	0.00	C
ATOM	46	C37	OCT	X	4	23.376	16.779	23.285	1.00	0.00	C
ATOM	47	C38	OCT	X	4	23.548	17.014	21.776	1.00	0.00	C
ATOM	48	O10	OCT	X	4	24.455	17.726	21.401	1.00	0.00	O
ATOM	49	C39	OCT	X	4	18.884	21.575	23.227	1.00	0.00	C
ATOM	50	C40	OCT	X	4	17.887	22.503	22.516	1.00	0.00	C
ATOM	51	C41	OCT	X	4	18.181	22.695	21.049	1.00	0.00	C
ATOM	52	O11	OCT	X	4	17.939	21.739	20.338	1.00	0.00	O
ATOM	53	C42	OCT	X	4	14.730	18.156	23.497	1.00	0.00	C
ATOM	54	C43	OCT	X	4	13.855	19.325	22.922	1.00	0.00	C
ATOM	55	C44	OCT	X	4	13.806	19.191	21.423	1.00	0.00	C
ATOM	56	O12	OCT	X	4	14.229	20.068	20.692	1.00	0.00	O
ATOM	57	C45	OCT	X	4	23.418	18.449	29.720	1.00	0.00	C
ATOM	58	C46	OCT	X	4	24.057	18.606	32.514	1.00	0.00	C
ATOM	59	C47	OCT	X	4	23.566	17.311	30.547	1.00	0.00	C
ATOM	60	C48	OCT	X	4	23.667	19.683	30.359	1.00	0.00	C
ATOM	61	C49	OCT	X	4	23.939	19.757	31.733	1.00	0.00	C
ATOM	62	C50	OCT	X	4	23.867	17.365	31.904	1.00	0.00	C
ATOM	63	C51	OCT	X	4	18.700	23.371	29.239	1.00	0.00	C
ATOM	64	C52	OCT	X	4	18.625	24.655	31.766	1.00	0.00	C
ATOM	65	C53	OCT	X	4	17.498	23.660	29.859	1.00	0.00	C
ATOM	66	C54	OCT	X	4	19.915	23.614	29.971	1.00	0.00	C
ATOM	67	C55	OCT	X	4	19.846	24.298	31.203	1.00	0.00	C
ATOM	68	C56	OCT	X	4	17.466	24.253	31.128	1.00	0.00	C
ATOM	69	C57	OCT	X	4	13.354	18.908	29.624	1.00	0.00	C
ATOM	70	C58	OCT	X	4	12.339	19.228	32.151	1.00	0.00	C
ATOM	71	C59	OCT	X	4	13.266	17.789	30.481	1.00	0.00	C
ATOM	72	C60	OCT	X	4	12.996	20.161	30.046	1.00	0.00	C
ATOM	73	C61	OCT	X	4	12.524	20.306	31.296	1.00	0.00	C
ATOM	74	C62	OCT	X	4	12.683	17.953	31.730	1.00	0.00	C
ATOM	75	C63	OCT	X	4	18.048	13.783	30.159	1.00	0.00	C

ATOM	76	C64	OCT	X	4	17.772	13.061	32.871	1.00	0.00	C
ATOM	77	C65	OCT	X	4	16.794	13.538	30.693	1.00	0.00	C
ATOM	78	C66	OCT	X	4	19.187	13.688	30.989	1.00	0.00	C
ATOM	79	C67	OCT	X	4	19.065	13.245	32.317	1.00	0.00	C
ATOM	80	C68	OCT	X	4	16.651	13.272	32.089	1.00	0.00	C
ATOM	81	O13	OCT	X	4	20.973	24.572	31.886	1.00	0.00	O
ATOM	82	O14	OCT	X	4	12.357	21.575	31.940	1.00	0.00	O
ATOM	83	O15	OCT	X	4	12.564	16.911	32.621	1.00	0.00	O
ATOM	84	O16	OCT	X	4	24.045	20.993	32.373	1.00	0.00	O
ATOM	85	O17	OCT	X	4	23.911	16.241	32.705	1.00	0.00	O
ATOM	86	O18	OCT	X	4	15.445	13.135	32.646	1.00	0.00	O
ATOM	87	O19	OCT	X	4	20.167	13.174	33.112	1.00	0.00	O
ATOM	88	C69	OCT	X	4	13.073	22.781	31.568	1.00	0.00	C
ATOM	89	C70	OCT	X	4	14.271	25.130	30.764	1.00	0.00	C
ATOM	90	C71	OCT	X	4	14.427	23.033	31.839	1.00	0.00	C
ATOM	91	C72	OCT	X	4	12.336	23.692	30.854	1.00	0.00	C
ATOM	92	C73	OCT	X	4	12.948	24.874	30.400	1.00	0.00	C
ATOM	93	C74	OCT	X	4	14.991	24.223	31.488	1.00	0.00	C
ATOM	94	O20	OCT	X	4	16.336	24.472	31.817	1.00	0.00	O
ATOM	95	C75	OCT	X	4	23.650	22.200	31.828	1.00	0.00	C
ATOM	96	C76	OCT	X	4	22.940	24.585	30.652	1.00	0.00	C
ATOM	97	C77	OCT	X	4	24.524	22.791	31.022	1.00	0.00	C
ATOM	98	C78	OCT	X	4	22.482	22.830	32.261	1.00	0.00	C
ATOM	99	C79	OCT	X	4	22.170	24.048	31.663	1.00	0.00	C
ATOM	100	C80	OCT	X	4	24.189	24.012	30.347	1.00	0.00	C
ATOM	101	C81	OCT	X	4	12.891	15.639	32.321	1.00	0.00	C
ATOM	102	C82	OCT	X	4	13.320	13.017	31.612	1.00	0.00	C
ATOM	103	C83	OCT	X	4	11.874	14.942	31.668	1.00	0.00	C
ATOM	104	C84	OCT	X	4	14.141	15.073	32.601	1.00	0.00	C
ATOM	105	C85	OCT	X	4	14.299	13.710	32.291	1.00	0.00	C
ATOM	106	C86	OCT	X	4	12.124	13.594	31.294	1.00	0.00	C
ATOM	107	C87	OCT	X	4	11.171	12.925	30.401	1.00	0.00	C
ATOM	108	O21	OCT	X	4	11.221	11.649	30.399	1.00	0.00	O
ATOM	109	C88	OCT	X	4	23.817	12.046	30.073	1.00	0.00	C
ATOM	110	O22	OCT	X	4	24.916	12.294	29.672	1.00	0.00	O
ATOM	111	C89	OCT	X	4	25.110	24.582	29.305	1.00	0.00	C
ATOM	112	O23	OCT	X	4	25.144	25.798	29.118	1.00	0.00	O
ATOM	113	O24	OCT	X	4	18.450	12.860	21.529	1.00	0.00	O
ATOM	114	O25	OCT	X	4	13.391	18.175	20.880	1.00	0.00	O
ATOM	115	O26	OCT	X	4	18.399	23.838	20.560	1.00	0.00	O
ATOM	116	C90	OCT	X	4	12.211	25.968	29.680	1.00	0.00	C
ATOM	117	O27	OCT	X	4	12.678	27.061	29.562	1.00	0.00	O
ATOM	118	O28	OCT	X	4	23.148	11.132	29.534	1.00	0.00	O
ATOM	119	O29	OCT	X	4	10.232	13.424	29.875	1.00	0.00	O
ATOM	120	O30	OCT	X	4	11.083	25.851	29.212	1.00	0.00	O
ATOM	121	O31	OCT	X	4	26.055	23.911	28.903	1.00	0.00	O
ATOM	122	O32	OCT	X	4	22.837	16.336	21.034	1.00	0.00	O
ATOM	123	C91	OCT	X	4	23.332	15.000	32.393	1.00	0.00	C
ATOM	124	C92	OCT	X	4	22.002	12.659	31.716	1.00	0.00	C
ATOM	125	C93	OCT	X	4	22.073	14.672	32.964	1.00	0.00	C
ATOM	126	C94	OCT	X	4	23.848	14.119	31.414	1.00	0.00	C
ATOM	127	C95	OCT	X	4	23.183	12.955	31.063	1.00	0.00	C
ATOM	128	C96	OCT	X	4	21.394	13.537	32.635	1.00	0.00	C
ATOM	129	H1	OCT	X	4	20.177	19.385	24.186	1.00	0.00	H
ATOM	130	H2	OCT	X	4	21.995	21.675	28.167	1.00	0.00	H
ATOM	131	H3	OCT	X	4	23.191	17.817	25.681	1.00	0.00	H
ATOM	132	H4	OCT	X	4	21.657	18.382	28.675	1.00	0.00	H
ATOM	133	H5	OCT	X	4	19.996	16.619	24.530	1.00	0.00	H
ATOM	134	H6	OCT	X	4	21.847	15.144	28.798	1.00	0.00	H
ATOM	135	H7	OCT	X	4	18.373	13.590	25.862	1.00	0.00	H

ATOM	136	H8	OCT	X	4	18.192	15.480	28.938	1.00	0.00	H
ATOM	137	H9	OCT	X	4	18.831	22.758	24.995	1.00	0.00	H
ATOM	138	H10	OCT	X	4	14.949	15.220	28.469	1.00	0.00	H
ATOM	139	H11	OCT	X	4	15.213	22.178	27.858	1.00	0.00	H
ATOM	140	H12	OCT	X	4	15.181	18.821	28.642	1.00	0.00	H
ATOM	141	H13	OCT	X	4	17.152	19.570	24.078	1.00	0.00	H
ATOM	142	H14	OCT	X	4	17.150	16.730	24.328	1.00	0.00	H
ATOM	143	H15	OCT	X	4	13.944	18.200	25.311	1.00	0.00	H
ATOM	144	H16	OCT	X	4	18.642	21.572	28.230	1.00	0.00	H
ATOM	145	H17	OCT	X	4	18.743	15.187	23.318	1.00	0.00	H
ATOM	146	H18	OCT	X	4	19.385	13.585	23.887	1.00	0.00	H
ATOM	147	H19	OCT	X	4	17.105	12.646	23.976	1.00	0.00	H
ATOM	148	H20	OCT	X	4	16.435	14.254	23.536	1.00	0.00	H
ATOM	149	H21	OCT	X	4	23.014	18.905	23.701	1.00	0.00	H
ATOM	150	H22	OCT	X	4	21.597	18.115	23.136	1.00	0.00	H
ATOM	151	H23	OCT	X	4	24.299	16.863	23.863	1.00	0.00	H
ATOM	152	H24	OCT	X	4	22.954	15.796	23.502	1.00	0.00	H
ATOM	153	H25	OCT	X	4	19.896	21.864	22.934	1.00	0.00	H
ATOM	154	H26	OCT	X	4	18.794	20.552	22.856	1.00	0.00	H
ATOM	155	H27	OCT	X	4	16.926	21.996	22.621	1.00	0.00	H
ATOM	156	H28	OCT	X	4	17.870	23.458	23.046	1.00	0.00	H
ATOM	157	H29	OCT	X	4	15.692	18.230	22.986	1.00	0.00	H
ATOM	158	H30	OCT	X	4	14.296	17.219	23.142	1.00	0.00	H
ATOM	159	H31	OCT	X	4	12.837	19.232	23.303	1.00	0.00	H
ATOM	160	H32	OCT	X	4	14.262	20.322	23.106	1.00	0.00	H
ATOM	161	H33	OCT	X	4	24.291	18.602	33.575	1.00	0.00	H
ATOM	162	H34	OCT	X	4	23.426	16.300	30.174	1.00	0.00	H
ATOM	163	H35	OCT	X	4	23.626	20.649	29.863	1.00	0.00	H
ATOM	164	H36	OCT	X	4	18.641	24.895	32.827	1.00	0.00	H
ATOM	165	H37	OCT	X	4	16.519	23.375	29.484	1.00	0.00	H
ATOM	166	H38	OCT	X	4	20.874	23.351	29.532	1.00	0.00	H
ATOM	167	H39	OCT	X	4	12.070	19.371	33.194	1.00	0.00	H
ATOM	168	H40	OCT	X	4	13.575	16.829	30.076	1.00	0.00	H
ATOM	169	H41	OCT	X	4	13.172	21.122	29.568	1.00	0.00	H
ATOM	170	H42	OCT	X	4	17.608	12.865	33.928	1.00	0.00	H
ATOM	171	H43	OCT	X	4	15.908	13.741	30.098	1.00	0.00	H
ATOM	172	H44	OCT	X	4	20.180	14.010	30.688	1.00	0.00	H
ATOM	173	H45	OCT	X	4	14.682	26.090	30.462	1.00	0.00	H
ATOM	174	H46	OCT	X	4	14.998	22.411	32.523	1.00	0.00	H
ATOM	175	H47	OCT	X	4	11.277	23.588	30.634	1.00	0.00	H
ATOM	176	H48	OCT	X	4	22.681	25.454	30.052	1.00	0.00	H
ATOM	177	H49	OCT	X	4	25.455	22.290	30.769	1.00	0.00	H
ATOM	178	H50	OCT	X	4	21.888	22.453	33.090	1.00	0.00	H
ATOM	179	H51	OCT	X	4	13.462	11.967	31.372	1.00	0.00	H
ATOM	180	H52	OCT	X	4	10.928	15.436	31.463	1.00	0.00	H
ATOM	181	H53	OCT	X	4	14.877	15.563	33.233	1.00	0.00	H
ATOM	182	H54	OCT	X	4	21.365	11.797	31.534	1.00	0.00	H
ATOM	183	H55	OCT	X	4	21.641	15.469	33.563	1.00	0.00	H
ATOM	184	H56	OCT	X	4	24.846	14.239	31.000	1.00	0.00	H
ATOM	185	C1	MOL	X	5	18.980	17.011	31.984	1.00	0.00	C
ATOM	186	C2	MOL	X	5	20.031	17.958	32.694	1.00	0.00	C
ATOM	187	C3	MOL	X	5	17.813	17.989	31.622	1.00	0.00	C
ATOM	188	C4	MOL	X	5	17.232	18.508	32.940	1.00	0.00	C
ATOM	189	C5	MOL	X	5	19.482	18.605	33.988	1.00	0.00	C
ATOM	190	C6	MOL	X	5	18.217	19.482	33.603	1.00	0.00	C
ATOM	191	C7	MOL	X	5	18.656	20.591	32.564	1.00	0.00	C
ATOM	192	C8	MOL	X	5	20.567	19.061	31.764	1.00	0.00	C
ATOM	193	C9	MOL	X	5	18.334	19.110	30.627	1.00	0.00	C
ATOM	194	C10	MOL	X	5	19.380	19.994	31.306	1.00	0.00	C
ATOM	195	C11	MOL	X	5	17.683	20.127	34.842	1.00	0.00	C

ATOM	196	O1	MOL	X	5	16.821	19.573	35.517	1.00	0.00	O
ATOM	197	O2	MOL	X	5	18.210	21.109	35.271	1.00	0.00	O
ATOM	198	Br1	MOL	X	5	16.838	20.116	29.817	1.00	0.00	BR
ATOM	199	H1	MOL	X	5	18.661	16.139	32.558	1.00	0.00	H
ATOM	200	H2	MOL	X	5	19.450	16.549	31.114	1.00	0.00	H
ATOM	201	H3	MOL	X	5	20.889	17.347	32.984	1.00	0.00	H
ATOM	202	H4	MOL	X	5	16.971	17.476	31.153	1.00	0.00	H
ATOM	203	H5	MOL	X	5	16.873	17.672	33.546	1.00	0.00	H
ATOM	204	H6	MOL	X	5	16.334	19.077	32.689	1.00	0.00	H
ATOM	205	H7	MOL	X	5	20.272	19.157	34.502	1.00	0.00	H
ATOM	206	H8	MOL	X	5	19.193	17.810	34.680	1.00	0.00	H
ATOM	207	H9	MOL	X	5	17.799	21.213	32.296	1.00	0.00	H
ATOM	208	H10	MOL	X	5	19.337	21.306	33.031	1.00	0.00	H
ATOM	209	H11	MOL	X	5	21.038	18.617	30.885	1.00	0.00	H
ATOM	210	H12	MOL	X	5	21.381	19.633	32.215	1.00	0.00	H
ATOM	211	H13	MOL	X	5	18.791	18.674	29.735	1.00	0.00	H
ATOM	212	H14	MOL	X	5	19.739	20.719	30.573	1.00	0.00	H
END											

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ATOM	1	C1	OCT	X	4	21.441	24.515	30.050	1.00	0.00	C
ATOM	2	C2	OCT	X	4	23.564	23.153	31.210	1.00	0.00	C
ATOM	3	C3	OCT	X	4	22.079	23.419	29.446	1.00	0.00	C
ATOM	4	C4	OCT	X	4	21.922	24.845	31.310	1.00	0.00	C
ATOM	5	C5	OCT	X	4	22.909	24.154	31.938	1.00	0.00	C
ATOM	6	C6	OCT	X	4	23.076	22.709	30.001	1.00	0.00	C
ATOM	7	O1	OCT	X	4	24.556	22.443	31.866	1.00	0.00	O
ATOM	8	C7	OCT	X	4	23.657	21.439	29.405	1.00	0.00	C
ATOM	9	C8	OCT	X	4	24.173	21.233	32.624	1.00	0.00	C
ATOM	10	O2	OCT	X	4	24.431	20.044	31.923	1.00	0.00	O
ATOM	11	C9	OCT	X	4	23.454	19.619	31.107	1.00	0.00	C
ATOM	12	C10	OCT	X	4	22.927	20.246	29.947	1.00	0.00	C
ATOM	13	C11	OCT	X	4	21.758	19.702	29.358	1.00	0.00	C
ATOM	14	C12	OCT	X	4	22.707	18.594	31.711	1.00	0.00	C
ATOM	15	C13	OCT	X	4	21.059	18.702	29.957	1.00	0.00	C
ATOM	16	C14	OCT	X	4	21.501	18.104	31.125	1.00	0.00	C
ATOM	17	O3	OCT	X	4	20.774	17.162	31.823	1.00	0.00	O
ATOM	18	C15	OCT	X	4	19.861	18.084	29.275	1.00	0.00	C
ATOM	19	C16	OCT	X	4	18.608	18.799	29.783	1.00	0.00	C
ATOM	20	C17	OCT	X	4	18.001	18.436	31.011	1.00	0.00	C
ATOM	21	C18	OCT	X	4	19.644	17.638	32.507	1.00	0.00	C
ATOM	22	O4	OCT	X	4	18.457	17.361	31.751	1.00	0.00	O
ATOM	23	O5	OCT	X	4	21.418	25.909	31.981	1.00	0.00	O
ATOM	24	C19	OCT	X	4	20.329	25.254	29.247	1.00	0.00	C
ATOM	25	C20	OCT	X	4	18.934	24.729	29.671	1.00	0.00	C
ATOM	26	O6	OCT	X	4	19.122	26.255	31.537	1.00	0.00	O
ATOM	27	C21	OCT	X	4	18.426	25.288	30.799	1.00	0.00	C
ATOM	28	C22	OCT	X	4	16.844	19.094	31.479	1.00	0.00	C
ATOM	29	C23	OCT	X	4	16.377	20.172	30.786	1.00	0.00	C
ATOM	30	C24	OCT	X	4	17.262	24.818	31.341	1.00	0.00	C
ATOM	31	C25	OCT	X	4	16.629	23.760	30.729	1.00	0.00	C
ATOM	32	O7	OCT	X	4	15.316	20.896	31.314	1.00	0.00	O
ATOM	33	O8	OCT	X	4	15.502	23.218	31.312	1.00	0.00	O
ATOM	34	C26	OCT	X	4	15.742	22.031	32.111	1.00	0.00	C
ATOM	35	C27	OCT	X	4	18.339	23.585	29.072	1.00	0.00	C
ATOM	36	C28	OCT	X	4	17.176	23.133	29.582	1.00	0.00	C
ATOM	37	C29	OCT	X	4	18.187	19.932	29.102	1.00	0.00	C

ATOM	38	C30	OCT	X	4	16.523	21.876	28.911	1.00	0.00	C
ATOM	39	C31	OCT	X	4	17.041	20.589	29.572	1.00	0.00	C
ATOM	40	C32	OCT	X	4	20.096	25.800	32.529	1.00	0.00	C
ATOM	41	C33	OCT	X	4	19.775	17.972	27.668	1.00	0.00	C
ATOM	42	C34	OCT	X	4	20.444	16.671	27.134	1.00	0.00	C
ATOM	43	C35	OCT	X	4	20.288	16.549	25.620	1.00	0.00	C
ATOM	44	O9	OCT	X	4	21.210	16.881	24.903	1.00	0.00	O
ATOM	45	C36	OCT	X	4	23.802	21.497	27.849	1.00	0.00	C
ATOM	46	C37	OCT	X	4	24.848	22.533	27.406	1.00	0.00	C
ATOM	47	C38	OCT	X	4	25.081	22.348	25.872	1.00	0.00	C
ATOM	48	O10	OCT	X	4	25.810	21.509	25.370	1.00	0.00	O
ATOM	49	C39	OCT	X	4	20.571	25.387	27.718	1.00	0.00	C
ATOM	50	C40	OCT	X	4	19.777	26.536	27.178	1.00	0.00	C
ATOM	51	C41	OCT	X	4	19.778	26.523	25.650	1.00	0.00	C
ATOM	52	O11	OCT	X	4	20.792	26.257	25.059	1.00	0.00	O
ATOM	53	C42	OCT	X	4	16.587	21.811	27.381	1.00	0.00	C
ATOM	54	C43	OCT	X	4	15.451	22.605	26.738	1.00	0.00	C
ATOM	55	C44	OCT	X	4	15.647	22.350	25.288	1.00	0.00	C
ATOM	56	O12	OCT	X	4	16.083	23.283	24.706	1.00	0.00	O
ATOM	57	C45	OCT	X	4	24.748	21.171	34.011	1.00	0.00	C
ATOM	58	C46	OCT	X	4	25.316	21.119	36.765	1.00	0.00	C
ATOM	59	C47	OCT	X	4	24.869	19.926	34.668	1.00	0.00	C
ATOM	60	C48	OCT	X	4	24.877	22.400	34.726	1.00	0.00	C
ATOM	61	C49	OCT	X	4	25.138	22.357	36.077	1.00	0.00	C
ATOM	62	C50	OCT	X	4	25.135	19.941	36.083	1.00	0.00	C
ATOM	63	C51	OCT	X	4	20.014	26.565	33.831	1.00	0.00	C
ATOM	64	C52	OCT	X	4	19.716	27.385	36.481	1.00	0.00	C
ATOM	65	C53	OCT	X	4	18.716	26.888	34.296	1.00	0.00	C
ATOM	66	C54	OCT	X	4	21.116	26.548	34.689	1.00	0.00	C
ATOM	67	C55	OCT	X	4	20.953	26.988	35.989	1.00	0.00	C
ATOM	68	C56	OCT	X	4	18.601	27.314	35.596	1.00	0.00	C
ATOM	69	C57	OCT	X	4	14.937	22.053	33.411	1.00	0.00	C
ATOM	70	C58	OCT	X	4	13.695	22.232	35.832	1.00	0.00	C
ATOM	71	C59	OCT	X	4	14.559	20.878	34.058	1.00	0.00	C
ATOM	72	C60	OCT	X	4	14.546	23.283	33.963	1.00	0.00	C
ATOM	73	C61	OCT	X	4	13.998	23.368	35.208	1.00	0.00	C
ATOM	74	C62	OCT	X	4	13.991	20.971	35.395	1.00	0.00	C
ATOM	75	C63	OCT	X	4	19.441	17.126	33.927	1.00	0.00	C
ATOM	76	C64	OCT	X	4	19.136	16.086	36.486	1.00	0.00	C
ATOM	77	C65	OCT	X	4	18.165	16.836	34.429	1.00	0.00	C
ATOM	78	C66	OCT	X	4	20.565	16.717	34.638	1.00	0.00	C
ATOM	79	C67	OCT	X	4	20.429	16.196	35.915	1.00	0.00	C
ATOM	80	C68	OCT	X	4	18.002	16.407	35.749	1.00	0.00	C
ATOM	81	O13	OCT	X	4	21.912	26.965	36.945	1.00	0.00	O
ATOM	82	O14	OCT	X	4	13.587	24.610	35.736	1.00	0.00	O
ATOM	83	O15	OCT	X	4	13.620	19.843	36.145	1.00	0.00	O
ATOM	84	O16	OCT	X	4	25.269	23.521	36.833	1.00	0.00	O
ATOM	85	O17	OCT	X	4	25.240	18.738	36.792	1.00	0.00	O
ATOM	86	O18	OCT	X	4	16.775	16.419	36.398	1.00	0.00	O
ATOM	87	O19	OCT	X	4	21.524	15.691	36.622	1.00	0.00	O
ATOM	88	C69	OCT	X	4	14.194	25.824	35.472	1.00	0.00	C
ATOM	89	C70	OCT	X	4	15.383	28.377	34.983	1.00	0.00	C
ATOM	90	C71	OCT	X	4	15.527	26.040	35.779	1.00	0.00	C
ATOM	91	C72	OCT	X	4	13.484	26.876	34.831	1.00	0.00	C
ATOM	92	C73	OCT	X	4	14.059	28.123	34.600	1.00	0.00	C
ATOM	93	C74	OCT	X	4	16.092	27.305	35.629	1.00	0.00	C
ATOM	94	O20	OCT	X	4	17.355	27.553	36.117	1.00	0.00	O
ATOM	95	C75	OCT	X	4	24.854	24.794	36.641	1.00	0.00	C
ATOM	96	C76	OCT	X	4	24.077	27.411	36.102	1.00	0.00	C
ATOM	97	C77	OCT	X	4	25.784	25.652	36.112	1.00	0.00	C

ATOM	98	C78	OCT	X	4	23.575	25.222	36.909	1.00	0.00	C
ATOM	99	C79	OCT	X	4	23.185	26.542	36.675	1.00	0.00	C
ATOM	100	C80	OCT	X	4	25.371	26.954	35.776	1.00	0.00	C
ATOM	101	C81	OCT	X	4	13.980	18.603	35.702	1.00	0.00	C
ATOM	102	C82	OCT	X	4	14.900	16.060	35.072	1.00	0.00	C
ATOM	103	C83	OCT	X	4	13.129	17.802	34.933	1.00	0.00	C
ATOM	104	C84	OCT	X	4	15.271	18.262	36.086	1.00	0.00	C
ATOM	105	C85	OCT	X	4	15.658	16.938	35.830	1.00	0.00	C
ATOM	106	C86	OCT	X	4	13.644	16.520	34.596	1.00	0.00	C
ATOM	107	C87	OCT	X	4	12.753	15.521	34.005	1.00	0.00	C
ATOM	108	O21	OCT	X	4	11.873	15.901	33.240	1.00	0.00	O
ATOM	109	C88	OCT	X	4	25.950	14.361	34.844	1.00	0.00	C
ATOM	110	O22	OCT	X	4	27.102	14.545	34.565	1.00	0.00	O
ATOM	111	C89	OCT	X	4	26.335	27.945	35.235	1.00	0.00	C
ATOM	112	O23	OCT	X	4	27.470	27.667	34.901	1.00	0.00	O
ATOM	113	O24	OCT	X	4	19.244	16.053	25.197	1.00	0.00	O
ATOM	114	O25	OCT	X	4	15.545	21.254	24.818	1.00	0.00	O
ATOM	115	O26	OCT	X	4	18.730	26.491	25.004	1.00	0.00	O
ATOM	116	C90	OCT	X	4	13.252	29.255	33.987	1.00	0.00	C
ATOM	117	O27	OCT	X	4	12.067	29.093	33.693	1.00	0.00	O
ATOM	118	O28	OCT	X	4	25.604	13.208	34.856	1.00	0.00	O
ATOM	119	O29	OCT	X	4	13.072	14.332	34.008	1.00	0.00	O
ATOM	120	O30	OCT	X	4	13.753	30.334	33.819	1.00	0.00	O
ATOM	121	O31	OCT	X	4	25.939	29.091	35.075	1.00	0.00	O
ATOM	122	O32	OCT	X	4	24.637	23.270	25.195	1.00	0.00	O
ATOM	123	C91	OCT	X	4	24.713	17.513	36.449	1.00	0.00	C
ATOM	124	C92	OCT	X	4	23.654	15.105	35.602	1.00	0.00	C
ATOM	125	C93	OCT	X	4	23.452	17.127	36.848	1.00	0.00	C
ATOM	126	C94	OCT	X	4	25.534	16.622	35.695	1.00	0.00	C
ATOM	127	C95	OCT	X	4	25.003	15.374	35.386	1.00	0.00	C
ATOM	128	C96	OCT	X	4	22.850	16.034	36.298	1.00	0.00	C
ATOM	129	H1	OCT	X	4	21.690	22.946	28.548	1.00	0.00	H
ATOM	130	H2	OCT	X	4	23.259	24.396	32.939	1.00	0.00	H
ATOM	131	H3	OCT	X	4	24.685	21.419	29.775	1.00	0.00	H
ATOM	132	H4	OCT	X	4	23.099	21.255	32.862	1.00	0.00	H
ATOM	133	H5	OCT	X	4	21.276	20.142	28.489	1.00	0.00	H
ATOM	134	H6	OCT	X	4	23.075	18.142	32.629	1.00	0.00	H
ATOM	135	H7	OCT	X	4	19.691	17.071	29.645	1.00	0.00	H
ATOM	136	H8	OCT	X	4	19.859	18.708	32.648	1.00	0.00	H
ATOM	137	H9	OCT	X	4	20.481	26.302	29.514	1.00	0.00	H
ATOM	138	H10	OCT	X	4	16.249	18.712	32.305	1.00	0.00	H
ATOM	139	H11	OCT	X	4	16.750	25.274	32.184	1.00	0.00	H
ATOM	140	H12	OCT	X	4	16.812	21.941	32.348	1.00	0.00	H
ATOM	141	H13	OCT	X	4	18.899	23.154	28.246	1.00	0.00	H
ATOM	142	H14	OCT	X	4	18.606	20.279	28.161	1.00	0.00	H
ATOM	143	H15	OCT	X	4	15.460	21.910	29.157	1.00	0.00	H
ATOM	144	H16	OCT	X	4	19.812	24.751	32.702	1.00	0.00	H
ATOM	145	H17	OCT	X	4	18.698	17.991	27.487	1.00	0.00	H
ATOM	146	H18	OCT	X	4	20.231	18.819	27.149	1.00	0.00	H
ATOM	147	H19	OCT	X	4	21.509	16.811	27.331	1.00	0.00	H
ATOM	148	H20	OCT	X	4	20.099	15.756	27.620	1.00	0.00	H
ATOM	149	H21	OCT	X	4	22.906	21.840	27.327	1.00	0.00	H
ATOM	150	H22	OCT	X	4	23.914	20.497	27.426	1.00	0.00	H
ATOM	151	H23	OCT	X	4	24.532	23.564	27.580	1.00	0.00	H
ATOM	152	H24	OCT	X	4	25.747	22.439	28.020	1.00	0.00	H
ATOM	153	H25	OCT	X	4	21.606	25.582	27.431	1.00	0.00	H
ATOM	154	H26	OCT	X	4	20.341	24.453	27.201	1.00	0.00	H
ATOM	155	H27	OCT	X	4	18.766	26.413	27.571	1.00	0.00	H
ATOM	156	H28	OCT	X	4	20.220	27.490	27.473	1.00	0.00	H
ATOM	157	H29	OCT	X	4	17.426	22.326	26.907	1.00	0.00	H

ATOM	158	H30	OCT	X	4	16.588	20.762	27.077	1.00	0.00	H
ATOM	159	H31	OCT	X	4	14.557	22.170	27.190	1.00	0.00	H
ATOM	160	H32	OCT	X	4	15.678	23.637	27.016	1.00	0.00	H
ATOM	161	H33	OCT	X	4	25.619	21.149	37.808	1.00	0.00	H
ATOM	162	H34	OCT	X	4	24.694	18.956	34.209	1.00	0.00	H
ATOM	163	H35	OCT	X	4	24.820	23.369	34.237	1.00	0.00	H
ATOM	164	H36	OCT	X	4	19.664	27.807	37.481	1.00	0.00	H
ATOM	165	H37	OCT	X	4	17.825	26.812	33.678	1.00	0.00	H
ATOM	166	H38	OCT	X	4	22.095	26.135	34.459	1.00	0.00	H
ATOM	167	H39	OCT	X	4	13.237	22.242	36.818	1.00	0.00	H
ATOM	168	H40	OCT	X	4	14.817	19.903	33.653	1.00	0.00	H
ATOM	169	H41	OCT	X	4	14.962	24.209	33.574	1.00	0.00	H
ATOM	170	H42	OCT	X	4	18.950	15.663	37.470	1.00	0.00	H
ATOM	171	H43	OCT	X	4	17.264	17.117	33.891	1.00	0.00	H
ATOM	172	H44	OCT	X	4	21.526	16.864	34.151	1.00	0.00	H
ATOM	173	H45	OCT	X	4	15.806	29.377	34.929	1.00	0.00	H
ATOM	174	H46	OCT	X	4	15.945	25.190	36.312	1.00	0.00	H
ATOM	175	H47	OCT	X	4	12.457	26.727	34.506	1.00	0.00	H
ATOM	176	H48	OCT	X	4	23.740	28.362	35.698	1.00	0.00	H
ATOM	177	H49	OCT	X	4	26.792	25.322	35.876	1.00	0.00	H
ATOM	178	H50	OCT	X	4	22.922	24.473	37.349	1.00	0.00	H
ATOM	179	H51	OCT	X	4	15.192	15.042	34.828	1.00	0.00	H
ATOM	180	H52	OCT	X	4	12.161	18.122	34.559	1.00	0.00	H
ATOM	181	H53	OCT	X	4	15.876	18.846	36.775	1.00	0.00	H
ATOM	182	H54	OCT	X	4	23.229	14.190	35.197	1.00	0.00	H
ATOM	183	H55	OCT	X	4	22.807	17.807	37.399	1.00	0.00	H
ATOM	184	H56	OCT	X	4	26.562	16.902	35.482	1.00	0.00	H
ATOM	185	C1	MOL	X	5	19.188	21.198	33.018	1.00	0.00	C
ATOM	186	C2	MOL	X	5	18.619	20.462	34.079	1.00	0.00	C
ATOM	187	C3	MOL	X	5	19.095	20.662	35.345	1.00	0.00	C
ATOM	188	C4	MOL	X	5	20.264	21.485	35.524	1.00	0.00	C
ATOM	189	C5	MOL	X	5	20.909	22.077	34.434	1.00	0.00	C
ATOM	190	C6	MOL	X	5	20.375	21.923	33.180	1.00	0.00	C
ATOM	191	C7	MOL	X	5	20.857	21.585	36.964	1.00	0.00	C
ATOM	192	C8	MOL	X	5	19.770	21.927	38.090	1.00	0.00	C
ATOM	193	N1	MOL	X	5	20.269	22.143	39.498	1.00	0.00	N
ATOM	194	C9	MOL	X	5	19.119	22.465	40.475	1.00	0.00	C
ATOM	195	C10	MOL	X	5	21.321	23.167	39.571	1.00	0.00	C
ATOM	196	C11	MOL	X	5	20.899	20.944	40.047	1.00	0.00	C
ATOM	197	H1	MOL	X	5	18.313	21.761	40.259	1.00	0.00	H
ATOM	198	H2	MOL	X	5	18.811	23.496	40.294	1.00	0.00	H
ATOM	199	H3	MOL	X	5	19.529	22.422	41.485	1.00	0.00	H
ATOM	200	H4	MOL	X	5	22.084	22.958	38.820	1.00	0.00	H
ATOM	201	H5	MOL	X	5	21.729	23.283	40.576	1.00	0.00	H
ATOM	202	H6	MOL	X	5	20.944	24.126	39.212	1.00	0.00	H
ATOM	203	H7	MOL	X	5	20.227	20.092	39.936	1.00	0.00	H
ATOM	204	H8	MOL	X	5	21.780	20.797	39.421	1.00	0.00	H
ATOM	205	H9	MOL	X	5	21.115	21.192	41.087	1.00	0.00	H
ATOM	206	H10	MOL	X	5	18.822	20.979	32.019	1.00	0.00	H
ATOM	207	H11	MOL	X	5	17.750	19.825	33.931	1.00	0.00	H
ATOM	208	H12	MOL	X	5	18.647	20.287	36.262	1.00	0.00	H
ATOM	209	H13	MOL	X	5	21.846	22.578	34.664	1.00	0.00	H
ATOM	210	H14	MOL	X	5	20.892	22.381	32.341	1.00	0.00	H
ATOM	211	H15	MOL	X	5	21.450	20.705	37.220	1.00	0.00	H
ATOM	212	H16	MOL	X	5	21.497	22.469	36.925	1.00	0.00	H
ATOM	213	H17	MOL	X	5	19.336	22.885	37.798	1.00	0.00	H
ATOM	214	H18	MOL	X	5	19.063	21.098	38.140	1.00	0.00	H
END											

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ATOM	1	C1	OCT	X	4	21.338	25.277	30.071	1.00	0.00	C
ATOM	2	C2	OCT	X	4	23.253	23.789	31.436	1.00	0.00	C
ATOM	3	C3	OCT	X	4	22.016	24.231	29.411	1.00	0.00	C
ATOM	4	C4	OCT	X	4	21.639	25.604	31.394	1.00	0.00	C
ATOM	5	C5	OCT	X	4	22.621	24.829	32.042	1.00	0.00	C
ATOM	6	C6	OCT	X	4	22.951	23.448	30.123	1.00	0.00	C
ATOM	7	O1	OCT	X	4	24.225	23.131	32.171	1.00	0.00	O
ATOM	8	C7	OCT	X	4	23.626	22.196	29.497	1.00	0.00	C
ATOM	9	C8	OCT	X	4	23.742	21.906	32.783	1.00	0.00	C
ATOM	10	O2	OCT	X	4	24.320	20.845	31.954	1.00	0.00	O
ATOM	11	C9	OCT	X	4	23.419	20.224	31.104	1.00	0.00	C
ATOM	12	C10	OCT	X	4	22.963	20.893	29.904	1.00	0.00	C
ATOM	13	C11	OCT	X	4	22.001	20.229	29.167	1.00	0.00	C
ATOM	14	C12	OCT	X	4	22.840	19.068	31.525	1.00	0.00	C
ATOM	15	C13	OCT	X	4	21.354	19.074	29.614	1.00	0.00	C
ATOM	16	C14	OCT	X	4	21.709	18.537	30.815	1.00	0.00	C
ATOM	17	O3	OCT	X	4	20.973	17.420	31.368	1.00	0.00	O
ATOM	18	C15	OCT	X	4	20.041	18.738	28.884	1.00	0.00	C
ATOM	19	C16	OCT	X	4	18.869	19.417	29.503	1.00	0.00	C
ATOM	20	C17	OCT	X	4	18.261	18.877	30.648	1.00	0.00	C
ATOM	21	C18	OCT	X	4	19.847	17.816	32.098	1.00	0.00	C
ATOM	22	O4	OCT	X	4	18.651	17.707	31.240	1.00	0.00	O
ATOM	23	O5	OCT	X	4	21.054	26.607	32.133	1.00	0.00	O
ATOM	24	C19	OCT	X	4	20.254	26.077	29.320	1.00	0.00	C
ATOM	25	C20	OCT	X	4	18.919	25.478	29.707	1.00	0.00	C
ATOM	26	O6	OCT	X	4	18.794	27.071	31.618	1.00	0.00	O
ATOM	27	C21	OCT	X	4	18.195	26.103	30.772	1.00	0.00	C
ATOM	28	C22	OCT	X	4	17.364	19.655	31.375	1.00	0.00	C
ATOM	29	C23	OCT	X	4	16.847	20.793	30.773	1.00	0.00	C
ATOM	30	C24	OCT	X	4	16.986	25.545	31.258	1.00	0.00	C
ATOM	31	C25	OCT	X	4	16.581	24.282	30.717	1.00	0.00	C
ATOM	32	O7	OCT	X	4	15.747	21.263	31.361	1.00	0.00	O
ATOM	33	O8	OCT	X	4	15.451	23.665	31.291	1.00	0.00	O
ATOM	34	C26	OCT	X	4	15.817	22.534	32.109	1.00	0.00	C
ATOM	35	C27	OCT	X	4	18.454	24.360	29.049	1.00	0.00	C
ATOM	36	C28	OCT	X	4	17.274	23.753	29.547	1.00	0.00	C
ATOM	37	C29	OCT	X	4	18.443	20.622	28.985	1.00	0.00	C
ATOM	38	C30	OCT	X	4	16.716	22.497	28.930	1.00	0.00	C
ATOM	39	C31	OCT	X	4	17.357	21.275	29.607	1.00	0.00	C
ATOM	40	C32	OCT	X	4	19.671	26.441	32.558	1.00	0.00	C
ATOM	41	C33	OCT	X	4	20.179	18.495	27.377	1.00	0.00	C
ATOM	42	C34	OCT	X	4	20.999	17.252	26.997	1.00	0.00	C
ATOM	43	C35	OCT	X	4	21.107	17.180	25.504	1.00	0.00	C
ATOM	44	O9	OCT	X	4	21.829	17.874	24.866	1.00	0.00	O
ATOM	45	C36	OCT	X	4	23.818	22.355	27.987	1.00	0.00	C
ATOM	46	C37	OCT	X	4	24.888	21.373	27.376	1.00	0.00	C
ATOM	47	C38	OCT	X	4	24.976	21.523	25.955	1.00	0.00	C
ATOM	48	O10	OCT	X	4	25.863	22.200	25.470	1.00	0.00	O
ATOM	49	C39	OCT	X	4	20.294	26.360	27.784	1.00	0.00	C
ATOM	50	C40	OCT	X	4	19.270	27.433	27.426	1.00	0.00	C
ATOM	51	C41	OCT	X	4	19.384	27.823	25.966	1.00	0.00	C
ATOM	52	O11	OCT	X	4	20.438	28.151	25.489	1.00	0.00	O
ATOM	53	C42	OCT	X	4	16.683	22.440	27.346	1.00	0.00	C
ATOM	54	C43	OCT	X	4	15.817	23.523	26.665	1.00	0.00	C
ATOM	55	C44	OCT	X	4	15.980	23.527	25.162	1.00	0.00	C
ATOM	56	O12	OCT	X	4	15.933	24.532	24.497	1.00	0.00	O
ATOM	57	C45	OCT	X	4	24.233	21.796	34.237	1.00	0.00	C
ATOM	58	C46	OCT	X	4	24.891	21.606	37.012	1.00	0.00	C

ATOM	59	C47	OCT	X	4	24.063	20.591	34.908	1.00	0.00	C
ATOM	60	C48	OCT	X	4	24.586	22.963	34.956	1.00	0.00	C
ATOM	61	C49	OCT	X	4	24.877	22.870	36.393	1.00	0.00	C
ATOM	62	C50	OCT	X	4	24.522	20.504	36.230	1.00	0.00	C
ATOM	63	C51	OCT	X	4	19.477	27.017	33.944	1.00	0.00	C
ATOM	64	C52	OCT	X	4	19.133	27.710	36.593	1.00	0.00	C
ATOM	65	C53	OCT	X	4	18.276	27.597	34.365	1.00	0.00	C
ATOM	66	C54	OCT	X	4	20.528	26.728	34.918	1.00	0.00	C
ATOM	67	C55	OCT	X	4	20.284	27.081	36.226	1.00	0.00	C
ATOM	68	C56	OCT	X	4	18.145	27.970	35.661	1.00	0.00	C
ATOM	69	C57	OCT	X	4	15.087	22.437	33.465	1.00	0.00	C
ATOM	70	C58	OCT	X	4	13.946	22.223	36.065	1.00	0.00	C
ATOM	71	C59	OCT	X	4	14.657	21.155	33.994	1.00	0.00	C
ATOM	72	C60	OCT	X	4	14.840	23.627	34.195	1.00	0.00	C
ATOM	73	C61	OCT	X	4	14.288	23.456	35.497	1.00	0.00	C
ATOM	74	C62	OCT	X	4	14.107	21.075	35.292	1.00	0.00	C
ATOM	75	C63	OCT	X	4	19.666	16.941	33.295	1.00	0.00	C
ATOM	76	C64	OCT	X	4	19.383	15.910	35.870	1.00	0.00	C
ATOM	77	C65	OCT	X	4	18.440	16.989	33.916	1.00	0.00	C
ATOM	78	C66	OCT	X	4	20.728	16.375	33.915	1.00	0.00	C
ATOM	79	C67	OCT	X	4	20.637	15.805	35.206	1.00	0.00	C
ATOM	80	C68	OCT	X	4	18.299	16.430	35.213	1.00	0.00	C
ATOM	81	O13	OCT	X	4	21.129	26.671	37.274	1.00	0.00	O
ATOM	82	O14	OCT	X	4	14.040	24.527	36.270	1.00	0.00	O
ATOM	83	O15	OCT	X	4	13.872	19.892	35.896	1.00	0.00	O
ATOM	84	O16	OCT	X	4	25.136	23.958	37.213	1.00	0.00	O
ATOM	85	O17	OCT	X	4	24.324	19.282	36.960	1.00	0.00	O
ATOM	86	O18	OCT	X	4	17.136	16.519	35.951	1.00	0.00	O
ATOM	87	O19	OCT	X	4	21.784	15.358	35.959	1.00	0.00	O
ATOM	88	C69	OCT	X	4	14.331	25.841	35.938	1.00	0.00	C
ATOM	89	C70	OCT	X	4	14.709	28.501	35.249	1.00	0.00	C
ATOM	90	C71	OCT	X	4	15.521	26.445	36.263	1.00	0.00	C
ATOM	91	C72	OCT	X	4	13.332	26.518	35.310	1.00	0.00	C
ATOM	92	C73	OCT	X	4	13.544	27.788	34.920	1.00	0.00	C
ATOM	93	C74	OCT	X	4	15.698	27.776	35.850	1.00	0.00	C
ATOM	94	O20	OCT	X	4	16.869	28.443	36.101	1.00	0.00	O
ATOM	95	C75	OCT	X	4	24.557	25.169	36.964	1.00	0.00	C
ATOM	96	C76	OCT	X	4	23.249	27.606	36.771	1.00	0.00	C
ATOM	97	C77	OCT	X	4	25.265	26.297	36.680	1.00	0.00	C
ATOM	98	C78	OCT	X	4	23.139	25.255	37.216	1.00	0.00	C
ATOM	99	C79	OCT	X	4	22.501	26.512	37.141	1.00	0.00	C
ATOM	100	C80	OCT	X	4	24.644	27.552	36.580	1.00	0.00	C
ATOM	101	C81	OCT	X	4	14.309	18.703	35.424	1.00	0.00	C
ATOM	102	C82	OCT	X	4	15.222	16.259	34.525	1.00	0.00	C
ATOM	103	C83	OCT	X	4	13.574	17.947	34.519	1.00	0.00	C
ATOM	104	C84	OCT	X	4	15.504	18.216	35.916	1.00	0.00	C
ATOM	105	C85	OCT	X	4	15.991	17.024	35.396	1.00	0.00	C
ATOM	106	C86	OCT	X	4	13.953	16.655	34.072	1.00	0.00	C
ATOM	107	C87	OCT	X	4	13.100	15.858	33.112	1.00	0.00	C
ATOM	108	O21	OCT	X	4	12.143	16.322	32.587	1.00	0.00	O
ATOM	109	C88	OCT	X	4	26.654	15.271	35.335	1.00	0.00	C
ATOM	110	O22	OCT	X	4	26.698	14.066	35.407	1.00	0.00	O
ATOM	111	C89	OCT	X	4	25.451	28.768	36.148	1.00	0.00	C
ATOM	112	O23	OCT	X	4	26.640	28.609	35.887	1.00	0.00	O
ATOM	113	O24	OCT	X	4	20.532	16.331	24.807	1.00	0.00	O
ATOM	114	O25	OCT	X	4	16.169	22.472	24.600	1.00	0.00	O
ATOM	115	O26	OCT	X	4	18.424	27.836	25.215	1.00	0.00	O
ATOM	116	C90	OCT	X	4	12.458	28.440	34.088	1.00	0.00	C
ATOM	117	O27	OCT	X	4	12.487	29.622	33.932	1.00	0.00	O
ATOM	118	O28	OCT	X	4	27.625	15.955	35.029	1.00	0.00	O

ATOM	119	O29	OCT	X	4	13.347	14.622	33.043	1.00	0.00	O
ATOM	120	O30	OCT	X	4	11.531	27.785	33.668	1.00	0.00	O
ATOM	121	O31	OCT	X	4	25.035	29.904	35.968	1.00	0.00	O
ATOM	122	O32	OCT	X	4	24.496	20.648	25.272	1.00	0.00	O
ATOM	123	C91	OCT	X	4	24.250	18.003	36.427	1.00	0.00	C
ATOM	124	C92	OCT	X	4	24.123	15.348	35.578	1.00	0.00	C
ATOM	125	C93	OCT	X	4	23.006	17.357	36.337	1.00	0.00	C
ATOM	126	C94	OCT	X	4	25.444	17.343	36.052	1.00	0.00	C
ATOM	127	C95	OCT	X	4	25.362	16.001	35.628	1.00	0.00	C
ATOM	128	C96	OCT	X	4	22.942	15.999	35.912	1.00	0.00	C
ATOM	129	H1	OCT	X	4	21.765	23.965	28.387	1.00	0.00	H
ATOM	130	H2	OCT	X	4	22.881	24.954	33.089	1.00	0.00	H
ATOM	131	H3	OCT	X	4	24.671	22.105	29.801	1.00	0.00	H
ATOM	132	H4	OCT	X	4	22.643	21.875	32.794	1.00	0.00	H
ATOM	133	H5	OCT	X	4	21.623	20.730	28.279	1.00	0.00	H
ATOM	134	H6	OCT	X	4	23.276	18.470	32.321	1.00	0.00	H
ATOM	135	H7	OCT	X	4	19.723	17.734	29.173	1.00	0.00	H
ATOM	136	H8	OCT	X	4	19.984	18.871	32.380	1.00	0.00	H
ATOM	137	H9	OCT	X	4	20.323	27.131	29.598	1.00	0.00	H
ATOM	138	H10	OCT	X	4	16.883	19.344	32.299	1.00	0.00	H
ATOM	139	H11	OCT	X	4	16.398	26.031	32.032	1.00	0.00	H
ATOM	140	H12	OCT	X	4	16.887	22.688	32.317	1.00	0.00	H
ATOM	141	H13	OCT	X	4	19.054	23.875	28.284	1.00	0.00	H
ATOM	142	H14	OCT	X	4	18.999	21.093	28.178	1.00	0.00	H
ATOM	143	H15	OCT	X	4	15.648	22.528	29.157	1.00	0.00	H
ATOM	144	H16	OCT	X	4	19.382	25.389	32.699	1.00	0.00	H
ATOM	145	H17	OCT	X	4	19.185	18.337	26.953	1.00	0.00	H
ATOM	146	H18	OCT	X	4	20.625	19.349	26.864	1.00	0.00	H
ATOM	147	H19	OCT	X	4	21.994	17.322	27.440	1.00	0.00	H
ATOM	148	H20	OCT	X	4	20.580	16.312	27.363	1.00	0.00	H
ATOM	149	H21	OCT	X	4	24.180	23.370	27.813	1.00	0.00	H
ATOM	150	H22	OCT	X	4	22.890	22.395	27.413	1.00	0.00	H
ATOM	151	H23	OCT	X	4	25.836	21.744	27.772	1.00	0.00	H
ATOM	152	H24	OCT	X	4	24.847	20.299	27.570	1.00	0.00	H
ATOM	153	H25	OCT	X	4	21.313	26.694	27.575	1.00	0.00	H
ATOM	154	H26	OCT	X	4	20.160	25.467	27.170	1.00	0.00	H
ATOM	155	H27	OCT	X	4	18.299	26.974	27.624	1.00	0.00	H
ATOM	156	H28	OCT	X	4	19.432	28.311	28.056	1.00	0.00	H
ATOM	157	H29	OCT	X	4	17.678	22.522	26.903	1.00	0.00	H
ATOM	158	H30	OCT	X	4	16.352	21.434	27.081	1.00	0.00	H
ATOM	159	H31	OCT	X	4	14.796	23.333	27.001	1.00	0.00	H
ATOM	160	H32	OCT	X	4	16.168	24.519	26.945	1.00	0.00	H
ATOM	161	H33	OCT	X	4	25.245	21.413	38.022	1.00	0.00	H
ATOM	162	H34	OCT	X	4	23.556	19.728	34.483	1.00	0.00	H
ATOM	163	H35	OCT	X	4	24.614	23.928	34.457	1.00	0.00	H
ATOM	164	H36	OCT	X	4	19.143	28.054	37.624	1.00	0.00	H
ATOM	165	H37	OCT	X	4	17.405	27.747	33.731	1.00	0.00	H
ATOM	166	H38	OCT	X	4	21.472	26.251	34.670	1.00	0.00	H
ATOM	167	H39	OCT	X	4	13.630	22.095	37.097	1.00	0.00	H
ATOM	168	H40	OCT	X	4	14.869	20.268	33.402	1.00	0.00	H
ATOM	169	H41	OCT	X	4	15.118	24.627	33.871	1.00	0.00	H
ATOM	170	H42	OCT	X	4	19.323	15.404	36.830	1.00	0.00	H
ATOM	171	H43	OCT	X	4	17.604	17.477	33.420	1.00	0.00	H
ATOM	172	H44	OCT	X	4	21.709	16.400	33.447	1.00	0.00	H
ATOM	173	H45	OCT	X	4	14.781	29.542	34.942	1.00	0.00	H
ATOM	174	H46	OCT	X	4	16.308	25.907	36.786	1.00	0.00	H
ATOM	175	H47	OCT	X	4	12.337	26.105	35.168	1.00	0.00	H
ATOM	176	H48	OCT	X	4	22.688	28.501	36.515	1.00	0.00	H
ATOM	177	H49	OCT	X	4	26.349	26.295	36.593	1.00	0.00	H
ATOM	178	H50	OCT	X	4	22.579	24.378	37.531	1.00	0.00	H

ATOM	179	H51	OCT	X	4	15.691	15.319	34.243	1.00	0.00	H
ATOM	180	H52	OCT	X	4	12.719	18.456	34.081	1.00	0.00	H
ATOM	181	H53	OCT	X	4	16.136	18.760	36.613	1.00	0.00	H
ATOM	182	H54	OCT	X	4	24.040	14.335	35.193	1.00	0.00	H
ATOM	183	H55	OCT	X	4	22.089	17.812	36.703	1.00	0.00	H
ATOM	184	H56	OCT	X	4	26.386	17.826	36.298	1.00	0.00	H
ATOM	185	O1	MOL	X	5	20.220	22.861	33.191	1.00	0.00	O
ATOM	186	O2	MOL	X	5	21.274	23.790	34.761	1.00	0.00	O
ATOM	187	N1	MOL	X	5	20.471	22.983	34.372	1.00	0.00	N
ATOM	188	C1	MOL	X	5	19.698	22.175	35.254	1.00	0.00	C
ATOM	189	C2	MOL	X	5	19.684	22.413	36.643	1.00	0.00	C
ATOM	190	C3	MOL	X	5	19.004	21.085	34.772	1.00	0.00	C
ATOM	191	C4	MOL	X	5	18.872	21.632	37.507	1.00	0.00	C
ATOM	192	C5	MOL	X	5	18.281	20.312	35.674	1.00	0.00	C
ATOM	193	C6	MOL	X	5	18.164	20.573	36.983	1.00	0.00	C
ATOM	194	C7	MOL	X	5	18.952	21.861	38.982	1.00	0.00	C
ATOM	195	O3	MOL	X	5	19.500	22.889	39.351	1.00	0.00	O
ATOM	196	O4	MOL	X	5	18.301	21.199	39.739	1.00	0.00	O
ATOM	197	H1	MOL	X	5	20.367	23.161	37.038	1.00	0.00	H
ATOM	198	H2	MOL	X	5	19.106	20.783	33.733	1.00	0.00	H
ATOM	199	H3	MOL	X	5	17.802	19.416	35.289	1.00	0.00	H
ATOM	200	H4	MOL	X	5	17.669	19.824	37.595	1.00	0.00	H
END											

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ATOM	1	C1	OCB	X	4	22.023	24.482	31.447	1.00	0.00	C
ATOM	2	C2	OCB	X	4	24.185	23.068	32.525	1.00	0.00	C
ATOM	3	C3	OCB	X	4	22.578	23.376	30.799	1.00	0.00	C
ATOM	4	C4	OCB	X	4	22.563	24.822	32.696	1.00	0.00	C
ATOM	5	C5	OCB	X	4	23.635	24.129	33.208	1.00	0.00	C
ATOM	6	C6	OCB	X	4	23.662	22.640	31.265	1.00	0.00	C
ATOM	7	O1	OCB	X	4	25.191	22.424	33.090	1.00	0.00	O
ATOM	8	C7	OCB	X	4	24.207	21.322	30.669	1.00	0.00	C
ATOM	9	C8	OCB	X	4	24.860	21.107	33.733	1.00	0.00	C
ATOM	10	O2	OCB	X	4	25.224	19.919	32.946	1.00	0.00	O
ATOM	11	C9	OCB	X	4	24.139	19.418	32.294	1.00	0.00	C
ATOM	12	C10	OCB	X	4	23.589	20.078	31.239	1.00	0.00	C
ATOM	13	C11	OCB	X	4	22.456	19.533	30.681	1.00	0.00	C
ATOM	14	C12	OCB	X	4	23.562	18.300	32.855	1.00	0.00	C
ATOM	15	C13	OCB	X	4	21.796	18.462	31.216	1.00	0.00	C
ATOM	16	C14	OCB	X	4	22.345	17.865	32.357	1.00	0.00	C
ATOM	17	O3	OCB	X	4	21.807	16.784	32.950	1.00	0.00	O
ATOM	18	C15	OCB	X	4	20.504	17.874	30.641	1.00	0.00	C
ATOM	19	C16	OCB	X	4	19.323	18.466	31.438	1.00	0.00	C
ATOM	20	C17	OCB	X	4	18.854	17.979	32.624	1.00	0.00	C
ATOM	21	C18	OCB	X	4	20.829	17.186	33.910	1.00	0.00	C
ATOM	22	O4	OCB	X	4	19.515	16.971	33.363	1.00	0.00	O
ATOM	23	O5	OCB	X	4	22.004	25.861	33.486	1.00	0.00	O
ATOM	24	C19	OCB	X	4	20.757	25.185	30.911	1.00	0.00	C
ATOM	25	C20	OCB	X	4	19.487	24.655	31.574	1.00	0.00	C
ATOM	26	O6	OCB	X	4	19.732	26.098	33.524	1.00	0.00	O
ATOM	27	C21	OCB	X	4	19.068	25.136	32.832	1.00	0.00	C
ATOM	28	C22	OCB	X	4	17.827	18.528	33.304	1.00	0.00	C
ATOM	29	C23	OCB	X	4	17.271	19.714	32.813	1.00	0.00	C
ATOM	30	C24	OCB	X	4	18.066	24.455	33.589	1.00	0.00	C
ATOM	31	C25	OCB	X	4	17.509	23.287	33.055	1.00	0.00	C
ATOM	32	O7	OCB	X	4	16.354	20.336	33.586	1.00	0.00	O

ATOM	33	O8	OCB	X	4	16.400	22.741	33.700	1.00	0.00	O
ATOM	34	C26	OCB	X	4	16.750	21.462	34.419	1.00	0.00	C
ATOM	35	C27	OCB	X	4	18.783	23.573	31.020	1.00	0.00	C
ATOM	36	C28	OCB	X	4	17.867	22.847	31.743	1.00	0.00	C
ATOM	37	C29	OCB	X	4	18.726	19.643	30.952	1.00	0.00	C
ATOM	38	C30	OCB	X	4	17.131	21.648	31.142	1.00	0.00	C
ATOM	39	C31	OCB	X	4	17.751	20.360	31.686	1.00	0.00	C
ATOM	40	C32	OCB	X	4	20.845	25.613	34.300	1.00	0.00	C
ATOM	41	C33	OCB	X	4	20.354	17.819	29.155	1.00	0.00	C
ATOM	42	C34	OCB	X	4	21.322	16.913	28.466	1.00	0.00	C
ATOM	43	C35	OCB	X	4	21.232	16.910	26.968	1.00	0.00	C
ATOM	44	O9	OCB	X	4	21.747	17.729	26.274	1.00	0.00	O
ATOM	45	C36	OCB	X	4	24.268	21.211	29.103	1.00	0.00	C
ATOM	46	C37	OCB	X	4	25.185	22.301	28.489	1.00	0.00	C
ATOM	47	C38	OCB	X	4	25.328	22.131	26.996	1.00	0.00	C
ATOM	48	O10	OCB	X	4	25.113	23.024	26.228	1.00	0.00	O
ATOM	49	C39	OCB	X	4	20.629	25.258	29.335	1.00	0.00	C
ATOM	50	C40	OCB	X	4	21.652	26.320	28.718	1.00	0.00	C
ATOM	51	C41	OCB	X	4	21.413	26.410	27.220	1.00	0.00	C
ATOM	52	O11	OCB	X	4	21.123	25.395	26.623	1.00	0.00	O
ATOM	53	C42	OCB	X	4	16.861	21.585	29.604	1.00	0.00	C
ATOM	54	C43	OCB	X	4	15.593	22.420	29.213	1.00	0.00	C
ATOM	55	C44	OCB	X	4	15.176	22.093	27.791	1.00	0.00	C
ATOM	56	O12	OCB	X	4	15.875	21.382	27.129	1.00	0.00	O
ATOM	57	C45	OCB	X	4	25.737	21.100	35.007	1.00	0.00	C
ATOM	58	C46	OCB	X	4	26.784	21.091	37.656	1.00	0.00	C
ATOM	59	C47	OCB	X	4	25.905	19.901	35.768	1.00	0.00	C
ATOM	60	C48	OCB	X	4	26.064	22.284	35.720	1.00	0.00	C
ATOM	61	C49	OCB	X	4	26.560	22.305	37.044	1.00	0.00	C
ATOM	62	C50	OCB	X	4	26.523	19.904	37.058	1.00	0.00	C
ATOM	63	C51	OCB	X	4	21.048	26.131	35.710	1.00	0.00	C
ATOM	64	C52	OCB	X	4	21.301	27.351	38.196	1.00	0.00	C
ATOM	65	C53	OCB	X	4	19.949	26.617	36.415	1.00	0.00	C
ATOM	66	C54	OCB	X	4	22.263	26.228	36.315	1.00	0.00	C
ATOM	67	C55	OCB	X	4	22.409	26.839	37.551	1.00	0.00	C
ATOM	68	C56	OCB	X	4	20.066	27.095	37.696	1.00	0.00	C
ATOM	69	C57	OCB	X	4	16.158	21.563	35.746	1.00	0.00	C
ATOM	70	C58	OCB	X	4	15.543	21.508	38.479	1.00	0.00	C
ATOM	71	C59	OCB	X	4	15.955	20.329	36.401	1.00	0.00	C
ATOM	72	C60	OCB	X	4	15.972	22.745	36.461	1.00	0.00	C
ATOM	73	C61	OCB	X	4	15.662	22.720	37.816	1.00	0.00	C
ATOM	74	C62	OCB	X	4	15.672	20.338	37.782	1.00	0.00	C
ATOM	75	C63	OCB	X	4	20.888	16.532	35.271	1.00	0.00	C
ATOM	76	C64	OCB	X	4	20.911	15.306	37.800	1.00	0.00	C
ATOM	77	C65	OCB	X	4	19.716	16.247	35.982	1.00	0.00	C
ATOM	78	C66	OCB	X	4	22.069	16.174	35.833	1.00	0.00	C
ATOM	79	C67	OCB	X	4	22.112	15.631	37.120	1.00	0.00	C
ATOM	80	C68	OCB	X	4	19.723	15.633	37.244	1.00	0.00	C
ATOM	81	O13	OCB	X	4	23.613	27.056	38.268	1.00	0.00	O
ATOM	82	O14	OCB	X	4	15.577	23.898	38.579	1.00	0.00	O
ATOM	83	O15	OCB	X	4	15.642	19.144	38.488	1.00	0.00	O
ATOM	84	O16	OCB	X	4	26.845	23.602	37.606	1.00	0.00	O
ATOM	85	O17	OCB	X	4	26.717	18.738	37.745	1.00	0.00	O
ATOM	86	O18	OCB	X	4	18.575	15.244	37.997	1.00	0.00	O
ATOM	87	O19	OCB	X	4	23.277	15.300	37.744	1.00	0.00	O
ATOM	88	C69	OCB	X	4	16.078	25.146	38.184	1.00	0.00	C
ATOM	89	C70	OCB	X	4	16.873	27.676	37.226	1.00	0.00	C
ATOM	90	C71	OCB	X	4	17.362	25.612	38.455	1.00	0.00	C
ATOM	91	C72	OCB	X	4	15.192	25.899	37.358	1.00	0.00	C
ATOM	92	C73	OCB	X	4	15.633	27.092	36.829	1.00	0.00	C

ATOM	93	C74	OCB	X	4	17.696	26.912	38.064	1.00	0.00	C
ATOM	94	O20	OCB	X	4	18.922	27.444	38.362	1.00	0.00	O
ATOM	95	C75	OCB	X	4	26.435	24.881	37.380	1.00	0.00	C
ATOM	96	C76	OCB	X	4	25.600	27.512	37.085	1.00	0.00	C
ATOM	97	C77	OCB	X	4	27.091	25.778	36.512	1.00	0.00	C
ATOM	98	C78	OCB	X	4	25.213	25.310	37.987	1.00	0.00	C
ATOM	99	C79	OCB	X	4	24.755	26.617	37.796	1.00	0.00	C
ATOM	100	C80	OCB	X	4	26.745	27.149	36.363	1.00	0.00	C
ATOM	101	C81	OCB	X	4	15.945	17.901	37.985	1.00	0.00	C
ATOM	102	C82	OCB	X	4	16.366	15.214	37.141	1.00	0.00	C
ATOM	103	C83	OCB	X	4	14.976	17.155	37.300	1.00	0.00	C
ATOM	104	C84	OCB	X	4	17.192	17.312	38.204	1.00	0.00	C
ATOM	105	C85	OCB	X	4	17.382	15.974	37.764	1.00	0.00	C
ATOM	106	C86	OCB	X	4	15.115	15.821	36.893	1.00	0.00	C
ATOM	107	C87	OCB	X	4	14.013	14.948	36.317	1.00	0.00	C
ATOM	108	O21	OCB	X	4	12.844	15.151	36.650	1.00	0.00	O
ATOM	109	C88	OCB	X	4	27.313	14.704	34.953	1.00	0.00	C
ATOM	110	O22	OCB	X	4	27.026	13.560	34.743	1.00	0.00	O
ATOM	111	C89	OCB	X	4	27.504	28.087	35.439	1.00	0.00	C
ATOM	112	O23	OCB	X	4	27.045	29.127	35.099	1.00	0.00	O
ATOM	113	O24	OCB	X	4	20.661	15.929	26.507	1.00	0.00	O
ATOM	114	O25	OCB	X	4	14.276	22.800	27.242	1.00	0.00	O
ATOM	115	O26	OCB	X	4	21.459	27.481	26.638	1.00	0.00	O
ATOM	116	C90	OCB	X	4	14.809	27.772	35.828	1.00	0.00	C
ATOM	117	O27	OCB	X	4	14.990	28.964	35.587	1.00	0.00	O
ATOM	118	O28	OCB	X	4	28.441	15.038	34.624	1.00	0.00	O
ATOM	119	O29	OCB	X	4	14.249	13.922	35.741	1.00	0.00	O
ATOM	120	O30	OCB	X	4	13.938	27.220	35.144	1.00	0.00	O
ATOM	121	O31	OCB	X	4	28.517	27.731	34.901	1.00	0.00	O
ATOM	122	O32	OCB	X	4	25.495	20.992	26.476	1.00	0.00	O
ATOM	123	C91	OCB	X	4	26.224	17.555	37.223	1.00	0.00	C
ATOM	124	C92	OCB	X	4	25.271	15.078	36.450	1.00	0.00	C
ATOM	125	C93	OCB	X	4	25.013	17.064	37.779	1.00	0.00	C
ATOM	126	C94	OCB	X	4	26.951	16.774	36.340	1.00	0.00	C
ATOM	127	C95	OCB	X	4	26.540	15.485	35.954	1.00	0.00	C
ATOM	128	C96	OCB	X	4	24.506	15.848	37.368	1.00	0.00	C
ATOM	129	C97	OCB	X	4	24.121	17.827	38.776	1.00	0.00	C
ATOM	130	C98	OCB	X	4	24.486	24.341	38.881	1.00	0.00	C
ATOM	131	C99	OCB	X	4	18.264	24.647	39.209	1.00	0.00	C
ATOM	132	C	OCB	X	4	18.243	18.063	38.898	1.00	0.00	C
ATOM	133	H1	OCB	X	4	22.072	23.097	29.879	1.00	0.00	H
ATOM	134	H2	OCB	X	4	23.989	24.351	34.211	1.00	0.00	H
ATOM	135	H3	OCB	X	4	25.258	21.259	30.957	1.00	0.00	H
ATOM	136	H4	OCB	X	4	23.787	21.108	33.972	1.00	0.00	H
ATOM	137	H5	OCB	X	4	22.006	20.019	29.819	1.00	0.00	H
ATOM	138	H6	OCB	X	4	23.922	17.857	33.780	1.00	0.00	H
ATOM	139	H7	OCB	X	4	20.556	16.811	30.888	1.00	0.00	H
ATOM	140	H8	OCB	X	4	20.925	18.260	34.123	1.00	0.00	H
ATOM	141	H9	OCB	X	4	20.831	26.223	31.242	1.00	0.00	H
ATOM	142	H10	OCB	X	4	17.435	18.099	34.222	1.00	0.00	H
ATOM	143	H11	OCB	X	4	17.769	24.743	34.594	1.00	0.00	H
ATOM	144	H12	OCB	X	4	17.847	21.424	34.478	1.00	0.00	H
ATOM	145	H13	OCB	X	4	19.119	23.098	30.101	1.00	0.00	H
ATOM	146	H14	OCB	X	4	19.169	20.121	30.082	1.00	0.00	H
ATOM	147	H15	OCB	X	4	16.199	21.766	31.697	1.00	0.00	H
ATOM	148	H16	OCB	X	4	20.696	24.528	34.404	1.00	0.00	H
ATOM	149	H17	OCB	X	4	19.371	17.526	28.779	1.00	0.00	H
ATOM	150	H18	OCB	X	4	20.443	18.770	28.626	1.00	0.00	H
ATOM	151	H19	OCB	X	4	22.318	17.312	28.671	1.00	0.00	H
ATOM	152	H20	OCB	X	4	21.384	15.917	28.909	1.00	0.00	H

ATOM	153	H21	OCB	X	4	23.316	21.450	28.624	1.00	0.00	H
ATOM	154	H22	OCB	X	4	24.514	20.189	28.808	1.00	0.00	H
ATOM	155	H23	OCB	X	4	24.899	23.318	28.764	1.00	0.00	H
ATOM	156	H24	OCB	X	4	26.202	22.083	28.821	1.00	0.00	H
ATOM	157	H25	OCB	X	4	20.706	24.276	28.864	1.00	0.00	H
ATOM	158	H26	OCB	X	4	19.614	25.637	29.197	1.00	0.00	H
ATOM	159	H27	OCB	X	4	21.489	27.272	29.228	1.00	0.00	H
ATOM	160	H28	OCB	X	4	22.694	26.071	28.930	1.00	0.00	H
ATOM	161	H29	OCB	X	4	17.787	21.759	29.051	1.00	0.00	H
ATOM	162	H30	OCB	X	4	16.635	20.547	29.353	1.00	0.00	H
ATOM	163	H31	OCB	X	4	14.847	22.084	29.936	1.00	0.00	H
ATOM	164	H32	OCB	X	4	15.680	23.494	29.390	1.00	0.00	H
ATOM	165	H33	OCB	X	4	27.251	21.052	38.637	1.00	0.00	H
ATOM	166	H34	OCB	X	4	25.523	18.974	35.349	1.00	0.00	H
ATOM	167	H35	OCB	X	4	25.876	23.255	35.269	1.00	0.00	H
ATOM	168	H36	OCB	X	4	21.435	27.894	39.128	1.00	0.00	H
ATOM	169	H37	OCB	X	4	18.965	26.548	35.957	1.00	0.00	H
ATOM	170	H38	OCB	X	4	23.150	25.846	35.817	1.00	0.00	H
ATOM	171	H39	OCB	X	4	15.489	21.459	39.563	1.00	0.00	H
ATOM	172	H40	OCB	X	4	16.182	19.387	35.909	1.00	0.00	H
ATOM	173	H41	OCB	X	4	16.055	23.663	35.886	1.00	0.00	H
ATOM	174	H42	OCB	X	4	20.974	14.901	38.806	1.00	0.00	H
ATOM	175	H43	OCB	X	4	18.696	16.527	35.730	1.00	0.00	H
ATOM	176	H44	OCB	X	4	22.972	16.321	35.247	1.00	0.00	H
ATOM	177	H45	OCB	X	4	17.274	28.574	36.763	1.00	0.00	H
ATOM	178	H46	OCB	X	4	14.198	25.528	37.122	1.00	0.00	H
ATOM	179	H47	OCB	X	4	25.326	28.560	37.000	1.00	0.00	H
ATOM	180	H48	OCB	X	4	27.890	25.390	35.884	1.00	0.00	H
ATOM	181	H49	OCB	X	4	16.508	14.184	36.824	1.00	0.00	H
ATOM	182	H50	OCB	X	4	14.026	17.637	37.082	1.00	0.00	H
ATOM	183	H51	OCB	X	4	24.881	14.086	36.239	1.00	0.00	H
ATOM	184	H52	OCB	X	4	27.870	17.148	35.898	1.00	0.00	H
ATOM	185	H53	OCB	X	4	23.078	18.007	38.509	1.00	0.00	H
ATOM	186	H54	OCB	X	4	24.139	17.286	39.724	1.00	0.00	H
ATOM	187	H55	OCB	X	4	24.603	18.773	39.032	1.00	0.00	H
ATOM	188	H56	OCB	X	4	23.474	24.683	39.108	1.00	0.00	H
ATOM	189	H57	OCB	X	4	24.368	23.396	38.347	1.00	0.00	H
ATOM	190	H58	OCB	X	4	25.001	24.139	39.823	1.00	0.00	H
ATOM	191	H59	OCB	X	4	17.787	24.059	39.996	1.00	0.00	H
ATOM	192	H60	OCB	X	4	18.686	23.984	38.451	1.00	0.00	H
ATOM	193	H61	OCB	X	4	19.019	25.177	39.794	1.00	0.00	H
ATOM	194	H62	OCB	X	4	17.934	19.012	39.341	1.00	0.00	H
ATOM	195	H63	OCB	X	4	18.591	17.475	39.749	1.00	0.00	H
ATOM	196	H64	OCB	X	4	19.019	18.154	38.134	1.00	0.00	H
ATOM	197	C1	MOL	X	5	20.961	21.716	34.012	1.00	0.00	C
ATOM	198	C2	MOL	X	5	21.017	21.114	35.000	1.00	0.00	C
ATOM	199	C3	MOL	X	5	21.003	20.351	36.215	1.00	0.00	C
ATOM	200	C4	MOL	X	5	20.592	21.092	37.479	1.00	0.00	C
ATOM	201	C5	MOL	X	5	21.159	20.327	38.697	1.00	0.00	C
ATOM	202	C6	MOL	X	5	20.727	21.002	39.958	1.00	0.00	C
ATOM	203	O1	MOL	X	5	20.962	22.167	40.155	1.00	0.00	O
ATOM	204	O2	MOL	X	5	20.067	20.343	40.721	1.00	0.00	O
ATOM	205	H1	MOL	X	5	20.827	22.161	33.052	1.00	0.00	H
ATOM	206	H2	MOL	X	5	20.253	19.568	36.086	1.00	0.00	H
ATOM	207	H3	MOL	X	5	22.030	20.006	36.350	1.00	0.00	H
ATOM	208	H4	MOL	X	5	21.084	22.067	37.461	1.00	0.00	H
ATOM	209	H5	MOL	X	5	19.533	21.347	37.561	1.00	0.00	H
ATOM	210	H6	MOL	X	5	20.696	19.340	38.633	1.00	0.00	H
ATOM	211	H7	MOL	X	5	22.237	20.236	38.544	1.00	0.00	H

END

OAMe-G2

ATOM	1	C1	OCB	X	4	21.513	24.979	29.928	1.00	0.00	C
ATOM	2	C2	OCB	X	4	23.845	24.168	31.247	1.00	0.00	C
ATOM	3	C3	OCB	X	4	22.140	23.850	29.509	1.00	0.00	C
ATOM	4	C4	OCB	X	4	22.023	25.737	30.986	1.00	0.00	C
ATOM	5	C5	OCB	X	4	23.212	25.309	31.622	1.00	0.00	C
ATOM	6	C6	OCB	X	4	23.305	23.395	30.178	1.00	0.00	C
ATOM	7	O1	OCB	X	4	24.874	23.603	31.922	1.00	0.00	O
ATOM	8	C7	OCB	X	4	23.983	22.089	29.692	1.00	0.00	C
ATOM	9	C8	OCB	X	4	24.354	22.516	32.734	1.00	0.00	C
ATOM	10	O2	OCB	X	4	24.804	21.234	32.345	1.00	0.00	O
ATOM	11	C9	OCB	X	4	23.798	20.561	31.732	1.00	0.00	C
ATOM	12	C10	OCB	X	4	23.343	20.916	30.439	1.00	0.00	C
ATOM	13	C11	OCB	X	4	22.217	20.196	29.970	1.00	0.00	C
ATOM	14	C12	OCB	X	4	23.194	19.532	32.401	1.00	0.00	C
ATOM	15	C13	OCB	X	4	21.580	19.205	30.640	1.00	0.00	C
ATOM	16	C14	OCB	X	4	22.064	18.925	31.944	1.00	0.00	C
ATOM	17	O3	OCB	X	4	21.441	17.973	32.751	1.00	0.00	O
ATOM	18	C15	OCB	X	4	20.342	18.469	30.131	1.00	0.00	C
ATOM	19	C16	OCB	X	4	19.028	19.166	30.534	1.00	0.00	C
ATOM	20	C17	OCB	X	4	18.500	18.929	31.781	1.00	0.00	C
ATOM	21	C18	OCB	X	4	20.263	18.500	33.370	1.00	0.00	C
ATOM	22	O4	OCB	X	4	19.148	18.028	32.657	1.00	0.00	O
ATOM	23	O5	OCB	X	4	21.348	26.792	31.492	1.00	0.00	O
ATOM	24	C19	OCB	X	4	20.329	25.523	29.125	1.00	0.00	C
ATOM	25	C20	OCB	X	4	19.033	25.022	29.803	1.00	0.00	C
ATOM	26	O6	OCB	X	4	18.998	26.851	31.511	1.00	0.00	O
ATOM	27	C21	OCB	X	4	18.466	25.748	30.866	1.00	0.00	C
ATOM	28	C22	OCB	X	4	17.320	19.565	32.281	1.00	0.00	C
ATOM	29	C23	OCB	X	4	16.722	20.469	31.444	1.00	0.00	C
ATOM	30	C24	OCB	X	4	17.422	25.197	31.573	1.00	0.00	C
ATOM	31	C25	OCB	X	4	16.847	24.016	31.122	1.00	0.00	C
ATOM	32	O7	OCB	X	4	15.671	21.081	32.055	1.00	0.00	O
ATOM	33	O8	OCB	X	4	15.816	23.443	31.855	1.00	0.00	O
ATOM	34	C26	OCB	X	4	16.101	22.326	32.689	1.00	0.00	C
ATOM	35	C27	OCB	X	4	18.425	23.821	29.342	1.00	0.00	C
ATOM	36	C28	OCB	X	4	17.297	23.367	29.992	1.00	0.00	C
ATOM	37	C29	OCB	X	4	18.448	20.226	29.735	1.00	0.00	C
ATOM	38	C30	OCB	X	4	16.671	22.026	29.497	1.00	0.00	C
ATOM	39	C31	OCB	X	4	17.269	20.836	30.201	1.00	0.00	C
ATOM	40	C32	OCB	X	4	20.162	26.541	32.272	1.00	0.00	C
ATOM	41	C33	OCB	X	4	20.504	18.030	28.671	1.00	0.00	C
ATOM	42	C34	OCB	X	4	19.429	16.943	28.375	1.00	0.00	C
ATOM	43	C35	OCB	X	4	19.457	16.546	26.965	1.00	0.00	C
ATOM	44	O9	OCB	X	4	18.760	17.166	26.205	1.00	0.00	O
ATOM	45	C36	OCB	X	4	24.160	21.984	28.190	1.00	0.00	C
ATOM	46	C37	OCB	X	4	24.892	20.722	27.873	1.00	0.00	C
ATOM	47	C38	OCB	X	4	25.247	20.709	26.386	1.00	0.00	C
ATOM	48	O10	OCB	X	4	26.352	21.014	26.024	1.00	0.00	O
ATOM	49	C39	OCB	X	4	20.348	25.349	27.582	1.00	0.00	C
ATOM	50	C40	OCB	X	4	21.643	25.869	26.956	1.00	0.00	C
ATOM	51	C41	OCB	X	4	21.330	26.116	25.462	1.00	0.00	C
ATOM	52	O11	OCB	X	4	21.275	25.194	24.657	1.00	0.00	O
ATOM	53	C42	OCB	X	4	16.476	21.929	27.906	1.00	0.00	C
ATOM	54	C43	OCB	X	4	15.593	20.727	27.478	1.00	0.00	C
ATOM	55	C44	OCB	X	4	15.202	20.869	25.993	1.00	0.00	C
ATOM	56	O12	OCB	X	4	15.798	20.392	25.121	1.00	0.00	O
ATOM	57	C45	OCB	X	4	24.763	22.773	34.217	1.00	0.00	C

ATOM	58	C46	OCB	X	4	25.797	23.264	36.896	1.00	0.00	C
ATOM	59	C47	OCB	X	4	25.121	21.732	35.095	1.00	0.00	C
ATOM	60	C48	OCB	X	4	25.012	24.030	34.722	1.00	0.00	C
ATOM	61	C49	OCB	X	4	25.446	24.315	36.022	1.00	0.00	C
ATOM	62	C50	OCB	X	4	25.638	21.982	36.414	1.00	0.00	C
ATOM	63	C51	OCB	X	4	20.202	27.434	33.493	1.00	0.00	C
ATOM	64	C52	OCB	X	4	20.230	28.899	35.833	1.00	0.00	C
ATOM	65	C53	OCB	X	4	19.056	27.898	34.069	1.00	0.00	C
ATOM	66	C54	OCB	X	4	21.387	27.823	34.024	1.00	0.00	C
ATOM	67	C55	OCB	X	4	21.366	28.704	35.118	1.00	0.00	C
ATOM	68	C56	OCB	X	4	19.037	28.558	35.252	1.00	0.00	C
ATOM	69	C57	OCB	X	4	15.569	22.583	34.080	1.00	0.00	C
ATOM	70	C58	OCB	X	4	14.590	23.020	36.710	1.00	0.00	C
ATOM	71	C59	OCB	X	4	15.409	21.506	34.955	1.00	0.00	C
ATOM	72	C60	OCB	X	4	15.302	23.884	34.543	1.00	0.00	C
ATOM	73	C61	OCB	X	4	14.785	24.123	35.818	1.00	0.00	C
ATOM	74	C62	OCB	X	4	14.939	21.742	36.304	1.00	0.00	C
ATOM	75	C63	OCB	X	4	20.162	17.990	34.808	1.00	0.00	C
ATOM	76	C64	OCB	X	4	20.187	17.267	37.558	1.00	0.00	C
ATOM	77	C65	OCB	X	4	18.998	17.648	35.460	1.00	0.00	C
ATOM	78	C66	OCB	X	4	21.356	17.969	35.578	1.00	0.00	C
ATOM	79	C67	OCB	X	4	21.381	17.635	36.913	1.00	0.00	C
ATOM	80	C68	OCB	X	4	18.991	17.388	36.855	1.00	0.00	C
ATOM	81	O13	OCB	X	4	22.540	29.192	35.646	1.00	0.00	O
ATOM	82	O14	OCB	X	4	14.504	25.338	36.381	1.00	0.00	O
ATOM	83	O15	OCB	X	4	14.749	20.696	37.183	1.00	0.00	O
ATOM	84	O16	OCB	X	4	25.630	25.549	36.525	1.00	0.00	O
ATOM	85	O17	OCB	X	4	25.880	20.861	37.226	1.00	0.00	O
ATOM	86	O18	OCB	X	4	17.863	17.178	37.570	1.00	0.00	O
ATOM	87	O19	OCB	X	4	22.556	17.497	37.670	1.00	0.00	O
ATOM	88	C69	OCB	X	4	14.946	26.528	35.762	1.00	0.00	C
ATOM	89	C70	OCB	X	4	15.731	28.906	34.724	1.00	0.00	C
ATOM	90	C71	OCB	X	4	16.249	27.006	36.169	1.00	0.00	C
ATOM	91	C72	OCB	X	4	14.142	27.135	34.830	1.00	0.00	C
ATOM	92	C73	OCB	X	4	14.540	28.319	34.249	1.00	0.00	C
ATOM	93	C74	OCB	X	4	16.587	28.272	35.591	1.00	0.00	C
ATOM	94	O20	OCB	X	4	17.832	28.879	35.892	1.00	0.00	O
ATOM	95	C75	OCB	X	4	25.216	26.683	35.880	1.00	0.00	C
ATOM	96	C76	OCB	X	4	24.723	29.155	34.690	1.00	0.00	C
ATOM	97	C77	OCB	X	4	26.207	27.289	35.058	1.00	0.00	C
ATOM	98	C78	OCB	X	4	23.971	27.286	36.125	1.00	0.00	C
ATOM	99	C79	OCB	X	4	23.771	28.485	35.482	1.00	0.00	C
ATOM	100	C80	OCB	X	4	25.946	28.523	34.395	1.00	0.00	C
ATOM	101	C81	OCB	X	4	15.098	19.444	36.958	1.00	0.00	C
ATOM	102	C82	OCB	X	4	15.753	16.751	36.553	1.00	0.00	C
ATOM	103	C83	OCB	X	4	14.132	18.554	36.392	1.00	0.00	C
ATOM	104	C84	OCB	X	4	16.296	18.953	37.389	1.00	0.00	C
ATOM	105	C85	OCB	X	4	16.592	17.628	37.226	1.00	0.00	C
ATOM	106	C86	OCB	X	4	14.491	17.234	36.149	1.00	0.00	C
ATOM	107	C87	OCB	X	4	13.657	16.323	35.236	1.00	0.00	C
ATOM	108	O21	OCB	X	4	14.139	15.447	34.517	1.00	0.00	O
ATOM	109	C88	OCB	X	4	26.635	16.406	35.214	1.00	0.00	C
ATOM	110	O22	OCB	X	4	25.999	15.429	34.880	1.00	0.00	O
ATOM	111	C89	OCB	X	4	27.030	29.204	33.624	1.00	0.00	C
ATOM	112	O23	OCB	X	4	26.797	30.265	33.109	1.00	0.00	O
ATOM	113	O24	OCB	X	4	20.133	15.589	26.647	1.00	0.00	O
ATOM	114	O25	OCB	X	4	14.166	21.453	25.736	1.00	0.00	O
ATOM	115	O26	OCB	X	4	20.832	27.189	25.104	1.00	0.00	O
ATOM	116	C90	OCB	X	4	13.733	28.981	33.189	1.00	0.00	C
ATOM	117	O27	OCB	X	4	12.598	28.493	32.876	1.00	0.00	O

ATOM	118	O28	OCB	X	4	27.661	16.737	34.703	1.00	0.00	O
ATOM	119	O29	OCB	X	4	12.447	16.393	35.149	1.00	0.00	O
ATOM	120	O30	OCB	X	4	14.034	30.027	32.658	1.00	0.00	O
ATOM	121	O31	OCB	X	4	28.189	28.855	33.916	1.00	0.00	O
ATOM	122	O32	OCB	X	4	24.338	20.554	25.563	1.00	0.00	O
ATOM	123	C91	OCB	X	4	25.395	19.616	37.068	1.00	0.00	C
ATOM	124	C92	OCB	X	4	24.566	17.145	36.410	1.00	0.00	C
ATOM	125	C93	OCB	X	4	24.172	19.192	37.537	1.00	0.00	C
ATOM	126	C94	OCB	X	4	26.331	18.765	36.454	1.00	0.00	C
ATOM	127	C95	OCB	X	4	25.901	17.459	36.076	1.00	0.00	C
ATOM	128	C96	OCB	X	4	23.757	17.951	37.210	1.00	0.00	C
ATOM	129	C97	OCB	X	4	23.332	20.159	38.269	1.00	0.00	C
ATOM	130	C98	OCB	X	4	22.946	26.784	37.140	1.00	0.00	C
ATOM	131	C99	OCB	X	4	17.163	26.247	37.142	1.00	0.00	C
ATOM	132	C	OCB	X	4	17.326	19.988	37.849	1.00	0.00	C
ATOM	133	H1	OCB	X	4	21.812	23.138	28.756	1.00	0.00	H
ATOM	134	H2	OCB	X	4	23.702	25.969	32.334	1.00	0.00	H
ATOM	135	H3	OCB	X	4	25.027	22.067	30.012	1.00	0.00	H
ATOM	136	H4	OCB	X	4	23.255	22.555	32.712	1.00	0.00	H
ATOM	137	H5	OCB	X	4	21.863	20.328	28.951	1.00	0.00	H
ATOM	138	H6	OCB	X	4	23.558	19.324	33.404	1.00	0.00	H
ATOM	139	H7	OCB	X	4	20.312	17.434	30.476	1.00	0.00	H
ATOM	140	H8	OCB	X	4	20.243	19.599	33.334	1.00	0.00	H
ATOM	141	H9	OCB	X	4	20.283	26.607	29.252	1.00	0.00	H
ATOM	142	H10	OCB	X	4	16.934	19.364	33.277	1.00	0.00	H
ATOM	143	H11	OCB	X	4	17.062	25.694	32.471	1.00	0.00	H
ATOM	144	H12	OCB	X	4	17.199	22.272	32.703	1.00	0.00	H
ATOM	145	H13	OCB	X	4	18.825	23.256	28.503	1.00	0.00	H
ATOM	146	H14	OCB	X	4	18.914	20.551	28.809	1.00	0.00	H
ATOM	147	H15	OCB	X	4	15.634	22.197	29.793	1.00	0.00	H
ATOM	148	H16	OCB	X	4	20.167	25.471	32.529	1.00	0.00	H
ATOM	149	H17	OCB	X	4	20.490	18.874	27.977	1.00	0.00	H
ATOM	150	H18	OCB	X	4	21.487	17.626	28.421	1.00	0.00	H
ATOM	151	H19	OCB	X	4	19.662	16.024	28.917	1.00	0.00	H
ATOM	152	H20	OCB	X	4	18.444	17.218	28.758	1.00	0.00	H
ATOM	153	H21	OCB	X	4	24.779	22.759	27.734	1.00	0.00	H
ATOM	154	H22	OCB	X	4	23.290	22.092	27.539	1.00	0.00	H
ATOM	155	H23	OCB	X	4	25.854	20.561	28.364	1.00	0.00	H
ATOM	156	H24	OCB	X	4	24.365	19.810	28.160	1.00	0.00	H
ATOM	157	H25	OCB	X	4	20.200	24.377	27.106	1.00	0.00	H
ATOM	158	H26	OCB	X	4	19.506	25.904	27.163	1.00	0.00	H
ATOM	159	H27	OCB	X	4	21.867	26.806	27.472	1.00	0.00	H
ATOM	160	H28	OCB	X	4	22.509	25.218	27.092	1.00	0.00	H
ATOM	161	H29	OCB	X	4	15.892	22.816	27.653	1.00	0.00	H
ATOM	162	H30	OCB	X	4	17.408	21.804	27.351	1.00	0.00	H
ATOM	163	H31	OCB	X	4	16.147	19.806	27.674	1.00	0.00	H
ATOM	164	H32	OCB	X	4	14.703	20.808	28.106	1.00	0.00	H
ATOM	165	H33	OCB	X	4	26.072	23.437	37.933	1.00	0.00	H
ATOM	166	H34	OCB	X	4	25.080	20.738	34.656	1.00	0.00	H
ATOM	167	H35	OCB	X	4	24.943	24.856	34.019	1.00	0.00	H
ATOM	168	H36	OCB	X	4	20.176	29.407	36.792	1.00	0.00	H
ATOM	169	H37	OCB	X	4	18.115	27.591	33.619	1.00	0.00	H
ATOM	170	H38	OCB	X	4	22.370	27.631	33.602	1.00	0.00	H
ATOM	171	H39	OCB	X	4	14.236	23.204	37.721	1.00	0.00	H
ATOM	172	H40	OCB	X	4	15.674	20.513	34.603	1.00	0.00	H
ATOM	173	H41	OCB	X	4	15.519	24.768	33.949	1.00	0.00	H
ATOM	174	H42	OCB	X	4	20.197	17.053	38.624	1.00	0.00	H
ATOM	175	H43	OCB	X	4	18.035	17.646	34.957	1.00	0.00	H
ATOM	176	H44	OCB	X	4	22.310	18.183	35.104	1.00	0.00	H
ATOM	177	H45	OCB	X	4	16.001	29.882	34.329	1.00	0.00	H

ATOM	178	H46	OCB	X	4	13.253	26.612	34.489	1.00	0.00	H
ATOM	179	H47	OCB	X	4	24.521	30.121	34.234	1.00	0.00	H
ATOM	180	H48	OCB	X	4	27.179	26.826	34.906	1.00	0.00	H
ATOM	181	H49	OCB	X	4	15.976	15.695	36.425	1.00	0.00	H
ATOM	182	H50	OCB	X	4	13.181	18.984	36.088	1.00	0.00	H
ATOM	183	H51	OCB	X	4	24.107	16.229	36.049	1.00	0.00	H
ATOM	184	H52	OCB	X	4	27.339	19.077	36.197	1.00	0.00	H
ATOM	185	H53	OCB	X	4	22.853	20.828	37.552	1.00	0.00	H
ATOM	186	H54	OCB	X	4	22.597	19.593	38.846	1.00	0.00	H
ATOM	187	H55	OCB	X	4	23.882	20.798	38.963	1.00	0.00	H
ATOM	188	H56	OCB	X	4	23.468	26.378	38.009	1.00	0.00	H
ATOM	189	H57	OCB	X	4	22.348	27.634	37.475	1.00	0.00	H
ATOM	190	H58	OCB	X	4	22.353	25.996	36.670	1.00	0.00	H
ATOM	191	H59	OCB	X	4	16.673	25.381	37.592	1.00	0.00	H
ATOM	192	H60	OCB	X	4	18.104	25.932	36.686	1.00	0.00	H
ATOM	193	H61	OCB	X	4	17.444	26.893	37.975	1.00	0.00	H
ATOM	194	H62	OCB	X	4	17.608	20.634	37.015	1.00	0.00	H
ATOM	195	H63	OCB	X	4	16.991	20.645	38.655	1.00	0.00	H
ATOM	196	H64	OCB	X	4	18.261	19.534	38.183	1.00	0.00	H
ATOM	197	C1	MOL	X	5	19.085	23.161	37.149	1.00	0.00	C
ATOM	198	C2	MOL	X	5	19.077	23.013	35.799	1.00	0.00	C
ATOM	199	C3	MOL	X	5	20.320	22.883	35.137	1.00	0.00	C
ATOM	200	C4	MOL	X	5	21.494	23.061	35.862	1.00	0.00	C
ATOM	201	C5	MOL	X	5	21.501	23.252	37.227	1.00	0.00	C
ATOM	202	C6	MOL	X	5	20.283	23.390	37.896	1.00	0.00	C
ATOM	203	C7	MOL	X	5	20.213	22.632	33.730	1.00	0.00	C
ATOM	204	N1	MOL	X	5	20.132	22.555	32.610	1.00	0.00	N
ATOM	205	C8	MOL	X	5	20.169	23.552	39.390	1.00	0.00	C
ATOM	206	O1	MOL	X	5	21.179	23.533	40.047	1.00	0.00	O
ATOM	207	O2	MOL	X	5	19.064	23.627	39.896	1.00	0.00	O
ATOM	208	H1	MOL	X	5	18.142	23.140	37.690	1.00	0.00	H
ATOM	209	H2	MOL	X	5	18.164	22.886	35.223	1.00	0.00	H
ATOM	210	H3	MOL	X	5	22.362	22.928	35.221	1.00	0.00	H
ATOM	211	H4	MOL	X	5	22.375	23.548	37.801	1.00	0.00	H
END											

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ATOM	1	C1	OCB	X	4	20.134	22.165	30.544	1.00	0.00	C
ATOM	2	C2	OCB	X	4	22.462	20.905	31.416	1.00	0.00	C
ATOM	3	C3	OCB	X	4	20.685	21.129	29.793	1.00	0.00	C
ATOM	4	C4	OCB	X	4	20.691	22.402	31.791	1.00	0.00	C
ATOM	5	C5	OCB	X	4	21.898	21.796	32.234	1.00	0.00	C
ATOM	6	C6	OCB	X	4	21.854	20.516	30.236	1.00	0.00	C
ATOM	7	O1	OCB	X	4	23.527	20.292	32.070	1.00	0.00	O
ATOM	8	C7	OCB	X	4	22.527	19.370	29.493	1.00	0.00	C
ATOM	9	C8	OCB	X	4	23.335	19.016	32.648	1.00	0.00	C
ATOM	10	O2	OCB	X	4	23.771	18.012	31.696	1.00	0.00	O
ATOM	11	C9	OCB	X	4	22.781	17.352	31.052	1.00	0.00	C
ATOM	12	C10	OCB	X	4	22.047	17.991	30.079	1.00	0.00	C
ATOM	13	C11	OCB	X	4	21.031	17.252	29.408	1.00	0.00	C
ATOM	14	C12	OCB	X	4	22.482	16.036	31.395	1.00	0.00	C
ATOM	15	C13	OCB	X	4	20.648	15.965	29.737	1.00	0.00	C
ATOM	16	C14	OCB	X	4	21.387	15.364	30.786	1.00	0.00	C
ATOM	17	O3	OCB	X	4	20.835	14.180	31.317	1.00	0.00	O
ATOM	18	C15	OCB	X	4	19.446	15.259	29.146	1.00	0.00	C
ATOM	19	C16	OCB	X	4	18.236	15.718	29.998	1.00	0.00	C
ATOM	20	C17	OCB	X	4	17.731	14.954	31.073	1.00	0.00	C

ATOM	21	C18	OCB	X	4	19.706	14.307	32.231	1.00	0.00	C
ATOM	22	O4	OCB	X	4	18.468	13.974	31.791	1.00	0.00	O
ATOM	23	O5	OCB	X	4	20.078	23.177	32.757	1.00	0.00	O
ATOM	24	C19	OCB	X	4	18.697	22.709	30.178	1.00	0.00	C
ATOM	25	C20	OCB	X	4	17.614	21.881	30.800	1.00	0.00	C
ATOM	26	O6	OCB	X	4	17.633	23.185	32.884	1.00	0.00	O
ATOM	27	C21	OCB	X	4	17.057	22.188	32.048	1.00	0.00	C
ATOM	28	C22	OCB	X	4	16.678	15.383	31.803	1.00	0.00	C
ATOM	29	C23	OCB	X	4	15.968	16.595	31.426	1.00	0.00	C
ATOM	30	C24	OCB	X	4	15.968	21.423	32.575	1.00	0.00	C
ATOM	31	C25	OCB	X	4	15.552	20.262	31.896	1.00	0.00	C
ATOM	32	O7	OCB	X	4	14.986	17.035	32.254	1.00	0.00	O
ATOM	33	O8	OCB	X	4	14.636	19.383	32.501	1.00	0.00	O
ATOM	34	C26	OCB	X	4	15.252	18.189	33.082	1.00	0.00	C
ATOM	35	C27	OCB	X	4	17.187	20.682	30.183	1.00	0.00	C
ATOM	36	C28	OCB	X	4	16.124	19.942	30.629	1.00	0.00	C
ATOM	37	C29	OCB	X	4	17.566	16.961	29.708	1.00	0.00	C
ATOM	38	C30	OCB	X	4	15.620	18.620	29.951	1.00	0.00	C
ATOM	39	C31	OCB	X	4	16.422	17.373	30.374	1.00	0.00	C
ATOM	40	C32	OCB	X	4	18.881	22.735	33.443	1.00	0.00	C
ATOM	41	C33	OCB	X	4	19.211	15.331	27.654	1.00	0.00	C
ATOM	42	C34	OCB	X	4	20.400	14.809	26.908	1.00	0.00	C
ATOM	43	C35	OCB	X	4	20.090	14.518	25.498	1.00	0.00	C
ATOM	44	O9	OCB	X	4	19.915	15.459	24.677	1.00	0.00	O
ATOM	45	C36	OCB	X	4	22.480	19.396	27.973	1.00	0.00	C
ATOM	46	C37	OCB	X	4	23.360	20.480	27.308	1.00	0.00	C
ATOM	47	C38	OCB	X	4	23.374	20.303	25.808	1.00	0.00	C
ATOM	48	O10	OCB	X	4	22.437	20.687	25.144	1.00	0.00	O
ATOM	49	C39	OCB	X	4	18.598	23.116	28.678	1.00	0.00	C
ATOM	50	C40	OCB	X	4	17.287	23.785	28.433	1.00	0.00	C
ATOM	51	C41	OCB	X	4	17.103	24.438	27.056	1.00	0.00	C
ATOM	52	O11	OCB	X	4	16.947	23.675	26.121	1.00	0.00	O
ATOM	53	C42	OCB	X	4	15.378	18.680	28.382	1.00	0.00	C
ATOM	54	C43	OCB	X	4	14.302	19.629	27.948	1.00	0.00	C
ATOM	55	C44	OCB	X	4	14.169	19.386	26.486	1.00	0.00	C
ATOM	56	O12	OCB	X	4	13.451	18.452	26.137	1.00	0.00	O
ATOM	57	C45	OCB	X	4	24.194	18.919	33.944	1.00	0.00	C
ATOM	58	C46	OCB	X	4	25.440	18.514	36.413	1.00	0.00	C
ATOM	59	C47	OCB	X	4	24.474	17.610	34.403	1.00	0.00	C
ATOM	60	C48	OCB	X	4	24.519	20.047	34.704	1.00	0.00	C
ATOM	61	C49	OCB	X	4	25.031	19.801	35.958	1.00	0.00	C
ATOM	62	C50	OCB	X	4	25.122	17.424	35.641	1.00	0.00	C
ATOM	63	C51	OCB	X	4	19.011	23.128	34.984	1.00	0.00	C
ATOM	64	C52	OCB	X	4	19.383	23.738	37.751	1.00	0.00	C
ATOM	65	C53	OCB	X	4	17.941	22.991	35.867	1.00	0.00	C
ATOM	66	C54	OCB	X	4	20.223	23.541	35.491	1.00	0.00	C
ATOM	67	C55	OCB	X	4	20.415	23.805	36.903	1.00	0.00	C
ATOM	68	C56	OCB	X	4	18.091	23.382	37.182	1.00	0.00	C
ATOM	69	C57	OCB	X	4	14.847	17.930	34.557	1.00	0.00	C
ATOM	70	C58	OCB	X	4	14.007	17.548	37.202	1.00	0.00	C
ATOM	71	C59	OCB	X	4	14.893	16.621	35.166	1.00	0.00	C
ATOM	72	C60	OCB	X	4	14.515	19.014	35.371	1.00	0.00	C
ATOM	73	C61	OCB	X	4	14.052	18.865	36.649	1.00	0.00	C
ATOM	74	C62	OCB	X	4	14.453	16.468	36.512	1.00	0.00	C
ATOM	75	C63	OCB	X	4	19.948	13.455	33.512	1.00	0.00	C
ATOM	76	C64	OCB	X	4	20.377	12.109	36.006	1.00	0.00	C
ATOM	77	C65	OCB	X	4	18.900	13.142	34.429	1.00	0.00	C
ATOM	78	C66	OCB	X	4	21.191	13.168	33.979	1.00	0.00	C
ATOM	79	C67	OCB	X	4	21.414	12.449	35.224	1.00	0.00	C
ATOM	80	C68	OCB	X	4	19.140	12.523	35.661	1.00	0.00	C

ATOM	81	O13	OCB	X	4	21.721	24.084	37.378	1.00	0.00	O
ATOM	82	O14	OCB	X	4	13.573	19.947	37.421	1.00	0.00	O
ATOM	83	O15	OCB	X	4	14.472	15.271	37.250	1.00	0.00	O
ATOM	84	O16	OCB	X	4	25.300	20.847	36.856	1.00	0.00	O
ATOM	85	O17	OCB	X	4	25.562	16.231	36.197	1.00	0.00	O
ATOM	86	O18	OCB	X	4	18.110	12.226	36.569	1.00	0.00	O
ATOM	87	O19	OCB	X	4	22.740	12.267	35.645	1.00	0.00	O
ATOM	88	C69	OCB	X	4	14.056	21.210	37.294	1.00	0.00	C
ATOM	89	C70	OCB	X	4	14.811	23.846	36.985	1.00	0.00	C
ATOM	90	C71	OCB	X	4	15.340	21.578	37.731	1.00	0.00	C
ATOM	91	C72	OCB	X	4	13.111	22.142	36.726	1.00	0.00	C
ATOM	92	C73	OCB	X	4	13.498	23.482	36.578	1.00	0.00	C
ATOM	93	C74	OCB	X	4	15.725	22.924	37.578	1.00	0.00	C
ATOM	94	O20	OCB	X	4	16.939	23.332	37.996	1.00	0.00	O
ATOM	95	C75	OCB	X	4	24.701	22.077	36.713	1.00	0.00	C
ATOM	96	C76	OCB	X	4	23.659	24.627	36.311	1.00	0.00	C
ATOM	97	C77	OCB	X	4	25.481	23.007	35.965	1.00	0.00	C
ATOM	98	C78	OCB	X	4	23.382	22.339	37.064	1.00	0.00	C
ATOM	99	C79	OCB	X	4	22.890	23.652	36.825	1.00	0.00	C
ATOM	100	C80	OCB	X	4	24.943	24.351	35.826	1.00	0.00	C
ATOM	101	C81	OCB	X	4	14.977	14.125	36.618	1.00	0.00	C
ATOM	102	C82	OCB	X	4	16.039	11.755	35.589	1.00	0.00	C
ATOM	103	C83	OCB	X	4	14.218	13.358	35.730	1.00	0.00	C
ATOM	104	C84	OCB	X	4	16.316	13.772	36.868	1.00	0.00	C
ATOM	105	C85	OCB	X	4	16.820	12.599	36.361	1.00	0.00	C
ATOM	106	C86	OCB	X	4	14.701	12.111	35.252	1.00	0.00	C
ATOM	107	C87	OCB	X	4	13.840	11.174	34.531	1.00	0.00	C
ATOM	108	O21	OCB	X	4	12.636	11.410	34.463	1.00	0.00	O
ATOM	109	C88	OCB	X	4	26.704	12.749	32.828	1.00	0.00	C
ATOM	110	O22	OCB	X	4	27.668	13.278	32.544	1.00	0.00	O
ATOM	111	C89	OCB	X	4	25.795	25.382	35.102	1.00	0.00	C
ATOM	112	O23	OCB	X	4	25.420	26.494	35.183	1.00	0.00	O
ATOM	113	O24	OCB	X	4	19.806	13.407	25.172	1.00	0.00	O
ATOM	114	O25	OCB	X	4	14.774	20.055	25.649	1.00	0.00	O
ATOM	115	O26	OCB	X	4	17.214	25.649	26.869	1.00	0.00	O
ATOM	116	C90	OCB	X	4	12.680	24.476	35.855	1.00	0.00	C
ATOM	117	O27	OCB	X	4	12.963	25.653	35.940	1.00	0.00	O
ATOM	118	O28	OCB	X	4	26.380	11.694	32.230	1.00	0.00	O
ATOM	119	O29	OCB	X	4	14.272	10.094	34.186	1.00	0.00	O
ATOM	120	O30	OCB	X	4	11.755	24.132	35.147	1.00	0.00	O
ATOM	121	O31	OCB	X	4	26.817	25.129	34.546	1.00	0.00	O
ATOM	122	O32	OCB	X	4	24.294	19.727	25.326	1.00	0.00	O
ATOM	123	C91	OCB	X	4	25.335	14.954	35.631	1.00	0.00	C
ATOM	124	C92	OCB	X	4	24.731	12.543	34.344	1.00	0.00	C
ATOM	125	C93	OCB	X	4	24.162	14.238	36.029	1.00	0.00	C
ATOM	126	C94	OCB	X	4	26.027	14.551	34.490	1.00	0.00	C
ATOM	127	C95	OCB	X	4	25.773	13.297	33.886	1.00	0.00	C
ATOM	128	C96	OCB	X	4	23.838	13.043	35.319	1.00	0.00	C
ATOM	129	C97	OCB	X	4	23.315	14.536	37.220	1.00	0.00	C
ATOM	130	C98	OCB	X	4	22.511	21.373	37.747	1.00	0.00	C
ATOM	131	C99	OCB	X	4	16.351	20.574	38.307	1.00	0.00	C
ATOM	132	C	OCB	X	4	17.155	14.712	37.787	1.00	0.00	C
ATOM	133	H1	OCB	X	4	20.197	20.745	28.901	1.00	0.00	H
ATOM	134	H2	OCB	X	4	22.358	21.991	33.199	1.00	0.00	H
ATOM	135	H3	OCB	X	4	23.600	19.458	29.672	1.00	0.00	H
ATOM	136	H4	OCB	X	4	22.317	18.842	33.027	1.00	0.00	H
ATOM	137	H5	OCB	X	4	20.442	17.610	28.567	1.00	0.00	H
ATOM	138	H6	OCB	X	4	23.063	15.560	32.181	1.00	0.00	H
ATOM	139	H7	OCB	X	4	19.374	14.184	29.322	1.00	0.00	H
ATOM	140	H8	OCB	X	4	19.606	15.337	32.603	1.00	0.00	H

ATOM	141	H9	OCB	X	4	18.642	23.663	30.708	1.00	0.00	H
ATOM	142	H10	OCB	X	4	16.297	14.796	32.635	1.00	0.00	H
ATOM	143	H11	OCB	X	4	15.622	21.629	33.584	1.00	0.00	H
ATOM	144	H12	OCB	X	4	16.335	18.369	33.158	1.00	0.00	H
ATOM	145	H13	OCB	X	4	17.751	20.299	29.335	1.00	0.00	H
ATOM	146	H14	OCB	X	4	17.955	17.574	28.899	1.00	0.00	H
ATOM	147	H15	OCB	X	4	14.579	18.510	30.262	1.00	0.00	H
ATOM	148	H16	OCB	X	4	18.951	21.643	33.329	1.00	0.00	H
ATOM	149	H17	OCB	X	4	18.327	14.786	27.318	1.00	0.00	H
ATOM	150	H18	OCB	X	4	19.123	16.397	27.432	1.00	0.00	H
ATOM	151	H19	OCB	X	4	21.134	15.617	26.945	1.00	0.00	H
ATOM	152	H20	OCB	X	4	20.915	13.935	27.312	1.00	0.00	H
ATOM	153	H21	OCB	X	4	21.454	19.459	27.604	1.00	0.00	H
ATOM	154	H22	OCB	X	4	22.809	18.483	27.471	1.00	0.00	H
ATOM	155	H23	OCB	X	4	23.090	21.454	27.723	1.00	0.00	H
ATOM	156	H24	OCB	X	4	24.395	20.410	27.649	1.00	0.00	H
ATOM	157	H25	OCB	X	4	19.399	23.818	28.435	1.00	0.00	H
ATOM	158	H26	OCB	X	4	18.631	22.211	28.069	1.00	0.00	H
ATOM	159	H27	OCB	X	4	16.534	22.997	28.506	1.00	0.00	H
ATOM	160	H28	OCB	X	4	17.042	24.499	29.221	1.00	0.00	H
ATOM	161	H29	OCB	X	4	16.367	18.847	27.950	1.00	0.00	H
ATOM	162	H30	OCB	X	4	15.026	17.664	28.193	1.00	0.00	H
ATOM	163	H31	OCB	X	4	13.368	19.432	28.479	1.00	0.00	H
ATOM	164	H32	OCB	X	4	14.573	20.668	28.146	1.00	0.00	H
ATOM	165	H33	OCB	X	4	25.882	18.426	37.402	1.00	0.00	H
ATOM	166	H34	OCB	X	4	24.079	16.745	33.876	1.00	0.00	H
ATOM	167	H35	OCB	X	4	24.421	21.061	34.323	1.00	0.00	H
ATOM	168	H36	OCB	X	4	19.524	23.903	38.816	1.00	0.00	H
ATOM	169	H37	OCB	X	4	16.965	22.769	35.441	1.00	0.00	H
ATOM	170	H38	OCB	X	4	21.047	23.656	34.791	1.00	0.00	H
ATOM	171	H39	OCB	X	4	13.624	17.444	38.214	1.00	0.00	H
ATOM	172	H40	OCB	X	4	15.066	15.773	34.509	1.00	0.00	H
ATOM	173	H41	OCB	X	4	14.628	20.030	34.999	1.00	0.00	H
ATOM	174	H42	OCB	X	4	20.603	11.645	36.962	1.00	0.00	H
ATOM	175	H43	OCB	X	4	17.867	13.415	34.227	1.00	0.00	H
ATOM	176	H44	OCB	X	4	22.040	13.603	33.459	1.00	0.00	H
ATOM	177	H45	OCB	X	4	15.145	24.868	36.827	1.00	0.00	H
ATOM	178	H46	OCB	X	4	12.103	21.833	36.459	1.00	0.00	H
ATOM	179	H47	OCB	X	4	23.185	25.605	36.317	1.00	0.00	H
ATOM	180	H48	OCB	X	4	26.514	22.743	35.752	1.00	0.00	H
ATOM	181	H49	OCB	X	4	16.424	10.784	35.288	1.00	0.00	H
ATOM	182	H50	OCB	X	4	13.215	13.747	35.573	1.00	0.00	H
ATOM	183	H51	OCB	X	4	24.399	11.606	33.904	1.00	0.00	H
ATOM	184	H52	OCB	X	4	26.782	15.183	34.029	1.00	0.00	H
ATOM	185	H53	OCB	X	4	23.282	13.684	37.902	1.00	0.00	H
ATOM	186	H54	OCB	X	4	23.672	15.405	37.777	1.00	0.00	H
ATOM	187	H55	OCB	X	4	22.283	14.793	36.972	1.00	0.00	H
ATOM	188	H56	OCB	X	4	21.984	21.667	38.656	1.00	0.00	H
ATOM	189	H57	OCB	X	4	21.703	20.983	37.125	1.00	0.00	H
ATOM	190	H58	OCB	X	4	23.070	20.500	38.091	1.00	0.00	H
ATOM	191	H59	OCB	X	4	15.693	19.858	38.803	1.00	0.00	H
ATOM	192	H60	OCB	X	4	16.856	20.277	37.385	1.00	0.00	H
ATOM	193	H61	OCB	X	4	17.018	21.041	39.035	1.00	0.00	H
ATOM	194	H62	OCB	X	4	16.699	15.702	37.851	1.00	0.00	H
ATOM	195	H63	OCB	X	4	17.278	14.158	38.720	1.00	0.00	H
ATOM	196	H64	OCB	X	4	18.061	14.895	37.206	1.00	0.00	H
ATOM	197	C1	MOL	X	5	19.074	18.629	32.615	1.00	0.00	C
ATOM	198	C2	MOL	X	5	19.497	19.215	34.012	1.00	0.00	C
ATOM	199	C3	MOL	X	5	19.982	18.148	34.860	1.00	0.00	C
ATOM	200	C4	MOL	X	5	19.859	18.594	36.370	1.00	0.00	C

ATOM	201	C5	MOL	X	5	20.342	17.504	37.322	1.00	0.00	C
ATOM	202	C6	MOL	X	5	20.044	17.936	38.813	1.00	0.00	C
ATOM	203	N1	MOL	X	5	20.462	16.998	39.918	1.00	0.00	N
ATOM	204	C7	MOL	X	5	21.959	16.917	40.124	1.00	0.00	C
ATOM	205	C8	MOL	X	5	19.977	15.621	39.635	1.00	0.00	C
ATOM	206	C9	MOL	X	5	19.777	17.492	41.152	1.00	0.00	C
ATOM	207	H1	MOL	X	5	18.341	19.325	32.202	1.00	0.00	H
ATOM	208	H2	MOL	X	5	19.931	18.526	31.946	1.00	0.00	H
ATOM	209	H3	MOL	X	5	18.593	19.582	34.503	1.00	0.00	H
ATOM	210	H4	MOL	X	5	20.213	20.040	34.028	1.00	0.00	H
ATOM	211	H5	MOL	X	5	20.960	17.874	34.460	1.00	0.00	H
ATOM	212	H6	MOL	X	5	19.330	17.272	34.876	1.00	0.00	H
ATOM	213	H7	MOL	X	5	18.831	18.861	36.625	1.00	0.00	H
ATOM	214	H8	MOL	X	5	20.489	19.476	36.497	1.00	0.00	H
ATOM	215	H9	MOL	X	5	21.432	17.536	37.276	1.00	0.00	H
ATOM	216	H10	MOL	X	5	19.960	16.504	37.105	1.00	0.00	H
ATOM	217	H11	MOL	X	5	18.971	18.126	38.856	1.00	0.00	H
ATOM	218	H12	MOL	X	5	20.531	18.881	39.056	1.00	0.00	H
ATOM	219	H13	MOL	X	5	18.557	17.667	32.597	1.00	0.00	H
ATOM	220	H14	MOL	X	5	22.448	16.397	39.300	1.00	0.00	H
ATOM	221	H15	MOL	X	5	22.355	17.912	40.331	1.00	0.00	H
ATOM	222	H16	MOL	X	5	22.066	16.275	41.000	1.00	0.00	H
ATOM	223	H17	MOL	X	5	20.284	14.899	40.392	1.00	0.00	H
ATOM	224	H18	MOL	X	5	18.891	15.629	39.533	1.00	0.00	H
ATOM	225	H19	MOL	X	5	20.341	15.369	38.638	1.00	0.00	H
ATOM	226	H20	MOL	X	5	20.307	18.436	41.289	1.00	0.00	H
ATOM	227	H21	MOL	X	5	18.701	17.616	41.016	1.00	0.00	H
ATOM	228	H22	MOL	X	5	20.068	16.830	41.968	1.00	0.00	H
END											

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ATOM	1	C1	OCB	X	4	21.059	17.850	26.407	1.00	0.00	C
ATOM	2	C2	OCB	X	4	19.737	15.742	27.463	1.00	0.00	C
ATOM	3	C3	OCB	X	4	19.924	17.308	25.727	1.00	0.00	C
ATOM	4	C4	OCB	X	4	21.469	17.380	27.605	1.00	0.00	C
ATOM	5	C5	OCB	X	4	20.742	16.315	28.137	1.00	0.00	C
ATOM	6	C6	OCB	X	4	19.304	16.153	26.192	1.00	0.00	C
ATOM	7	O1	OCB	X	4	19.216	14.586	28.057	1.00	0.00	O
ATOM	8	C7	OCB	X	4	18.127	15.426	25.568	1.00	0.00	C
ATOM	9	C8	OCB	X	4	17.989	14.703	28.677	1.00	0.00	C
ATOM	10	O2	OCB	X	4	16.877	14.406	27.875	1.00	0.00	O
ATOM	11	C9	OCB	X	4	16.256	15.428	27.274	1.00	0.00	C
ATOM	12	C10	OCB	X	4	16.844	16.032	26.169	1.00	0.00	C
ATOM	13	C11	OCB	X	4	16.277	17.153	25.588	1.00	0.00	C
ATOM	14	C12	OCB	X	4	15.051	15.852	27.734	1.00	0.00	C
ATOM	15	C13	OCB	X	4	15.069	17.610	26.061	1.00	0.00	C
ATOM	16	C14	OCB	X	4	14.428	16.916	27.136	1.00	0.00	C
ATOM	17	O3	OCB	X	4	13.428	17.551	27.854	1.00	0.00	O
ATOM	18	C15	OCB	X	4	14.559	18.907	25.534	1.00	0.00	C
ATOM	19	C16	OCB	X	4	15.212	20.053	26.206	1.00	0.00	C
ATOM	20	C17	OCB	X	4	14.724	20.443	27.500	1.00	0.00	C
ATOM	21	C18	OCB	X	4	13.857	18.599	28.799	1.00	0.00	C
ATOM	22	O4	OCB	X	4	13.651	19.823	28.130	1.00	0.00	O
ATOM	23	O5	OCB	X	4	22.479	17.913	28.364	1.00	0.00	O
ATOM	24	C19	OCB	X	4	21.745	19.070	25.842	1.00	0.00	C
ATOM	25	C20	OCB	X	4	21.040	20.305	26.452	1.00	0.00	C
ATOM	26	O6	OCB	X	4	22.537	20.294	28.365	1.00	0.00	O

ATOM	27	C21	OCB	X	4	21.552	20.861	27.636	1.00	0.00	C
ATOM	28	C22	OCB	X	4	15.306	21.512	28.212	1.00	0.00	C
ATOM	29	C23	OCB	X	4	16.398	22.116	27.638	1.00	0.00	C
ATOM	30	C24	OCB	X	4	20.948	21.908	28.209	1.00	0.00	C
ATOM	31	C25	OCB	X	4	19.821	22.462	27.624	1.00	0.00	C
ATOM	32	O7	OCB	X	4	16.882	23.228	28.310	1.00	0.00	O
ATOM	33	O8	OCB	X	4	19.172	23.489	28.285	1.00	0.00	O
ATOM	34	C26	OCB	X	4	18.115	23.022	29.087	1.00	0.00	C
ATOM	35	C27	OCB	X	4	19.906	20.818	25.862	1.00	0.00	C
ATOM	36	C28	OCB	X	4	19.305	21.949	26.425	1.00	0.00	C
ATOM	37	C29	OCB	X	4	16.253	20.756	25.655	1.00	0.00	C
ATOM	38	C30	OCB	X	4	18.048	22.611	25.839	1.00	0.00	C
ATOM	39	C31	OCB	X	4	16.820	21.851	26.316	1.00	0.00	C
ATOM	40	C32	OCB	X	4	22.217	19.108	29.166	1.00	0.00	C
ATOM	41	C33	OCB	X	4	14.516	19.156	24.015	1.00	0.00	C
ATOM	42	C34	OCB	X	4	13.542	18.230	23.195	1.00	0.00	C
ATOM	43	C35	OCB	X	4	13.262	18.747	21.773	1.00	0.00	C
ATOM	44	O9	OCB	X	4	13.825	18.366	20.741	1.00	0.00	O
ATOM	45	C36	OCB	X	4	18.142	15.513	24.005	1.00	0.00	C
ATOM	46	C37	OCB	X	4	19.048	14.501	23.362	1.00	0.00	C
ATOM	47	C38	OCB	X	4	18.776	14.289	21.869	1.00	0.00	C
ATOM	48	O10	OCB	X	4	17.833	13.548	21.600	1.00	0.00	O
ATOM	49	C39	OCB	X	4	22.043	19.013	24.349	1.00	0.00	C
ATOM	50	C40	OCB	X	4	22.819	20.240	23.755	1.00	0.00	C
ATOM	51	C41	OCB	X	4	23.660	20.008	22.533	1.00	0.00	C
ATOM	52	O11	OCB	X	4	23.359	19.189	21.695	1.00	0.00	O
ATOM	53	C42	OCB	X	4	18.066	22.655	24.290	1.00	0.00	C
ATOM	54	C43	OCB	X	4	19.159	23.664	23.849	1.00	0.00	C
ATOM	55	C44	OCB	X	4	19.078	24.066	22.377	1.00	0.00	C
ATOM	56	O12	OCB	X	4	19.506	23.414	21.483	1.00	0.00	O
ATOM	57	C45	OCB	X	4	17.867	14.012	30.014	1.00	0.00	C
ATOM	58	C46	OCB	X	4	17.804	12.854	32.612	1.00	0.00	C
ATOM	59	C47	OCB	X	4	16.669	13.501	30.514	1.00	0.00	C
ATOM	60	C48	OCB	X	4	18.981	13.944	30.797	1.00	0.00	C
ATOM	61	C49	OCB	X	4	19.000	13.331	32.068	1.00	0.00	C
ATOM	62	C50	OCB	X	4	16.593	12.976	31.885	1.00	0.00	C
ATOM	63	C51	OCB	X	4	22.865	19.139	30.542	1.00	0.00	C
ATOM	64	C52	OCB	X	4	23.676	18.991	33.220	1.00	0.00	C
ATOM	65	C53	OCB	X	4	22.962	20.326	31.280	1.00	0.00	C
ATOM	66	C54	OCB	X	4	23.269	17.920	31.101	1.00	0.00	C
ATOM	67	C55	OCB	X	4	23.622	17.856	32.462	1.00	0.00	C
ATOM	68	C56	OCB	X	4	23.332	20.237	32.609	1.00	0.00	C
ATOM	69	C57	OCB	X	4	17.944	23.829	30.393	1.00	0.00	C
ATOM	70	C58	OCB	X	4	17.519	24.489	33.049	1.00	0.00	C
ATOM	71	C59	OCB	X	4	16.653	23.896	30.872	1.00	0.00	C
ATOM	72	C60	OCB	X	4	19.022	24.134	31.189	1.00	0.00	C
ATOM	73	C61	OCB	X	4	18.808	24.430	32.531	1.00	0.00	C
ATOM	74	C62	OCB	X	4	16.435	24.256	32.206	1.00	0.00	C
ATOM	75	C63	OCB	X	4	13.010	18.541	30.082	1.00	0.00	C
ATOM	76	C64	OCB	X	4	11.729	18.470	32.526	1.00	0.00	C
ATOM	77	C65	OCB	X	4	12.671	19.756	30.721	1.00	0.00	C
ATOM	78	C66	OCB	X	4	12.728	17.371	30.706	1.00	0.00	C
ATOM	79	C67	OCB	X	4	12.168	17.298	31.928	1.00	0.00	C
ATOM	80	C68	OCB	X	4	11.988	19.711	31.937	1.00	0.00	C
ATOM	81	O13	OCB	X	4	23.791	16.592	33.075	1.00	0.00	O
ATOM	82	O14	OCB	X	4	19.890	24.581	33.443	1.00	0.00	O
ATOM	83	O15	OCB	X	4	15.214	24.080	32.809	1.00	0.00	O
ATOM	84	O16	OCB	X	4	20.209	13.175	32.724	1.00	0.00	O
ATOM	85	O17	OCB	X	4	15.418	12.620	32.456	1.00	0.00	O
ATOM	86	O18	OCB	X	4	11.576	20.852	32.571	1.00	0.00	O

ATOM	87	O19	OCB	X	4	12.048	16.085	32.599	1.00	0.00	O
ATOM	88	C69	OCB	X	4	21.174	24.145	33.080	1.00	0.00	C
ATOM	89	C70	OCB	X	4	23.838	23.482	32.445	1.00	0.00	C
ATOM	90	C71	OCB	X	4	21.704	22.957	33.567	1.00	0.00	C
ATOM	91	C72	OCB	X	4	21.998	25.035	32.399	1.00	0.00	C
ATOM	92	C73	OCB	X	4	23.302	24.655	31.962	1.00	0.00	C
ATOM	93	C74	OCB	X	4	23.003	22.565	33.123	1.00	0.00	C
ATOM	94	O20	OCB	X	4	23.539	21.334	33.366	1.00	0.00	O
ATOM	95	C75	OCB	X	4	21.453	13.777	32.331	1.00	0.00	C
ATOM	96	C76	OCB	X	4	24.059	14.650	31.614	1.00	0.00	C
ATOM	97	C77	OCB	X	4	22.266	13.045	31.436	1.00	0.00	C
ATOM	98	C78	OCB	X	4	22.050	14.915	32.932	1.00	0.00	C
ATOM	99	C79	OCB	X	4	23.320	15.355	32.560	1.00	0.00	C
ATOM	100	C80	OCB	X	4	23.574	13.492	31.140	1.00	0.00	C
ATOM	101	C81	OCB	X	4	14.016	23.633	32.261	1.00	0.00	C
ATOM	102	C82	OCB	X	4	11.553	22.808	31.217	1.00	0.00	C
ATOM	103	C83	OCB	X	4	13.354	24.428	31.222	1.00	0.00	C
ATOM	104	C84	OCB	X	4	13.319	22.536	32.842	1.00	0.00	C
ATOM	105	C85	OCB	X	4	12.170	22.066	32.237	1.00	0.00	C
ATOM	106	C86	OCB	X	4	12.045	24.040	30.786	1.00	0.00	C
ATOM	107	C87	OCB	X	4	11.114	24.839	29.835	1.00	0.00	C
ATOM	108	O21	OCB	X	4	11.256	26.010	29.571	1.00	0.00	O
ATOM	109	C88	OCB	X	4	11.351	12.310	29.613	1.00	0.00	C
ATOM	110	O22	OCB	X	4	11.355	11.063	29.536	1.00	0.00	O
ATOM	111	C89	OCB	X	4	24.298	12.709	30.080	1.00	0.00	C
ATOM	112	O23	OCB	X	4	23.851	11.702	29.628	1.00	0.00	O
ATOM	113	O24	OCB	X	4	12.323	19.478	21.577	1.00	0.00	O
ATOM	114	O25	OCB	X	4	18.418	25.039	22.108	1.00	0.00	O
ATOM	115	O26	OCB	X	4	24.671	20.639	22.457	1.00	0.00	O
ATOM	116	C90	OCB	X	4	24.130	25.557	31.093	1.00	0.00	C
ATOM	117	O27	OCB	X	4	25.265	25.271	30.805	1.00	0.00	O
ATOM	118	O28	OCB	X	4	10.506	12.866	28.995	1.00	0.00	O
ATOM	119	O29	OCB	X	4	10.242	24.327	29.249	1.00	0.00	O
ATOM	120	O30	OCB	X	4	23.647	26.502	30.548	1.00	0.00	O
ATOM	121	O31	OCB	X	4	25.315	13.214	29.675	1.00	0.00	O
ATOM	122	O32	OCB	X	4	19.507	14.717	21.010	1.00	0.00	O
ATOM	123	C91	OCB	X	4	14.193	13.184	32.011	1.00	0.00	C
ATOM	124	C92	OCB	X	4	11.721	14.205	31.177	1.00	0.00	C
ATOM	125	C93	OCB	X	4	13.680	14.422	32.530	1.00	0.00	C
ATOM	126	C94	OCB	X	4	13.383	12.443	31.157	1.00	0.00	C
ATOM	127	C95	OCB	X	4	12.185	13.022	30.684	1.00	0.00	C
ATOM	128	C96	OCB	X	4	12.478	14.943	32.103	1.00	0.00	C
ATOM	129	C97	OCB	X	4	14.483	14.998	33.680	1.00	0.00	C
ATOM	130	C98	OCB	X	4	21.389	15.611	34.054	1.00	0.00	C
ATOM	131	C99	OCB	X	4	20.911	21.897	34.346	1.00	0.00	C
ATOM	132	C	OCB	X	4	13.826	21.958	34.203	1.00	0.00	C
ATOM	133	H1	OCB	X	4	19.402	17.826	24.927	1.00	0.00	H
ATOM	134	H2	OCB	X	4	21.118	15.865	29.053	1.00	0.00	H
ATOM	135	H3	OCB	X	4	18.221	14.378	25.863	1.00	0.00	H
ATOM	136	H4	OCB	X	4	17.905	15.746	29.016	1.00	0.00	H
ATOM	137	H5	OCB	X	4	16.670	17.555	24.658	1.00	0.00	H
ATOM	138	H6	OCB	X	4	14.684	15.550	28.712	1.00	0.00	H
ATOM	139	H7	OCB	X	4	13.514	18.993	25.841	1.00	0.00	H
ATOM	140	H8	OCB	X	4	14.929	18.485	29.018	1.00	0.00	H
ATOM	141	H9	OCB	X	4	22.761	19.082	26.242	1.00	0.00	H
ATOM	142	H10	OCB	X	4	15.065	21.841	29.219	1.00	0.00	H
ATOM	143	H11	OCB	X	4	21.393	22.290	29.125	1.00	0.00	H
ATOM	144	H12	OCB	X	4	18.218	21.954	29.330	1.00	0.00	H
ATOM	145	H13	OCB	X	4	19.664	20.393	24.891	1.00	0.00	H
ATOM	146	H14	OCB	X	4	16.564	20.464	24.655	1.00	0.00	H

ATOM	147	H15	OCB	X	4	17.943	23.660	26.122	1.00	0.00	H
ATOM	148	H16	OCB	X	4	21.128	19.094	29.319	1.00	0.00	H
ATOM	149	H17	OCB	X	4	14.275	20.201	23.815	1.00	0.00	H
ATOM	150	H18	OCB	X	4	15.492	18.937	23.575	1.00	0.00	H
ATOM	151	H19	OCB	X	4	13.947	17.219	23.124	1.00	0.00	H
ATOM	152	H20	OCB	X	4	12.604	18.190	23.754	1.00	0.00	H
ATOM	153	H21	OCB	X	4	18.313	16.544	23.690	1.00	0.00	H
ATOM	154	H22	OCB	X	4	17.178	15.254	23.563	1.00	0.00	H
ATOM	155	H23	OCB	X	4	20.099	14.743	23.530	1.00	0.00	H
ATOM	156	H24	OCB	X	4	18.840	13.559	23.874	1.00	0.00	H
ATOM	157	H25	OCB	X	4	22.670	18.122	24.281	1.00	0.00	H
ATOM	158	H26	OCB	X	4	21.172	18.725	23.757	1.00	0.00	H
ATOM	159	H27	OCB	X	4	22.071	21.007	23.543	1.00	0.00	H
ATOM	160	H28	OCB	X	4	23.503	20.638	24.508	1.00	0.00	H
ATOM	161	H29	OCB	X	4	18.116	21.640	23.890	1.00	0.00	H
ATOM	162	H30	OCB	X	4	17.074	22.937	23.932	1.00	0.00	H
ATOM	163	H31	OCB	X	4	18.887	24.531	24.454	1.00	0.00	H
ATOM	164	H32	OCB	X	4	20.161	23.276	24.045	1.00	0.00	H
ATOM	165	H33	OCB	X	4	17.774	12.534	33.650	1.00	0.00	H
ATOM	166	H34	OCB	X	4	15.764	13.500	29.912	1.00	0.00	H
ATOM	167	H35	OCB	X	4	19.983	14.138	30.421	1.00	0.00	H
ATOM	168	H36	OCB	X	4	23.820	18.840	34.287	1.00	0.00	H
ATOM	169	H37	OCB	X	4	22.708	21.303	30.877	1.00	0.00	H
ATOM	170	H38	OCB	X	4	23.059	16.969	30.619	1.00	0.00	H
ATOM	171	H39	OCB	X	4	17.375	24.608	34.119	1.00	0.00	H
ATOM	172	H40	OCB	X	4	15.783	23.595	30.294	1.00	0.00	H
ATOM	173	H41	OCB	X	4	20.007	23.971	30.760	1.00	0.00	H
ATOM	174	H42	OCB	X	4	11.186	18.420	33.467	1.00	0.00	H
ATOM	175	H43	OCB	X	4	12.938	20.689	30.233	1.00	0.00	H
ATOM	176	H44	OCB	X	4	13.103	16.514	30.152	1.00	0.00	H
ATOM	177	H45	OCB	X	4	24.811	23.205	32.047	1.00	0.00	H
ATOM	178	H46	OCB	X	4	21.501	25.949	32.085	1.00	0.00	H
ATOM	179	H47	OCB	X	4	25.019	15.023	31.266	1.00	0.00	H
ATOM	180	H48	OCB	X	4	21.747	12.223	30.951	1.00	0.00	H
ATOM	181	H49	OCB	X	4	10.543	22.507	30.952	1.00	0.00	H
ATOM	182	H50	OCB	X	4	13.889	25.176	30.643	1.00	0.00	H
ATOM	183	H51	OCB	X	4	10.789	14.592	30.773	1.00	0.00	H
ATOM	184	H52	OCB	X	4	13.745	11.526	30.700	1.00	0.00	H
ATOM	185	H53	OCB	X	4	14.590	14.332	34.539	1.00	0.00	H
ATOM	186	H54	OCB	X	4	15.479	15.234	33.300	1.00	0.00	H
ATOM	187	H55	OCB	X	4	13.902	15.870	33.987	1.00	0.00	H
ATOM	188	H56	OCB	X	4	21.895	15.348	34.985	1.00	0.00	H
ATOM	189	H57	OCB	X	4	21.477	16.696	33.959	1.00	0.00	H
ATOM	190	H58	OCB	X	4	20.353	15.300	34.203	1.00	0.00	H
ATOM	191	H59	OCB	X	4	19.967	22.285	34.734	1.00	0.00	H
ATOM	192	H60	OCB	X	4	20.651	21.049	33.709	1.00	0.00	H
ATOM	193	H61	OCB	X	4	21.598	21.511	35.103	1.00	0.00	H
ATOM	194	H62	OCB	X	4	13.350	21.047	34.569	1.00	0.00	H
ATOM	195	H63	OCB	X	4	14.895	21.741	34.260	1.00	0.00	H
ATOM	196	H64	OCB	X	4	13.696	22.715	34.979	1.00	0.00	H
ATOM	197	C1	MOL	X	5	15.764	19.550	31.959	1.00	0.00	C
ATOM	198	C2	MOL	X	5	15.931	18.200	32.701	1.00	0.00	C
ATOM	199	C3	MOL	X	5	17.090	20.350	32.006	1.00	0.00	C
ATOM	200	C4	MOL	X	5	17.560	20.510	33.482	1.00	0.00	C
ATOM	201	C5	MOL	X	5	16.371	18.425	34.145	1.00	0.00	C
ATOM	202	C6	MOL	X	5	17.753	19.187	34.285	1.00	0.00	C
ATOM	203	C7	MOL	X	5	18.793	18.284	33.416	1.00	0.00	C
ATOM	204	C8	MOL	X	5	16.998	17.385	31.936	1.00	0.00	C
ATOM	205	C9	MOL	X	5	18.131	19.571	31.268	1.00	0.00	C
ATOM	206	C10	MOL	X	5	18.348	18.165	31.975	1.00	0.00	C

ATOM	207	C11	MOL	X	5	18.151	19.288	35.719	1.00	0.00	C
ATOM	208	O1	MOL	X	5	18.973	18.568	36.215	1.00	0.00	O
ATOM	209	O2	MOL	X	5	17.512	19.958	36.528	1.00	0.00	O
ATOM	210	Br1	MOL	X	5	19.840	20.574	31.044	1.00	0.00	BR
ATOM	211	H1	MOL	X	5	15.086	20.242	32.463	1.00	0.00	H
ATOM	212	H2	MOL	X	5	15.399	19.422	30.937	1.00	0.00	H
ATOM	213	H3	MOL	X	5	14.962	17.697	32.697	1.00	0.00	H
ATOM	214	H4	MOL	X	5	16.952	21.287	31.463	1.00	0.00	H
ATOM	215	H5	MOL	X	5	16.833	21.198	33.919	1.00	0.00	H
ATOM	216	H6	MOL	X	5	18.473	21.104	33.403	1.00	0.00	H
ATOM	217	H7	MOL	X	5	16.528	17.491	34.687	1.00	0.00	H
ATOM	218	H8	MOL	X	5	15.566	18.955	34.658	1.00	0.00	H
ATOM	219	H9	MOL	X	5	19.792	18.720	33.357	1.00	0.00	H
ATOM	220	H10	MOL	X	5	18.960	17.335	33.931	1.00	0.00	H
ATOM	221	H11	MOL	X	5	16.810	17.190	30.878	1.00	0.00	H
ATOM	222	H12	MOL	X	5	17.215	16.407	32.371	1.00	0.00	H
ATOM	223	H13	MOL	X	5	17.730	19.465	30.257	1.00	0.00	H
ATOM	224	H14	MOL	X	5	18.984	17.499	31.389	1.00	0.00	H
END											

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ATOM	1	C1	OCB	X	4	22.134	24.202	29.705	1.00	0.00	C
ATOM	2	C2	OCB	X	4	24.311	22.658	30.609	1.00	0.00	C
ATOM	3	C3	OCB	X	4	22.630	23.086	28.994	1.00	0.00	C
ATOM	4	C4	OCB	X	4	22.828	24.535	30.819	1.00	0.00	C
ATOM	5	C5	OCB	X	4	24.016	23.864	31.229	1.00	0.00	C
ATOM	6	C6	OCB	X	4	23.663	22.274	29.446	1.00	0.00	C
ATOM	7	O1	OCB	X	4	25.313	21.815	31.154	1.00	0.00	O
ATOM	8	C7	OCB	X	4	23.933	20.935	28.848	1.00	0.00	C
ATOM	9	C8	OCB	X	4	24.986	20.653	31.869	1.00	0.00	C
ATOM	10	O2	OCB	X	4	25.004	19.473	31.168	1.00	0.00	O
ATOM	11	C9	OCB	X	4	23.893	19.016	30.524	1.00	0.00	C
ATOM	12	C10	OCB	X	4	23.243	19.725	29.494	1.00	0.00	C
ATOM	13	C11	OCB	X	4	22.004	19.336	28.992	1.00	0.00	C
ATOM	14	C12	OCB	X	4	23.299	17.880	31.095	1.00	0.00	C
ATOM	15	C13	OCB	X	4	21.384	18.174	29.492	1.00	0.00	C
ATOM	16	C14	OCB	X	4	22.071	17.481	30.598	1.00	0.00	C
ATOM	17	O3	OCB	X	4	21.352	16.608	31.272	1.00	0.00	O
ATOM	18	C15	OCB	X	4	19.995	17.757	28.940	1.00	0.00	C
ATOM	19	C16	OCB	X	4	18.933	18.561	29.673	1.00	0.00	C
ATOM	20	C17	OCB	X	4	18.529	18.111	30.915	1.00	0.00	C
ATOM	21	C18	OCB	X	4	20.349	17.056	32.192	1.00	0.00	C
ATOM	22	O4	OCB	X	4	19.093	16.953	31.474	1.00	0.00	O
ATOM	23	O5	OCB	X	4	22.446	25.579	31.615	1.00	0.00	O
ATOM	24	C19	OCB	X	4	20.934	24.996	29.283	1.00	0.00	C
ATOM	25	C20	OCB	X	4	19.660	24.486	29.951	1.00	0.00	C
ATOM	26	O6	OCB	X	4	19.994	26.006	31.744	1.00	0.00	O
ATOM	27	C21	OCB	X	4	19.173	25.072	31.148	1.00	0.00	C
ATOM	28	C22	OCB	X	4	17.464	18.715	31.595	1.00	0.00	C
ATOM	29	C23	OCB	X	4	16.956	19.875	31.065	1.00	0.00	C
ATOM	30	C24	OCB	X	4	18.051	24.609	31.780	1.00	0.00	C
ATOM	31	C25	OCB	X	4	17.441	23.496	31.340	1.00	0.00	C
ATOM	32	O7	OCB	X	4	16.191	20.592	31.926	1.00	0.00	O
ATOM	33	O8	OCB	X	4	16.504	23.001	32.120	1.00	0.00	O
ATOM	34	C26	OCB	X	4	16.837	21.688	32.686	1.00	0.00	C
ATOM	35	C27	OCB	X	4	18.995	23.328	29.475	1.00	0.00	C
ATOM	36	C28	OCB	X	4	17.800	22.910	30.096	1.00	0.00	C

ATOM	37	C29	OCB	X	4	18.345	19.699	29.133	1.00	0.00	C
ATOM	38	C30	OCB	X	4	16.938	21.808	29.459	1.00	0.00	C
ATOM	39	C31	OCB	X	4	17.347	20.385	29.856	1.00	0.00	C
ATOM	40	C32	OCB	X	4	21.222	25.436	32.406	1.00	0.00	C
ATOM	41	C33	OCB	X	4	19.939	17.739	27.357	1.00	0.00	C
ATOM	42	C34	OCB	X	4	19.202	16.510	26.834	1.00	0.00	C
ATOM	43	C35	OCB	X	4	18.981	16.630	25.357	1.00	0.00	C
ATOM	44	O9	OCB	X	4	19.925	16.798	24.644	1.00	0.00	O
ATOM	45	C36	OCB	X	4	23.993	20.939	27.237	1.00	0.00	C
ATOM	46	C37	OCB	X	4	24.862	22.024	26.591	1.00	0.00	C
ATOM	47	C38	OCB	X	4	25.039	21.902	25.084	1.00	0.00	C
ATOM	48	O10	OCB	X	4	25.922	21.137	24.664	1.00	0.00	O
ATOM	49	C39	OCB	X	4	20.745	25.238	27.780	1.00	0.00	C
ATOM	50	C40	OCB	X	4	21.994	25.635	26.988	1.00	0.00	C
ATOM	51	C41	OCB	X	4	21.546	26.049	25.568	1.00	0.00	C
ATOM	52	O11	OCB	X	4	21.315	27.250	25.433	1.00	0.00	O
ATOM	53	C42	OCB	X	4	16.645	22.057	27.966	1.00	0.00	C
ATOM	54	C43	OCB	X	4	15.648	21.107	27.359	1.00	0.00	C
ATOM	55	C44	OCB	X	4	15.312	21.778	26.041	1.00	0.00	C
ATOM	56	O12	OCB	X	4	14.542	22.721	26.026	1.00	0.00	O
ATOM	57	C45	OCB	X	4	25.641	20.511	33.253	1.00	0.00	C
ATOM	58	C46	OCB	X	4	26.797	20.400	35.821	1.00	0.00	C
ATOM	59	C47	OCB	X	4	25.672	19.292	33.975	1.00	0.00	C
ATOM	60	C48	OCB	X	4	26.137	21.610	33.799	1.00	0.00	C
ATOM	61	C49	OCB	X	4	26.707	21.587	35.100	1.00	0.00	C
ATOM	62	C50	OCB	X	4	26.231	19.224	35.267	1.00	0.00	C
ATOM	63	C51	OCB	X	4	21.488	26.096	33.803	1.00	0.00	C
ATOM	64	C52	OCB	X	4	21.874	26.958	36.433	1.00	0.00	C
ATOM	65	C53	OCB	X	4	20.321	26.406	34.613	1.00	0.00	C
ATOM	66	C54	OCB	X	4	22.761	26.053	34.353	1.00	0.00	C
ATOM	67	C55	OCB	X	4	22.967	26.502	35.642	1.00	0.00	C
ATOM	68	C56	OCB	X	4	20.597	26.821	35.944	1.00	0.00	C
ATOM	69	C57	OCB	X	4	16.346	21.722	34.153	1.00	0.00	C
ATOM	70	C58	OCB	X	4	15.389	21.705	36.831	1.00	0.00	C
ATOM	71	C59	OCB	X	4	16.027	20.497	34.807	1.00	0.00	C
ATOM	72	C60	OCB	X	4	16.335	22.879	34.909	1.00	0.00	C
ATOM	73	C61	OCB	X	4	15.864	22.895	36.244	1.00	0.00	C
ATOM	74	C62	OCB	X	4	15.473	20.516	36.083	1.00	0.00	C
ATOM	75	C63	OCB	X	4	20.413	16.409	33.560	1.00	0.00	C
ATOM	76	C64	OCB	X	4	20.417	15.280	36.093	1.00	0.00	C
ATOM	77	C65	OCB	X	4	19.247	16.466	34.373	1.00	0.00	C
ATOM	78	C66	OCB	X	4	21.592	15.845	34.097	1.00	0.00	C
ATOM	79	C67	OCB	X	4	21.624	15.428	35.377	1.00	0.00	C
ATOM	80	C68	OCB	X	4	19.271	15.884	35.664	1.00	0.00	C
ATOM	81	O13	OCB	X	4	24.238	26.571	36.143	1.00	0.00	O
ATOM	82	O14	OCB	X	4	15.839	24.029	36.975	1.00	0.00	O
ATOM	83	O15	OCB	X	4	15.031	19.340	36.619	1.00	0.00	O
ATOM	84	O16	OCB	X	4	27.314	22.721	35.562	1.00	0.00	O
ATOM	85	O17	OCB	X	4	26.495	17.997	35.821	1.00	0.00	O
ATOM	86	O18	OCB	X	4	18.210	15.765	36.469	1.00	0.00	O
ATOM	87	O19	OCB	X	4	22.771	15.008	36.017	1.00	0.00	O
ATOM	88	C69	OCB	X	4	16.516	25.150	36.571	1.00	0.00	C
ATOM	89	C70	OCB	X	4	17.564	27.552	35.876	1.00	0.00	C
ATOM	90	C71	OCB	X	4	17.781	25.452	36.964	1.00	0.00	C
ATOM	91	C72	OCB	X	4	15.692	26.060	35.816	1.00	0.00	C
ATOM	92	C73	OCB	X	4	16.229	27.286	35.491	1.00	0.00	C
ATOM	93	C74	OCB	X	4	18.324	26.650	36.571	1.00	0.00	C
ATOM	94	O20	OCB	X	4	19.588	27.067	36.812	1.00	0.00	O
ATOM	95	C75	OCB	X	4	26.849	24.079	35.295	1.00	0.00	C
ATOM	96	C76	OCB	X	4	26.184	26.832	34.973	1.00	0.00	C

ATOM	97	C77	OCB	X	4	27.643	24.970	34.566	1.00	0.00	C
ATOM	98	C78	OCB	X	4	25.712	24.653	35.953	1.00	0.00	C
ATOM	99	C79	OCB	X	4	25.379	25.996	35.726	1.00	0.00	C
ATOM	100	C80	OCB	X	4	27.325	26.306	34.331	1.00	0.00	C
ATOM	101	C81	OCB	X	4	15.399	18.067	36.251	1.00	0.00	C
ATOM	102	C82	OCB	X	4	15.982	15.353	36.006	1.00	0.00	C
ATOM	103	C83	OCB	X	4	14.385	17.129	35.922	1.00	0.00	C
ATOM	104	C84	OCB	X	4	16.703	17.623	36.481	1.00	0.00	C
ATOM	105	C85	OCB	X	4	16.956	16.245	36.357	1.00	0.00	C
ATOM	106	C86	OCB	X	4	14.690	15.790	35.708	1.00	0.00	C
ATOM	107	C87	OCB	X	4	13.667	14.746	35.357	1.00	0.00	C
ATOM	108	O21	OCB	X	4	13.828	13.605	35.696	1.00	0.00	O
ATOM	109	C88	OCB	X	4	26.882	13.652	33.494	1.00	0.00	C
ATOM	110	O22	OCB	X	4	28.014	13.947	33.075	1.00	0.00	O
ATOM	111	C89	OCB	X	4	28.186	27.246	33.438	1.00	0.00	C
ATOM	112	O23	OCB	X	4	29.098	26.758	32.769	1.00	0.00	O
ATOM	113	O24	OCB	X	4	17.811	16.389	24.896	1.00	0.00	O
ATOM	114	O25	OCB	X	4	15.656	21.269	24.926	1.00	0.00	O
ATOM	115	O26	OCB	X	4	21.164	25.268	24.708	1.00	0.00	O
ATOM	116	C90	OCB	X	4	15.301	28.352	34.832	1.00	0.00	C
ATOM	117	O27	OCB	X	4	15.770	29.462	34.553	1.00	0.00	O
ATOM	118	O28	OCB	X	4	26.351	12.653	33.093	1.00	0.00	O
ATOM	119	O29	OCB	X	4	12.733	15.028	34.667	1.00	0.00	O
ATOM	120	O30	OCB	X	4	14.101	28.217	34.876	1.00	0.00	O
ATOM	121	O31	OCB	X	4	27.946	28.417	33.477	1.00	0.00	O
ATOM	122	O32	OCB	X	4	24.243	22.490	24.379	1.00	0.00	O
ATOM	123	C91	OCB	X	4	25.908	16.780	35.460	1.00	0.00	C
ATOM	124	C92	OCB	X	4	24.778	14.271	34.820	1.00	0.00	C
ATOM	125	C93	OCB	X	4	24.668	16.429	35.941	1.00	0.00	C
ATOM	126	C94	OCB	X	4	26.564	15.890	34.604	1.00	0.00	C
ATOM	127	C95	OCB	X	4	26.094	14.625	34.320	1.00	0.00	C
ATOM	128	C96	OCB	X	4	24.096	15.186	35.645	1.00	0.00	C
ATOM	129	C97	OCB	X	4	23.838	17.431	36.877	1.00	0.00	C
ATOM	130	C98	OCB	X	4	24.770	23.689	36.683	1.00	0.00	C
ATOM	131	C99	OCB	X	4	18.694	24.496	37.830	1.00	0.00	C
ATOM	132	C	OCB	X	4	17.803	18.510	36.954	1.00	0.00	C
ATOM	133	H1	OCB	X	4	22.055	22.805	28.115	1.00	0.00	H
ATOM	134	H2	OCB	X	4	24.486	24.151	32.166	1.00	0.00	H
ATOM	135	H3	OCB	X	4	24.990	20.809	29.091	1.00	0.00	H
ATOM	136	H4	OCB	X	4	23.947	20.916	32.117	1.00	0.00	H
ATOM	137	H5	OCB	X	4	21.615	19.808	28.093	1.00	0.00	H
ATOM	138	H6	OCB	X	4	23.873	17.462	31.917	1.00	0.00	H
ATOM	139	H7	OCB	X	4	19.750	16.720	29.177	1.00	0.00	H
ATOM	140	H8	OCB	X	4	20.451	18.147	32.293	1.00	0.00	H
ATOM	141	H9	OCB	X	4	21.037	26.027	29.628	1.00	0.00	H
ATOM	142	H10	OCB	X	4	17.075	18.394	32.558	1.00	0.00	H
ATOM	143	H11	OCB	X	4	17.686	25.119	32.667	1.00	0.00	H
ATOM	144	H12	OCB	X	4	17.923	21.539	32.779	1.00	0.00	H
ATOM	145	H13	OCB	X	4	19.336	22.677	28.674	1.00	0.00	H
ATOM	146	H14	OCB	X	4	18.696	20.041	28.163	1.00	0.00	H
ATOM	147	H15	OCB	X	4	15.961	21.988	29.912	1.00	0.00	H
ATOM	148	H16	OCB	X	4	21.062	24.369	32.619	1.00	0.00	H
ATOM	149	H17	OCB	X	4	19.469	18.632	26.940	1.00	0.00	H
ATOM	150	H18	OCB	X	4	20.894	17.785	26.828	1.00	0.00	H
ATOM	151	H19	OCB	X	4	19.834	15.654	27.077	1.00	0.00	H
ATOM	152	H20	OCB	X	4	18.264	16.289	27.348	1.00	0.00	H
ATOM	153	H21	OCB	X	4	22.969	21.141	26.914	1.00	0.00	H
ATOM	154	H22	OCB	X	4	24.269	19.941	26.892	1.00	0.00	H
ATOM	155	H23	OCB	X	4	24.456	22.981	26.927	1.00	0.00	H
ATOM	156	H24	OCB	X	4	25.902	22.006	26.925	1.00	0.00	H

ATOM	157	H25	OCB	X	4	20.304	24.324	27.379	1.00	0.00	H
ATOM	158	H26	OCB	X	4	20.084	26.100	27.662	1.00	0.00	H
ATOM	159	H27	OCB	X	4	22.514	26.464	27.473	1.00	0.00	H
ATOM	160	H28	OCB	X	4	22.691	24.795	26.943	1.00	0.00	H
ATOM	161	H29	OCB	X	4	16.331	23.094	27.827	1.00	0.00	H
ATOM	162	H30	OCB	X	4	17.535	22.016	27.335	1.00	0.00	H
ATOM	163	H31	OCB	X	4	15.955	20.067	27.228	1.00	0.00	H
ATOM	164	H32	OCB	X	4	14.761	21.101	27.996	1.00	0.00	H
ATOM	165	H33	OCB	X	4	27.413	20.402	36.718	1.00	0.00	H
ATOM	166	H34	OCB	X	4	25.325	18.341	33.577	1.00	0.00	H
ATOM	167	H35	OCB	X	4	26.068	22.567	33.290	1.00	0.00	H
ATOM	168	H36	OCB	X	4	22.107	27.231	37.459	1.00	0.00	H
ATOM	169	H37	OCB	X	4	19.318	26.257	34.221	1.00	0.00	H
ATOM	170	H38	OCB	X	4	23.651	25.766	33.799	1.00	0.00	H
ATOM	171	H39	OCB	X	4	14.838	21.795	37.764	1.00	0.00	H
ATOM	172	H40	OCB	X	4	16.174	19.590	34.226	1.00	0.00	H
ATOM	173	H41	OCB	X	4	16.630	23.818	34.449	1.00	0.00	H
ATOM	174	H42	OCB	X	4	20.392	14.909	37.114	1.00	0.00	H
ATOM	175	H43	OCB	X	4	18.333	17.004	34.133	1.00	0.00	H
ATOM	176	H44	OCB	X	4	22.492	15.745	33.496	1.00	0.00	H
ATOM	177	H45	OCB	X	4	17.985	28.490	35.524	1.00	0.00	H
ATOM	178	H46	OCB	X	4	14.655	25.801	35.621	1.00	0.00	H
ATOM	179	H47	OCB	X	4	25.754	27.772	34.637	1.00	0.00	H
ATOM	180	H48	OCB	X	4	28.608	24.674	34.163	1.00	0.00	H
ATOM	181	H49	OCB	X	4	16.092	14.272	36.014	1.00	0.00	H
ATOM	182	H50	OCB	X	4	13.382	17.516	35.760	1.00	0.00	H
ATOM	183	H51	OCB	X	4	24.272	13.380	34.457	1.00	0.00	H
ATOM	184	H52	OCB	X	4	27.572	16.147	34.288	1.00	0.00	H
ATOM	185	H53	OCB	X	4	22.813	17.423	36.500	1.00	0.00	H
ATOM	186	H54	OCB	X	4	24.004	16.922	37.829	1.00	0.00	H
ATOM	187	H55	OCB	X	4	24.249	18.434	37.010	1.00	0.00	H
ATOM	188	H56	OCB	X	4	24.082	23.234	35.967	1.00	0.00	H
ATOM	189	H57	OCB	X	4	25.294	22.893	37.217	1.00	0.00	H
ATOM	190	H58	OCB	X	4	24.142	24.291	37.342	1.00	0.00	H
ATOM	191	H59	OCB	X	4	18.431	23.438	37.757	1.00	0.00	H
ATOM	192	H60	OCB	X	4	19.742	24.575	37.533	1.00	0.00	H
ATOM	193	H61	OCB	X	4	18.657	24.782	38.883	1.00	0.00	H
ATOM	194	H62	OCB	X	4	17.502	19.370	37.557	1.00	0.00	H
ATOM	195	H63	OCB	X	4	18.529	17.927	37.523	1.00	0.00	H
ATOM	196	H64	OCB	X	4	18.272	18.868	36.035	1.00	0.00	H
ATOM	197	C1	MOL	X	5	20.542	21.530	32.908	1.00	0.00	C
ATOM	198	C2	MOL	X	5	19.898	22.331	33.880	1.00	0.00	C
ATOM	199	C3	MOL	X	5	20.061	22.074	35.222	1.00	0.00	C
ATOM	200	C4	MOL	X	5	20.850	20.985	35.634	1.00	0.00	C
ATOM	201	C5	MOL	X	5	21.524	20.267	34.671	1.00	0.00	C
ATOM	202	C6	MOL	X	5	21.397	20.531	33.267	1.00	0.00	C
ATOM	203	C7	MOL	X	5	21.019	20.605	37.120	1.00	0.00	C
ATOM	204	C8	MOL	X	5	21.987	21.637	37.767	1.00	0.00	C
ATOM	205	N1	MOL	X	5	22.348	21.391	39.236	1.00	0.00	N
ATOM	206	C9	MOL	X	5	23.171	22.546	39.829	1.00	0.00	C
ATOM	207	C10	MOL	X	5	23.207	20.124	39.335	1.00	0.00	C
ATOM	208	C11	MOL	X	5	21.098	21.053	40.042	1.00	0.00	C
ATOM	209	H1	MOL	X	5	22.558	23.448	39.819	1.00	0.00	H
ATOM	210	H2	MOL	X	5	24.059	22.763	39.235	1.00	0.00	H
ATOM	211	H3	MOL	X	5	23.432	22.313	40.863	1.00	0.00	H
ATOM	212	H4	MOL	X	5	23.987	20.042	38.577	1.00	0.00	H
ATOM	213	H5	MOL	X	5	22.674	19.193	39.137	1.00	0.00	H
ATOM	214	H6	MOL	X	5	23.669	20.124	40.323	1.00	0.00	H
ATOM	215	H7	MOL	X	5	20.419	21.903	39.960	1.00	0.00	H
ATOM	216	H8	MOL	X	5	21.346	20.847	41.085	1.00	0.00	H

ATOM	217	H9	MOL	X	5	20.685	20.154	39.582	1.00	0.00	H
ATOM	218	H10	MOL	X	5	20.537	21.762	31.847	1.00	0.00	H
ATOM	219	H11	MOL	X	5	19.221	23.142	33.623	1.00	0.00	H
ATOM	220	H12	MOL	X	5	19.603	22.708	35.977	1.00	0.00	H
ATOM	221	H13	MOL	X	5	22.234	19.480	34.912	1.00	0.00	H
ATOM	222	H14	MOL	X	5	22.029	19.952	32.599	1.00	0.00	H
ATOM	223	H15	MOL	X	5	20.014	20.629	37.547	1.00	0.00	H
ATOM	224	H16	MOL	X	5	21.321	19.558	37.198	1.00	0.00	H
ATOM	225	H17	MOL	X	5	22.873	21.654	37.131	1.00	0.00	H
ATOM	226	H18	MOL	X	5	21.421	22.565	37.863	1.00	0.00	H
END											

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ATOM	1	C1	OCB	X	4	21.698	23.929	29.364	1.00	0.00	C
ATOM	2	C2	OCB	X	4	23.942	22.554	30.387	1.00	0.00	C
ATOM	3	C3	OCB	X	4	22.278	22.887	28.686	1.00	0.00	C
ATOM	4	C4	OCB	X	4	22.305	24.303	30.565	1.00	0.00	C
ATOM	5	C5	OCB	X	4	23.414	23.641	31.085	1.00	0.00	C
ATOM	6	C6	OCB	X	4	23.324	22.155	29.175	1.00	0.00	C
ATOM	7	O1	OCB	X	4	25.071	21.942	30.868	1.00	0.00	O
ATOM	8	C7	OCB	X	4	23.906	20.991	28.378	1.00	0.00	C
ATOM	9	C8	OCB	X	4	24.885	20.621	31.519	1.00	0.00	C
ATOM	10	O2	OCB	X	4	25.106	19.580	30.601	1.00	0.00	O
ATOM	11	C9	OCB	X	4	24.031	19.045	29.964	1.00	0.00	C
ATOM	12	C10	OCB	X	4	23.358	19.711	28.950	1.00	0.00	C
ATOM	13	C11	OCB	X	4	22.162	19.148	28.389	1.00	0.00	C
ATOM	14	C12	OCB	X	4	23.412	17.986	30.599	1.00	0.00	C
ATOM	15	C13	OCB	X	4	21.604	18.039	29.031	1.00	0.00	C
ATOM	16	C14	OCB	X	4	22.236	17.466	30.195	1.00	0.00	C
ATOM	17	O3	OCB	X	4	21.643	16.424	30.886	1.00	0.00	O
ATOM	18	C15	OCB	X	4	20.315	17.546	28.498	1.00	0.00	C
ATOM	19	C16	OCB	X	4	19.233	18.228	29.305	1.00	0.00	C
ATOM	20	C17	OCB	X	4	18.671	17.617	30.438	1.00	0.00	C
ATOM	21	C18	OCB	X	4	20.535	16.796	31.818	1.00	0.00	C
ATOM	22	O4	OCB	X	4	19.273	16.547	31.074	1.00	0.00	O
ATOM	23	O5	OCB	X	4	21.977	25.447	31.286	1.00	0.00	O
ATOM	24	C19	OCB	X	4	20.530	24.833	28.811	1.00	0.00	C
ATOM	25	C20	OCB	X	4	19.275	24.276	29.450	1.00	0.00	C
ATOM	26	O6	OCB	X	4	19.654	25.625	31.486	1.00	0.00	O
ATOM	27	C21	OCB	X	4	18.979	24.693	30.768	1.00	0.00	C
ATOM	28	C22	OCB	X	4	17.703	18.283	31.248	1.00	0.00	C
ATOM	29	C23	OCB	X	4	17.143	19.447	30.855	1.00	0.00	C
ATOM	30	C24	OCB	X	4	17.872	24.119	31.487	1.00	0.00	C
ATOM	31	C25	OCB	X	4	17.228	23.026	30.921	1.00	0.00	C
ATOM	32	O7	OCB	X	4	16.290	20.068	31.750	1.00	0.00	O
ATOM	33	O8	OCB	X	4	16.344	22.406	31.828	1.00	0.00	O
ATOM	34	C26	OCB	X	4	16.827	21.174	32.445	1.00	0.00	C
ATOM	35	C27	OCB	X	4	18.627	23.117	28.962	1.00	0.00	C
ATOM	36	C28	OCB	X	4	17.541	22.494	29.660	1.00	0.00	C
ATOM	37	C29	OCB	X	4	18.636	19.413	28.870	1.00	0.00	C
ATOM	38	C30	OCB	X	4	16.828	21.259	29.144	1.00	0.00	C
ATOM	39	C31	OCB	X	4	17.549	19.982	29.638	1.00	0.00	C
ATOM	40	C32	OCB	X	4	20.840	25.205	32.094	1.00	0.00	C
ATOM	41	C33	OCB	X	4	20.286	17.540	26.924	1.00	0.00	C
ATOM	42	C34	OCB	X	4	19.144	16.724	26.379	1.00	0.00	C
ATOM	43	C35	OCB	X	4	19.255	16.565	24.897	1.00	0.00	C
ATOM	44	O9	OCB	X	4	20.251	16.079	24.391	1.00	0.00	O

ATOM	45	C36	OCB	X	4	23.789	21.053	26.794	1.00	0.00	C
ATOM	46	C37	OCB	X	4	24.780	22.052	26.300	1.00	0.00	C
ATOM	47	C38	OCB	X	4	24.903	22.039	24.792	1.00	0.00	C
ATOM	48	O10	OCB	X	4	24.139	22.710	24.120	1.00	0.00	O
ATOM	49	C39	OCB	X	4	20.539	24.903	27.279	1.00	0.00	C
ATOM	50	C40	OCB	X	4	19.526	26.010	26.793	1.00	0.00	C
ATOM	51	C41	OCB	X	4	20.015	26.692	25.524	1.00	0.00	C
ATOM	52	O11	OCB	X	4	19.498	26.533	24.464	1.00	0.00	O
ATOM	53	C42	OCB	X	4	16.478	21.543	27.677	1.00	0.00	C
ATOM	54	C43	OCB	X	4	15.769	20.314	26.998	1.00	0.00	C
ATOM	55	C44	OCB	X	4	15.133	20.760	25.714	1.00	0.00	C
ATOM	56	O12	OCB	X	4	14.194	21.565	25.636	1.00	0.00	O
ATOM	57	C45	OCB	X	4	25.772	20.484	32.766	1.00	0.00	C
ATOM	58	C46	OCB	X	4	27.125	20.389	35.232	1.00	0.00	C
ATOM	59	C47	OCB	X	4	26.096	19.267	33.338	1.00	0.00	C
ATOM	60	C48	OCB	X	4	26.083	21.648	33.466	1.00	0.00	C
ATOM	61	C49	OCB	X	4	26.706	21.594	34.719	1.00	0.00	C
ATOM	62	C50	OCB	X	4	26.798	19.206	34.520	1.00	0.00	C
ATOM	63	C51	OCB	X	4	20.964	25.838	33.490	1.00	0.00	C
ATOM	64	C52	OCB	X	4	21.080	26.353	36.242	1.00	0.00	C
ATOM	65	C53	OCB	X	4	19.804	26.156	34.219	1.00	0.00	C
ATOM	66	C54	OCB	X	4	22.174	25.774	34.124	1.00	0.00	C
ATOM	67	C55	OCB	X	4	22.213	26.039	35.468	1.00	0.00	C
ATOM	68	C56	OCB	X	4	19.890	26.400	35.577	1.00	0.00	C
ATOM	69	C57	OCB	X	4	16.380	21.105	33.930	1.00	0.00	C
ATOM	70	C58	OCB	X	4	15.475	21.001	36.595	1.00	0.00	C
ATOM	71	C59	OCB	X	4	16.360	19.897	34.632	1.00	0.00	C
ATOM	72	C60	OCB	X	4	15.885	22.279	34.550	1.00	0.00	C
ATOM	73	C61	OCB	X	4	15.463	22.195	35.883	1.00	0.00	C
ATOM	74	C62	OCB	X	4	15.971	19.867	35.941	1.00	0.00	C
ATOM	75	C63	OCB	X	4	20.752	16.035	33.118	1.00	0.00	C
ATOM	76	C64	OCB	X	4	21.009	14.807	35.679	1.00	0.00	C
ATOM	77	C65	OCB	X	4	19.648	15.603	33.829	1.00	0.00	C
ATOM	78	C66	OCB	X	4	22.047	15.812	33.631	1.00	0.00	C
ATOM	79	C67	OCB	X	4	22.095	15.233	34.927	1.00	0.00	C
ATOM	80	C68	OCB	X	4	19.796	14.998	35.101	1.00	0.00	C
ATOM	81	O13	OCB	X	4	23.350	25.960	36.190	1.00	0.00	O
ATOM	82	O14	OCB	X	4	15.175	23.381	36.526	1.00	0.00	O
ATOM	83	O15	OCB	X	4	16.059	18.710	36.671	1.00	0.00	O
ATOM	84	O16	OCB	X	4	26.910	22.711	35.441	1.00	0.00	O
ATOM	85	O17	OCB	X	4	27.109	18.009	35.061	1.00	0.00	O
ATOM	86	O18	OCB	X	4	18.697	14.685	35.887	1.00	0.00	O
ATOM	87	O19	OCB	X	4	23.300	15.161	35.630	1.00	0.00	O
ATOM	88	C69	OCB	X	4	15.746	24.536	36.188	1.00	0.00	C
ATOM	89	C70	OCB	X	4	16.573	27.115	35.512	1.00	0.00	C
ATOM	90	C71	OCB	X	4	17.059	24.945	36.548	1.00	0.00	C
ATOM	91	C72	OCB	X	4	14.853	25.425	35.675	1.00	0.00	C
ATOM	92	C73	OCB	X	4	15.256	26.731	35.216	1.00	0.00	C
ATOM	93	C74	OCB	X	4	17.473	26.236	36.169	1.00	0.00	C
ATOM	94	O20	OCB	X	4	18.776	26.622	36.358	1.00	0.00	O
ATOM	95	C75	OCB	X	4	26.339	23.971	35.348	1.00	0.00	C
ATOM	96	C76	OCB	X	4	25.281	26.500	34.897	1.00	0.00	C
ATOM	97	C77	OCB	X	4	27.048	24.905	34.603	1.00	0.00	C
ATOM	98	C78	OCB	X	4	25.074	24.303	35.763	1.00	0.00	C
ATOM	99	C79	OCB	X	4	24.583	25.595	35.616	1.00	0.00	C
ATOM	100	C80	OCB	X	4	26.476	26.126	34.283	1.00	0.00	C
ATOM	101	C81	OCB	X	4	16.323	17.428	36.255	1.00	0.00	C
ATOM	102	C82	OCB	X	4	16.497	14.927	35.308	1.00	0.00	C
ATOM	103	C83	OCB	X	4	15.199	16.875	35.504	1.00	0.00	C
ATOM	104	C84	OCB	X	4	17.532	16.790	36.467	1.00	0.00	C

ATOM	105	C85	OCB	X	4	17.586	15.468	36.026	1.00	0.00	C
ATOM	106	C86	OCB	X	4	15.337	15.607	34.984	1.00	0.00	C
ATOM	107	C87	OCB	X	4	14.178	14.934	34.253	1.00	0.00	C
ATOM	108	O21	OCB	X	4	13.149	15.534	34.012	1.00	0.00	O
ATOM	109	C88	OCB	X	4	26.693	13.805	32.238	1.00	0.00	C
ATOM	110	O22	OCB	X	4	27.596	14.021	31.468	1.00	0.00	O
ATOM	111	C89	OCB	X	4	27.346	27.143	33.560	1.00	0.00	C
ATOM	112	O23	OCB	X	4	26.956	28.252	33.457	1.00	0.00	O
ATOM	113	O24	OCB	X	4	18.482	17.131	24.162	1.00	0.00	O
ATOM	114	O25	OCB	X	4	15.641	20.430	24.668	1.00	0.00	O
ATOM	115	O26	OCB	X	4	20.932	27.462	25.534	1.00	0.00	O
ATOM	116	C90	OCB	X	4	14.329	27.636	34.552	1.00	0.00	C
ATOM	117	O27	OCB	X	4	13.246	27.213	34.215	1.00	0.00	O
ATOM	118	O28	OCB	X	4	26.054	12.798	32.029	1.00	0.00	O
ATOM	119	O29	OCB	X	4	14.298	13.774	33.891	1.00	0.00	O
ATOM	120	O30	OCB	X	4	14.634	28.719	34.240	1.00	0.00	O
ATOM	121	O31	OCB	X	4	28.481	26.975	33.234	1.00	0.00	O
ATOM	122	O32	OCB	X	4	25.610	21.241	24.172	1.00	0.00	O
ATOM	123	C91	OCB	X	4	26.428	16.857	34.731	1.00	0.00	C
ATOM	124	C92	OCB	X	4	25.040	14.560	34.083	1.00	0.00	C
ATOM	125	C93	OCB	X	4	25.288	16.504	35.406	1.00	0.00	C
ATOM	126	C94	OCB	X	4	26.908	16.041	33.661	1.00	0.00	C
ATOM	127	C95	OCB	X	4	26.243	14.846	33.310	1.00	0.00	C
ATOM	128	C96	OCB	X	4	24.501	15.421	34.988	1.00	0.00	C
ATOM	129	C97	OCB	X	4	24.848	17.347	36.600	1.00	0.00	C
ATOM	130	C98	OCB	X	4	24.371	23.266	36.608	1.00	0.00	C
ATOM	131	C99	OCB	X	4	18.043	23.981	37.166	1.00	0.00	C
ATOM	132	C	OCB	X	4	18.674	17.439	37.252	1.00	0.00	C
ATOM	133	H1	OCB	X	4	21.878	22.597	27.718	1.00	0.00	H
ATOM	134	H2	OCB	X	4	23.938	24.014	31.961	1.00	0.00	H
ATOM	135	H3	OCB	X	4	24.976	20.948	28.590	1.00	0.00	H
ATOM	136	H4	OCB	X	4	23.864	20.564	31.925	1.00	0.00	H
ATOM	137	H5	OCB	X	4	21.717	19.570	27.492	1.00	0.00	H
ATOM	138	H6	OCB	X	4	23.953	17.502	31.408	1.00	0.00	H
ATOM	139	H7	OCB	X	4	20.259	16.510	28.839	1.00	0.00	H
ATOM	140	H8	OCB	X	4	20.624	17.849	32.123	1.00	0.00	H
ATOM	141	H9	OCB	X	4	20.769	25.834	29.176	1.00	0.00	H
ATOM	142	H10	OCB	X	4	17.474	17.885	32.234	1.00	0.00	H
ATOM	143	H11	OCB	X	4	17.737	24.411	32.526	1.00	0.00	H
ATOM	144	H12	OCB	X	4	17.918	21.105	32.572	1.00	0.00	H
ATOM	145	H13	OCB	X	4	18.921	22.690	28.007	1.00	0.00	H
ATOM	146	H14	OCB	X	4	19.002	19.862	27.950	1.00	0.00	H
ATOM	147	H15	OCB	X	4	15.857	21.357	29.635	1.00	0.00	H
ATOM	148	H16	OCB	X	4	20.856	24.109	32.180	1.00	0.00	H
ATOM	149	H17	OCB	X	4	20.265	18.547	26.502	1.00	0.00	H
ATOM	150	H18	OCB	X	4	21.202	17.045	26.595	1.00	0.00	H
ATOM	151	H19	OCB	X	4	19.165	15.730	26.832	1.00	0.00	H
ATOM	152	H20	OCB	X	4	18.152	17.122	26.604	1.00	0.00	H
ATOM	153	H21	OCB	X	4	22.809	21.402	26.460	1.00	0.00	H
ATOM	154	H22	OCB	X	4	24.102	20.088	26.390	1.00	0.00	H
ATOM	155	H23	OCB	X	4	24.418	23.005	26.692	1.00	0.00	H
ATOM	156	H24	OCB	X	4	25.761	21.798	26.707	1.00	0.00	H
ATOM	157	H25	OCB	X	4	21.555	25.109	26.935	1.00	0.00	H
ATOM	158	H26	OCB	X	4	20.244	23.931	26.877	1.00	0.00	H
ATOM	159	H27	OCB	X	4	18.564	25.517	26.636	1.00	0.00	H
ATOM	160	H28	OCB	X	4	19.539	26.829	27.516	1.00	0.00	H
ATOM	161	H29	OCB	X	4	15.824	22.416	27.723	1.00	0.00	H
ATOM	162	H30	OCB	X	4	17.342	21.750	27.042	1.00	0.00	H
ATOM	163	H31	OCB	X	4	16.433	19.471	26.795	1.00	0.00	H
ATOM	164	H32	OCB	X	4	14.949	19.940	27.614	1.00	0.00	H

ATOM	165	H33	OCB	X	4	27.634	20.435	36.191	1.00	0.00	H
ATOM	166	H34	OCB	X	4	25.768	18.344	32.868	1.00	0.00	H
ATOM	167	H35	OCB	X	4	25.701	22.604	33.116	1.00	0.00	H
ATOM	168	H36	OCB	X	4	20.920	26.557	37.297	1.00	0.00	H
ATOM	169	H37	OCB	X	4	18.818	26.167	33.762	1.00	0.00	H
ATOM	170	H38	OCB	X	4	23.007	25.345	33.573	1.00	0.00	H
ATOM	171	H39	OCB	X	4	15.286	20.992	37.665	1.00	0.00	H
ATOM	172	H40	OCB	X	4	16.716	19.058	34.039	1.00	0.00	H
ATOM	173	H41	OCB	X	4	15.766	23.251	34.077	1.00	0.00	H
ATOM	174	H42	OCB	X	4	21.150	14.517	36.718	1.00	0.00	H
ATOM	175	H43	OCB	X	4	18.640	15.819	33.484	1.00	0.00	H
ATOM	176	H44	OCB	X	4	22.914	16.261	33.153	1.00	0.00	H
ATOM	177	H45	OCB	X	4	16.881	28.127	35.263	1.00	0.00	H
ATOM	178	H46	OCB	X	4	13.837	25.062	35.542	1.00	0.00	H
ATOM	179	H47	OCB	X	4	24.959	27.537	34.949	1.00	0.00	H
ATOM	180	H48	OCB	X	4	28.026	24.713	34.170	1.00	0.00	H
ATOM	181	H49	OCB	X	4	16.706	13.900	35.019	1.00	0.00	H
ATOM	182	H50	OCB	X	4	14.289	17.449	35.346	1.00	0.00	H
ATOM	183	H51	OCB	X	4	24.588	13.573	34.031	1.00	0.00	H
ATOM	184	H52	OCB	X	4	27.856	16.327	33.211	1.00	0.00	H
ATOM	185	H53	OCB	X	4	24.055	16.990	37.261	1.00	0.00	H
ATOM	186	H54	OCB	X	4	25.757	17.226	37.192	1.00	0.00	H
ATOM	187	H55	OCB	X	4	24.763	18.374	36.238	1.00	0.00	H
ATOM	188	H56	OCB	X	4	23.480	23.522	37.185	1.00	0.00	H
ATOM	189	H57	OCB	X	4	24.107	22.481	35.895	1.00	0.00	H
ATOM	190	H58	OCB	X	4	25.090	22.878	37.332	1.00	0.00	H
ATOM	191	H59	OCB	X	4	18.078	23.058	36.583	1.00	0.00	H
ATOM	192	H60	OCB	X	4	19.020	24.379	37.449	1.00	0.00	H
ATOM	193	H61	OCB	X	4	17.595	23.709	38.124	1.00	0.00	H
ATOM	194	H62	OCB	X	4	19.612	16.945	36.991	1.00	0.00	H
ATOM	195	H63	OCB	X	4	18.764	18.489	36.964	1.00	0.00	H
ATOM	196	H64	OCB	X	4	18.421	17.354	38.311	1.00	0.00	H
ATOM	197	O1	MOL	X	5	19.531	22.558	34.023	1.00	0.00	O
ATOM	198	O2	MOL	X	5	20.990	21.783	32.668	1.00	0.00	O
ATOM	199	N1	MOL	X	5	20.331	21.687	33.681	1.00	0.00	N
ATOM	200	C1	MOL	X	5	20.935	20.863	34.785	1.00	0.00	C
ATOM	201	C2	MOL	X	5	20.660	21.134	36.163	1.00	0.00	C
ATOM	202	C3	MOL	X	5	21.710	19.686	34.563	1.00	0.00	C
ATOM	203	C4	MOL	X	5	21.142	20.244	37.218	1.00	0.00	C
ATOM	204	C5	MOL	X	5	22.083	18.793	35.574	1.00	0.00	C
ATOM	205	C6	MOL	X	5	21.773	19.042	36.880	1.00	0.00	C
ATOM	206	C7	MOL	X	5	20.774	20.569	38.560	1.00	0.00	C
ATOM	207	O3	MOL	X	5	20.158	21.591	38.798	1.00	0.00	O
ATOM	208	O4	MOL	X	5	21.080	19.850	39.499	1.00	0.00	O
ATOM	209	H1	MOL	X	5	20.122	21.993	36.554	1.00	0.00	H
ATOM	210	H2	MOL	X	5	21.956	19.468	33.527	1.00	0.00	H
ATOM	211	H3	MOL	X	5	22.560	17.848	35.329	1.00	0.00	H
ATOM	212	H4	MOL	X	5	22.077	18.327	37.641	1.00	0.00	H
END											