

The Catalytic Formation of Leukotriene C₄: A Tale of Two Orientations

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Supporting Information

Discussion S1, Table S1, Table S2, Figure S1-S6 and Table S3 (198 pages total)

Discussion S1: Complete discussion of the QM/MM model for the second binding orientation ('head-to-tail').

QM/MM Calculations for the 'head-to-tail' model: The calculations were repeated for the 'head-to-tail' orientation with all appropriate bond lengths and bond angles for the reactant and products shown in **Figure S1**.

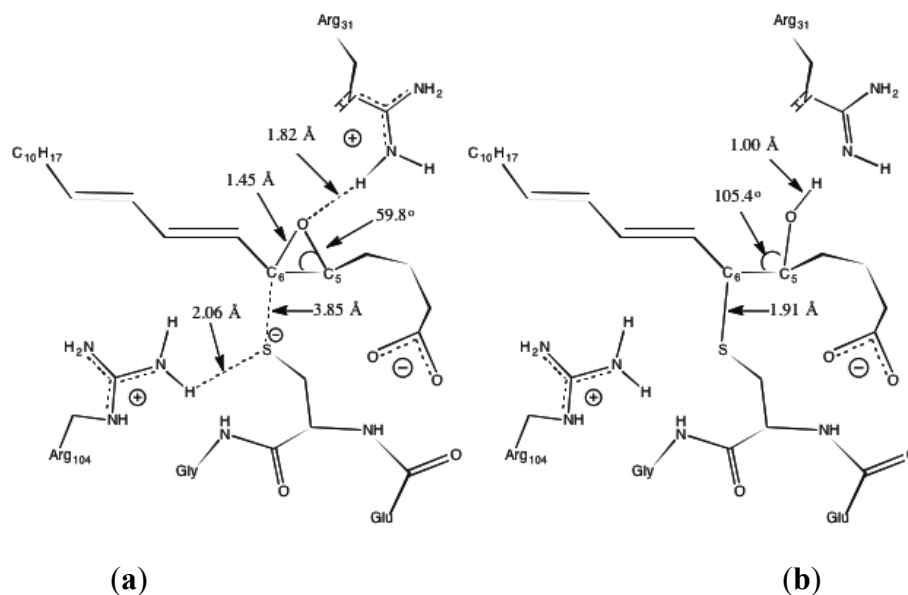


Figure S1. Optimized structures of (a) reactant and (b) product complexes of the 'head-to-tail' substrate orientation obtained at the ONIOM(ω B97XD/6-311+G(2df,p)//AMBER96)-ME level of theory with selected distances (in angstroms) and bond angles (in degrees) shown.

While it was found from the MD simulations that the 'head-to-tail' orientation results in the unbinding of the substrate at approximately 7 ns, we have chosen to calculate the reaction mechanism. Specifically, we have used an average structure prior to the substrate leaving the active site. The 'head-to-tail' substrate orientation in the reactant complex had very similar bond lengths to the 'tail-to-head' orientation (**Figure S1a**). The exception of the $r_{S...C6}$ bond distance which was slightly longer (3.85 vs. 3.78 Å) and the significantly shorter $r_{N-H...O}$ bond distance (1.82 vs. 3.08 Å). Thus, in the case of the 'head-to-tail' orientation, a strong interaction is seen between Arg31 and the epoxide functional group. However, as seen in **Figure S1** (and as

discussed in the MD section) no interaction between the carboxylate head and Arg104 is formed for the ‘head-to-tail’ model.

It is noted that at the current level of theory a transition state (with a single imaginary frequency) for the ‘head-to-tail’ model could not be obtained. However, we did perform a scan whereby $r(\text{glutathione-S}^-\cdots\text{C6})$ was shortened in increments of 0.15 Å. Along this scan the greatest energy cost was 79.6 kJ mol⁻¹ which corresponded to $r(\text{glutathione-S}^-\cdots\text{C6})$ being 2.46 Å. Similar to that seen in the ‘tail-to-head’ model $r(\text{Arg31}^+\cdots\text{O})$ is slightly longer and is now 1.62 Å. In the case of the breaking C6–O bond of the epoxide a lengthening of 1.98 Å is observed which results in the increase of the C6–C5–O angle by 87.8°.

For the optimized product complex (**Figure S1b**) $r(\text{C–S})$ is 1.91 Å thus, indicating the formation of the C–S bond. As a results of the C–S bond formation $r(\text{GSH}^-\cdots^+\text{Arg}_{104})$ has lengthened by 0.27 Å to a final length of 2.33 Å. With the opening of the epoxide the C6–C5–O angle is now 105.4°, which is slightly smaller than that observed for the ‘tail-to-head’ model. Similar to the previous model, optimization of the product complex results in a proton transfer Arg31 to the alkoxide forming the alcohol without energy barrier. The relative energy of the product complex with respect to the reactant complex was found to be only 0.1 kJ mol⁻¹. Thus, it appears that with respect to the ‘tail-to-head’ model S–C bond formation is considerably less energetically favourable.

Table S1: Table of bond lengths for ‘tail-to-head’ orientation.

Reactant (0.0 kJ/mol)		Transition State (102.0 kJ/mol)		Product (-135.5 kJ/mol)	
Bond	Bond Length	Bond	Bond Length	Bond	Bond Length
S..C6	3.78	S..C6	2.75	S..C6	1.87
C5..O	1.44	C5..O	1.40	C5..O	1.41
O..H	3.08	O..H	1.58	O..H	1.00
H..N	1.02	H..N	1.07	H..N	1.75

Table S2: Table of bond lengths for ‘head-to-tail’ orientation.

Reactant (0.0 kJ/mol)		Transition State* (79.6 kJ/mol)		Product (0.1 kJ/mol)	
Bond	Bond Length	Bond	Bond Length	Bond	Bond Length
S..C6	3.85	S..C6	2.56	S..C6	1.91
C5..O	1.43	C5..O	1.41	C5..O	1.39
O..H	1.82	O..H	1.77	O..H	1.00
H..N	1.02	H..N	1.03	H..N	1.79

*The transition state of the 'head-to-tail' orientation was not optimized.

Figure S1: Reactant complex (RC) for the 'tail-to-head' orientation.

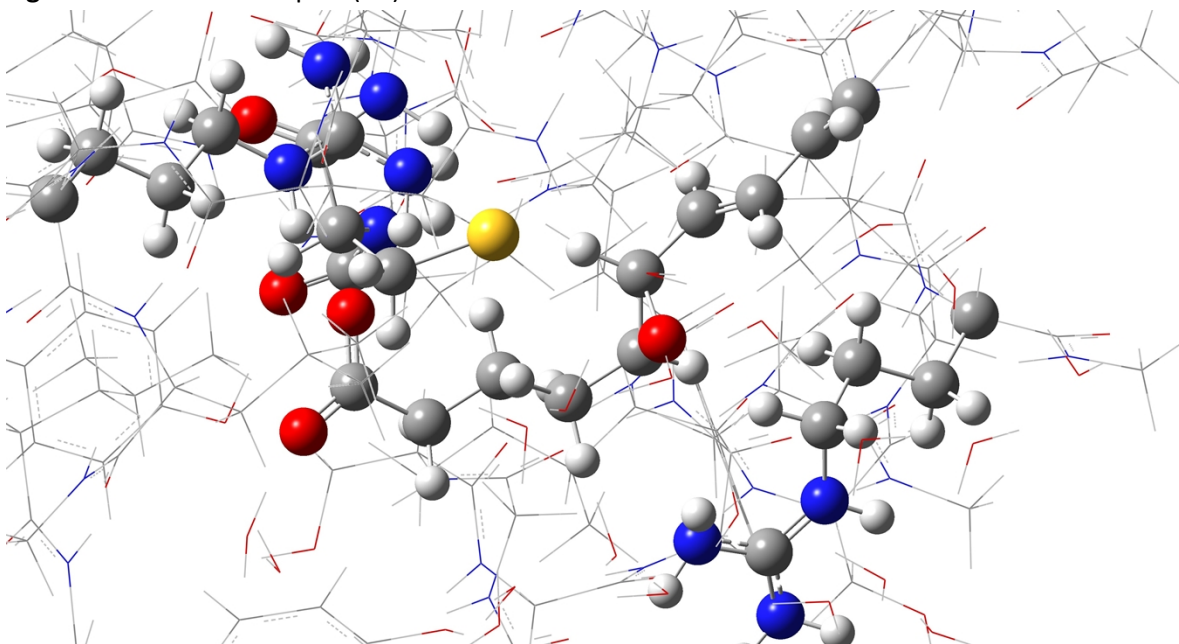


Figure S2: Transition state (TS) for the 'tail-to-head' orientation.

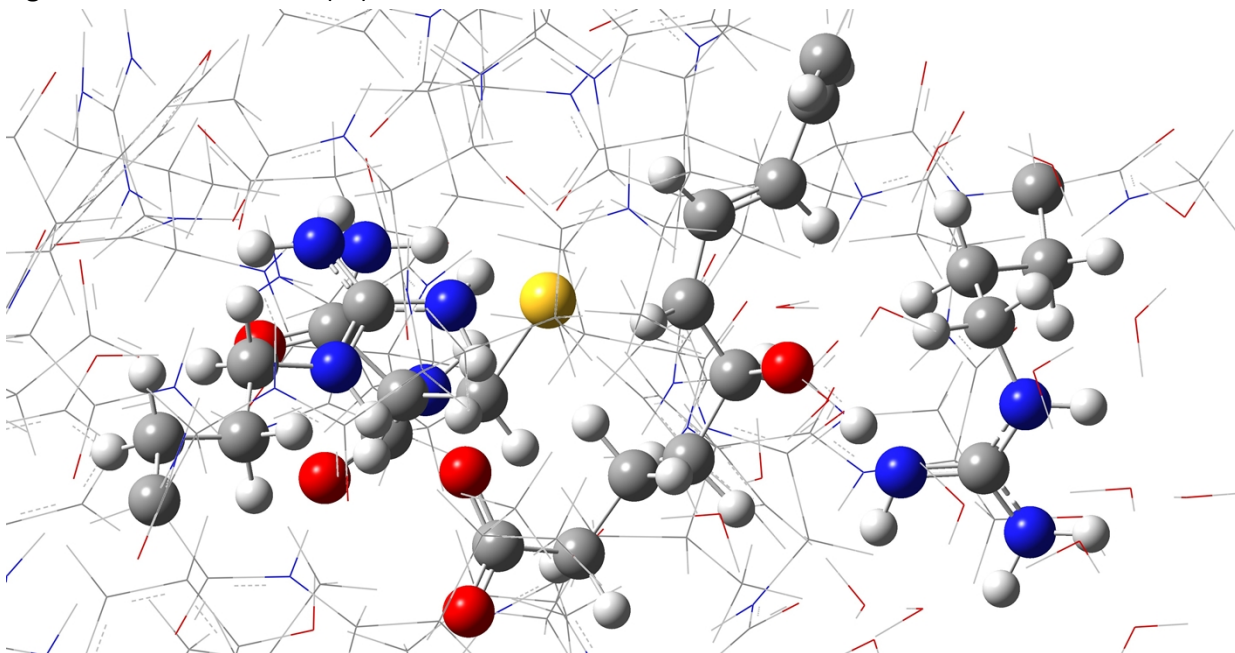


Figure S3: Product complex (PC) for the 'tail-to-head' orientation.

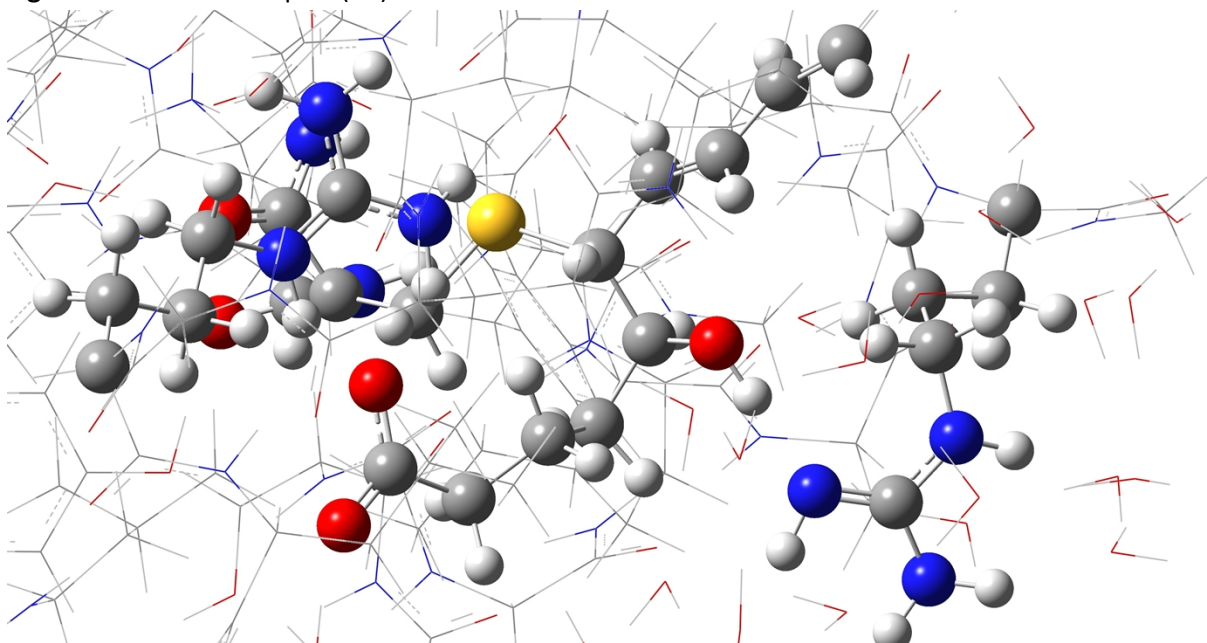


Figure S4: Reactant complex (RC) for the 'head-to-tail' orientation.

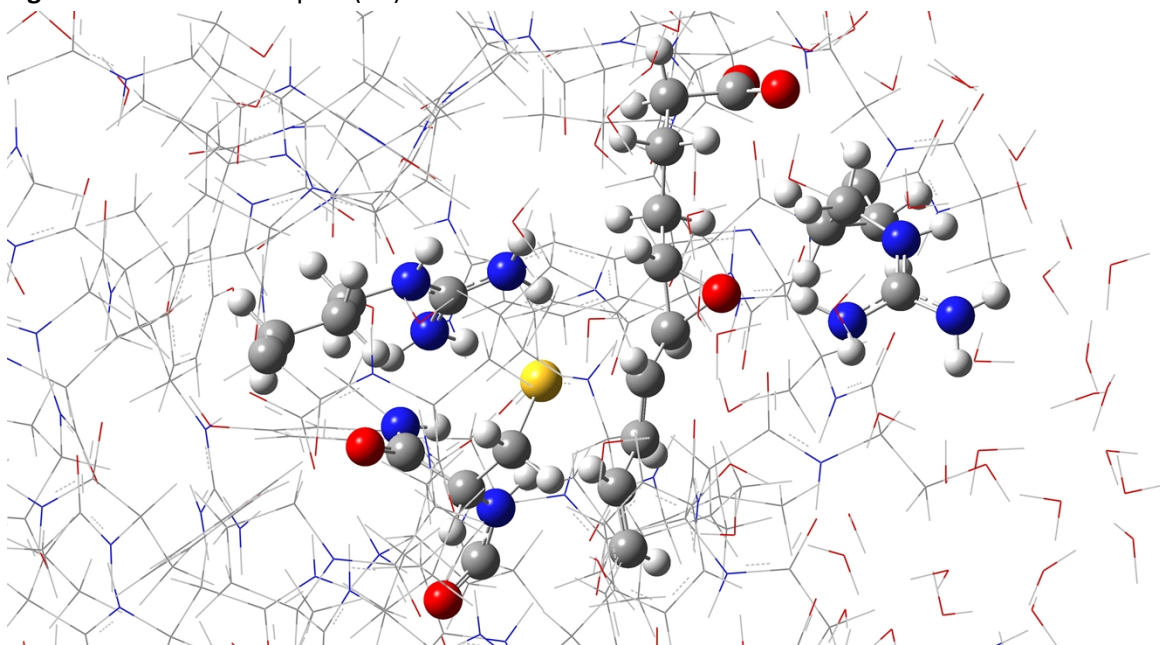


Figure S5: Transition state (TS) for the 'head-to-tail' orientation.

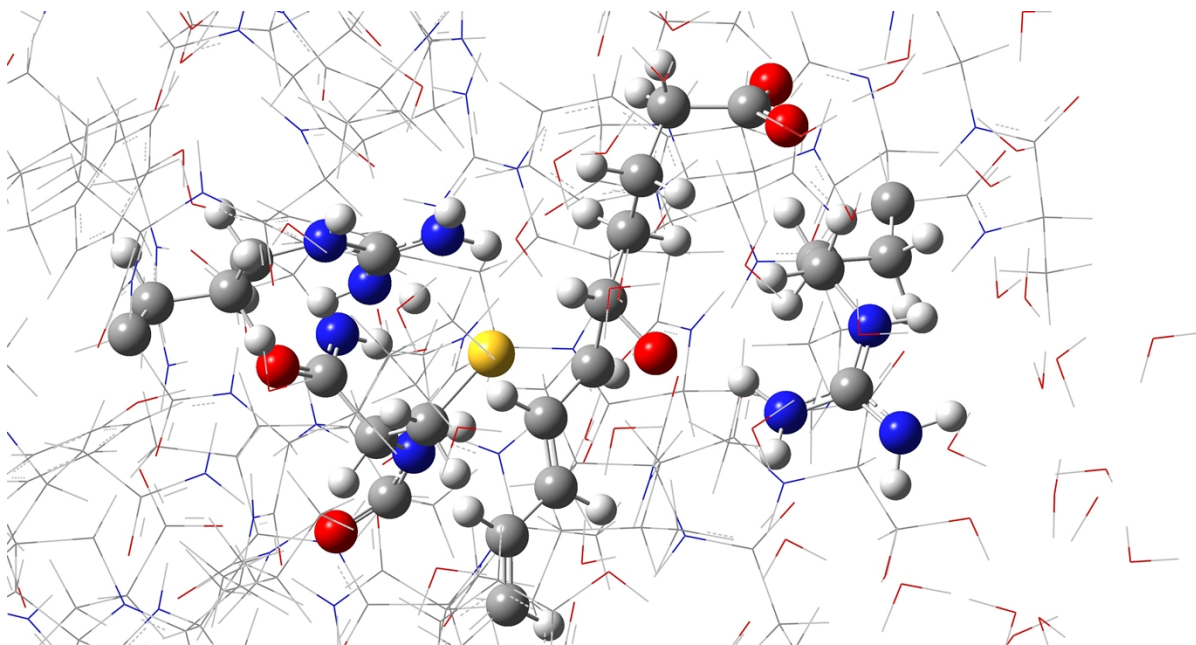


Figure S6: Product complex (PC) for the 'head-to-tail' orientation.

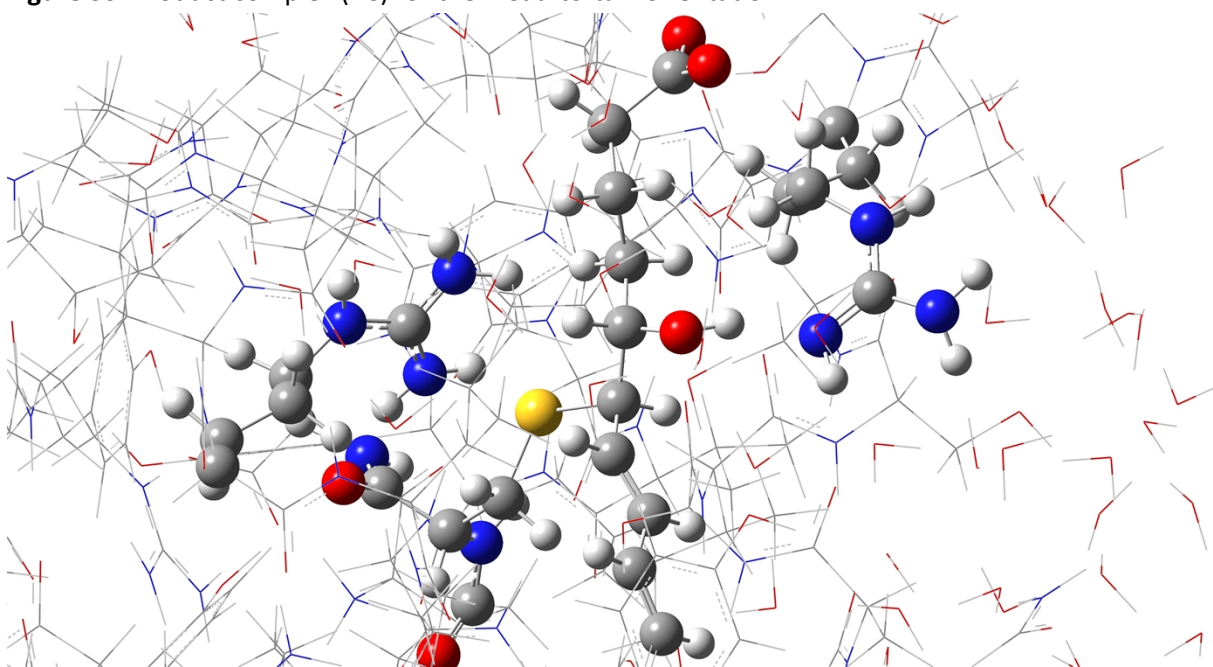


Table S3: Reactant complex (RC), transition state (TS), and product complex (PC) for the 'tail-to-head' and 'head-to-tail' orientations. Corresponding electronic energies included when calculated.

RC (Tail-to-head orientation)

E = -2159.39873250 hartrees

HETATM	1	C	0	5.285	-5.539	9.448	C
HETATM	2	H	0	5.605	-4.965	10.292	H
HETATM	3	H	0	5.620	-6.549	9.556	H
HETATM	4	H	0	4.217	-5.521	9.388	H

HETATM	5	C	0	5.882	-4.925	8.204	C
HETATM	6	O	0	5.912	-3.705	8.111	O
HETATM	7	N	0	6.337	-5.739	7.247	N
HETATM	8	C	0	6.835	-5.271	5.940	C
HETATM	9	H	0	7.085	-6.123	5.308	H
HETATM	10	C	0	5.792	-4.413	5.224	C
HETATM	11	O	0	6.073	-3.269	4.894	O
HETATM	12	H	0	6.306	-6.731	7.426	H
HETATM	13	H	0	7.736	-4.675	6.088	H
HETATM	14	N	0	4.574	-4.936	5.029	N
HETATM	15	C	0	3.414	-4.217	4.468	C
HETATM	16	C	0	3.160	-2.879	5.152	C
HETATM	17	O	0	3.083	-1.853	4.485	O
HETATM	18	C	0	2.164	-5.100	4.522	C
HETATM	19	O	0	2.004	-5.657	5.816	O
HETATM	20	H	0	4.393	-5.867	5.375	H
HETATM	21	H	0	3.617	-3.999	3.419	H
HETATM	22	H	0	2.260	-5.906	3.793	H
HETATM	23	H	0	1.294	-4.496	4.269	H
HETATM	24	H	0	1.182	-6.163	5.812	H
HETATM	25	N	0	3.071	-2.881	6.481	N
HETATM	26	C	0	2.921	-1.685	7.309	C
HETATM	27	C	0	4.065	-0.677	7.159	C
HETATM	28	O	0	3.837	0.531	7.152	O
HETATM	29	C	0	2.748	-2.094	8.784	C
HETATM	30	C	0	1.522	-2.982	9.076	C
HETATM	31	C	0	1.513	-3.360	10.557	C
HETATM	32	C	0	0.196	-2.286	8.755	C
HETATM	33	H	0	3.094	-3.793	6.914	H
HETATM	34	H	0	2.013	-1.171	7.003	H
HETATM	35	H	0	3.645	-2.621	9.108	H
HETATM	36	H	0	2.667	-1.186	9.385	H
HETATM	37	H	0	1.589	-3.901	8.493	H
HETATM	38	H	0	1.423	-2.466	11.174	H
HETATM	39	H	0	2.437	-3.878	10.813	H
HETATM	40	H	0	0.673	-4.025	10.764	H
HETATM	41	H	0	0.136	-1.335	9.285	H
HETATM	42	H	0	-0.634	-2.925	9.057	H
HETATM	43	H	0	0.117	-2.112	7.682	H
HETATM	44	N	0	5.291	-1.170	7.024	N
HETATM	45	C	0	6.464	-0.368	6.720	C
HETATM	46	H	0	7.354	-0.992	6.781	H
HETATM	47	C	0	6.399	0.240	5.325	C
HETATM	48	O	0	6.679	1.423	5.207	O
HETATM	49	H	0	5.398	-2.176	7.077	H
HETATM	50	H	0	6.553	0.438	7.450	H
HETATM	51	N	0	6.003	-0.516	4.290	N
HETATM	52	C	0	5.669	0.041	2.964	C
HETATM	53	C	0	4.604	1.122	3.120	C

HETATM	54	O	0	4.856	2.234	2.695	O
HETATM	55	C	0	5.295	-1.002	1.910	C
HETATM	56	C	0	5.124	-0.326	0.548	C
HETATM	57	C	0	6.392	-2.042	1.695	C
HETATM	58	H	0	5.828	-1.499	4.471	H
HETATM	59	H	0	6.563	0.547	2.601	H
HETATM	60	H	0	4.376	-1.500	2.204	H
HETATM	61	H	0	6.031	0.222	0.294	H
HETATM	62	H	0	4.283	0.366	0.573	H
HETATM	63	H	0	4.944	-1.071	-0.224	H
HETATM	64	H	0	7.275	-1.593	1.254	H
HETATM	65	H	0	6.028	-2.790	1.002	H
HETATM	66	H	0	6.670	-2.518	2.629	H
HETATM	67	N	0	3.474	0.851	3.779	N
HETATM	68	C	0	2.395	1.802	4.118	C
HETATM	69	C	0	2.898	3.119	4.733	C
HETATM	70	O	0	2.595	4.200	4.229	O
HETATM	71	C	0	1.327	1.074	4.973	C
HETATM	72	C	0	0.381	0.294	4.037	C
HETATM	73	C	0	0.532	1.989	5.924	C
HETATM	74	C	0	-0.367	-0.863	4.709	C
HETATM	75	H	0	3.364	-0.107	4.090	H
HETATM	76	H	0	1.905	2.096	3.189	H
HETATM	77	H	0	1.842	0.352	5.594	H
HETATM	78	H	0	-0.341	0.982	3.604	H
HETATM	79	H	0	0.960	-0.129	3.220	H
HETATM	80	H	0	0.111	2.827	5.374	H
HETATM	81	H	0	1.184	2.371	6.709	H
HETATM	82	H	0	-0.263	1.426	6.408	H
HETATM	83	H	0	-1.017	-0.490	5.497	H
HETATM	84	H	0	0.344	-1.574	5.128	H
HETATM	85	H	0	-0.978	-1.375	3.964	H
HETATM	86	N	0	3.666	3.047	5.820	N
HETATM	87	C	0	4.315	4.200	6.455	C
HETATM	88	C	0	5.281	4.881	5.477	C
HETATM	89	O	0	5.159	6.075	5.229	O
HETATM	90	C	0	5.041	3.718	7.712	C
HETATM	91	O	0	5.525	4.811	8.457	O
HETATM	92	H	0	3.835	2.119	6.194	H
HETATM	93	H	0	3.555	4.925	6.746	H
HETATM	94	H	0	5.870	3.064	7.435	H
HETATM	95	H	0	4.344	3.153	8.333	H
HETATM	96	H	0	5.981	4.446	9.244	H
HETATM	97	N	0	6.202	4.135	4.858	N
HETATM	98	C	0	7.179	4.612	3.876	C
HETATM	99	C	0	6.564	5.257	2.622	C
HETATM	100	O	0	7.147	6.192	2.076	O
HETATM	101	C	0	8.133	3.476	3.486	C
HETATM	102	H	0	6.222	3.144	5.067	H

HETATM 103 H	0	7.775	5.387	4.359	H
HETATM 104 H	0	8.900	3.858	2.811	H
HETATM 105 H	0	7.583	2.681	2.982	H
HETATM 106 H	0	8.618	3.075	4.377	H
HETATM 107 N	0	5.380	4.807	2.180	N
HETATM 108 C	0	4.575	5.459	1.142	C
HETATM 109 C	0	4.297	6.925	1.514	C
HETATM 110 O	0	4.140	7.757	0.632	O
HETATM 111 C	0	3.193	4.819	0.910	C
HETATM 112 C	0	3.146	3.351	0.474	C
HETATM 113 C	0	2.063	3.112	-0.580	C
HETATM 114 N	0	2.490	3.581	-1.907	N
HETATM 115 C	0	2.940	2.845	-2.901	C
HETATM 116 N	0	3.029	1.555	-2.827	N
HETATM 117 N	0	3.310	3.409	-4.006	N
HETATM 118 H	0	5.005	3.987	2.647	H
HETATM 119 H	0	5.131	5.463	0.205	H
HETATM 120 H	0	2.580	4.930	1.804	H
HETATM 121 H	0	2.714	5.417	0.136	H
HETATM 122 H	0	2.891	2.742	1.335	H
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HETATM 124 H	0	1.155	3.637	-0.283	H
HETATM 125 H	0	1.820	2.051	-0.601	H
HETATM 126 H	0	2.552	4.582	-2.044	H
HETATM 127 H	0	3.303	0.974	-3.597	H
HETATM 128 H	0	2.752	1.057	-1.978	H
HETATM 129 H	0	3.092	4.377	-4.174	H
HETATM 130 H	0	3.727	2.846	-4.737	H
HETATM 131 N	0	4.177	7.242	2.805	N
HETATM 132 C	0	3.833	8.569	3.377	C
HETATM 133 C	0	5.035	9.299	3.982	C
HETATM 134 O	0	5.005	10.527	4.053	O
HETATM 135 C	0	2.723	8.407	4.409	C
HETATM 136 C	0	1.437	7.864	3.794	C
HETATM 137 C	0	0.241	7.953	4.728	C
HETATM 138 N	0	0.590	7.370	6.029	N
HETATM 139 C	0	-0.056	6.482	6.753	C
HETATM 140 N	0	-1.229	5.952	6.347	N
HETATM 141 N	0	0.522	5.999	7.884	N
HETATM 142 H	0	4.294	6.467	3.449	H
HETATM 143 H	0	3.476	9.213	2.566	H
HETATM 144 H	0	3.077	7.742	5.211	H
HETATM 145 H	0	2.516	9.376	4.883	H
HETATM 146 H	0	1.570	6.825	3.477	H
HETATM 147 H	0	1.187	8.428	2.891	H
HETATM 148 H	0	-0.609	7.430	4.285	H
HETATM 149 H	0	-0.037	8.997	4.902	H
HETATM 150 H	0	1.422	7.755	6.469	H
HETATM 151 H	0	-1.705	5.463	7.104	H

HETATM 152 H	0	-1.834	6.617	5.868	H
HETATM 153 H	0	1.147	6.672	8.334	H
HETATM 154 H	0	-0.131	5.572	8.535	H
HETATM 155 N	0	6.065	8.556	4.397	N
HETATM 156 C	0	7.367	9.017	4.864	C
HETATM 157 H	0	7.538	9.989	4.452	H
HETATM 158 H	0	8.131	8.348	4.528	H
HETATM 159 H	0	7.386	9.073	5.932	H
HETATM 160 H	0	5.893	7.559	4.382	H
HETATM 161 C	0	5.530	10.837	-0.560	C
HETATM 162 H	0	5.495	11.894	-0.725	H
HETATM 163 H	0	6.510	10.559	-0.234	H
HETATM 164 H	0	4.815	10.569	0.189	H
HETATM 165 C	0	5.262	10.083	-1.862	C
HETATM 166 O	0	5.493	10.622	-2.937	O
HETATM 167 N	0	4.805	8.828	-1.780	N
HETATM 168 C	0	4.677	7.845	-2.881	C
HETATM 169 C	0	3.253	7.306	-3.032	C
HETATM 170 O	0	2.864	6.322	-2.405	O
HETATM 171 C	0	5.742	6.735	-2.787	C
HETATM 172 C	0	5.793	5.987	-4.119	C
HETATM 173 C	0	7.151	7.291	-2.532	C
HETATM 174 H	0	4.629	8.494	-0.841	H
HETATM 175 H	0	4.896	8.383	-3.804	H
HETATM 176 H	0	5.491	6.036	-1.990	H
HETATM 177 H	0	6.067	6.661	-4.930	H
HETATM 178 H	0	4.826	5.546	-4.325	H
HETATM 179 H	0	6.521	5.184	-4.067	H
HETATM 180 H	0	7.376	8.085	-3.244	H
HETATM 181 H	0	7.888	6.497	-2.633	H
HETATM 182 H	0	7.214	7.687	-1.518	H
HETATM 183 N	0	2.467	7.943	-3.905	N
HETATM 184 C	0	1.062	7.610	-4.194	C
HETATM 185 C	0	0.878	6.128	-4.606	C
HETATM 186 O	0	1.776	5.551	-5.222	O
HETATM 187 C	0	0.530	8.536	-5.293	C
HETATM 188 O	0	0.860	9.887	-5.029	O
HETATM 189 H	0	2.833	8.772	-4.353	H
HETATM 190 H	0	0.499	7.802	-3.281	H
HETATM 191 H	0	-0.553	8.432	-5.370	H
HETATM 192 H	0	0.977	8.250	-6.246	H
HETATM 193 H	0	0.438	10.193	-4.213	H
HETATM 194 N	0	-0.252	5.472	-4.274	N
HETATM 195 C	0	-0.363	4.007	-4.259	C
HETATM 196 C	0	0.023	3.199	-5.518	C
HETATM 197 O	0	0.861	2.310	-5.377	O
HETATM 198 C	0	-1.738	3.674	-3.689	C
HETATM 199 C	0	-2.469	5.004	-3.520	C
HETATM 200 C	0	-1.356	6.046	-3.521	C

HETATM 201 H	0	0.343	3.677	-3.499	H
HETATM 202 H	0	-2.289	3.010	-4.348	H
HETATM 203 H	0	-1.601	3.210	-2.712	H
HETATM 204 H	0	-3.039	5.030	-2.591	H
HETATM 205 H	0	-3.132	5.175	-4.368	H
HETATM 206 H	0	-1.030	6.224	-2.494	H
HETATM 207 H	0	-1.712	6.974	-3.969	H
HETATM 208 N	0	-0.515	3.451	-6.732	N
HETATM 209 C	0	-0.163	2.688	-7.950	C
HETATM 210 C	0	1.316	2.675	-8.310	C
HETATM 211 O	0	1.728	1.915	-9.188	O
HETATM 212 C	0	-0.959	3.344	-9.086	C
HETATM 213 C	0	-2.134	4.010	-8.381	C
HETATM 214 C	0	-1.537	4.439	-7.042	C
HETATM 215 H	0	-0.493	1.658	-7.838	H
HETATM 216 H	0	-0.356	4.113	-9.573	H
HETATM 217 H	0	-1.293	2.607	-9.817	H
HETATM 218 H	0	-2.923	3.275	-8.218	H
HETATM 219 H	0	-2.516	4.862	-8.944	H
HETATM 220 H	0	-2.319	4.465	-6.289	H
HETATM 221 H	0	-1.072	5.421	-7.141	H
HETATM 222 N	0	2.112	3.541	-7.680	N
HETATM 223 C	0	3.543	3.585	-7.867	C
HETATM 224 C	0	4.203	2.296	-7.341	C
HETATM 225 O	0	4.659	2.213	-6.203	O
HETATM 226 C	0	4.122	4.907	-7.341	C
HETATM 227 C	0	3.465	6.189	-7.894	C
HETATM 228 C	0	4.094	7.415	-7.231	C
HETATM 229 C	0	3.648	6.329	-9.408	C
HETATM 230 H	0	1.718	4.095	-6.932	H
HETATM 231 H	0	3.725	3.588	-8.943	H
HETATM 232 H	0	4.053	4.907	-6.259	H
HETATM 233 H	0	5.169	4.944	-7.620	H
HETATM 234 H	0	2.399	6.193	-7.675	H
HETATM 235 H	0	5.160	7.459	-7.454	H
HETATM 236 H	0	3.956	7.351	-6.154	H
HETATM 237 H	0	3.609	8.322	-7.591	H
HETATM 238 H	0	4.707	6.295	-9.663	H
HETATM 239 H	0	3.231	7.278	-9.742	H
HETATM 240 H	0	3.122	5.526	-9.923	H
HETATM 241 N	0	4.306	1.299	-8.228	N
HETATM 242 C	0	5.271	0.179	-8.220	C
HETATM 243 C	0	6.715	0.719	-8.452	C
HETATM 244 O	0	7.504	0.146	-9.203	O
HETATM 245 C	0	4.864	-0.861	-9.289	C
HETATM 246 O	0	5.771	-1.938	-9.309	O
HETATM 247 C	0	4.751	-0.321	-10.718	C
HETATM 248 H	0	3.726	1.427	-9.050	H
HETATM 249 H	0	5.252	-0.305	-7.244	H

HETATM 250 H	0	3.887	-1.255	-9.023	H
HETATM 251 H	0	5.699	0.101	-11.052	H
HETATM 252 H	0	3.975	0.441	-10.775	H
HETATM 253 H	0	4.478	-1.137	-11.387	H
HETATM 254 H	0	6.628	-1.542	-9.543	H
HETATM 255 N	0	7.060	1.862	-7.847	N
HETATM 256 C	0	8.202	2.741	-8.141	C
HETATM 257 H	0	8.174	3.036	-9.190	H
HETATM 258 C	0	8.151	3.998	-7.264	C
HETATM 259 O	0	7.167	4.215	-6.568	O
HETATM 260 H	0	6.405	2.228	-7.161	H
HETATM 261 H	0	9.130	2.204	-7.943	H
HETATM 262 N	0	9.184	4.840	-7.290	N
HETATM 263 C	0	9.209	6.105	-6.540	C
HETATM 264 C	0	10.317	6.173	-5.487	C
HETATM 265 O	0	10.894	5.156	-5.098	O
HETATM 266 H	0	9.999	4.581	-7.824	H
HETATM 267 H	0	9.355	6.922	-7.247	H
HETATM 268 H	0	8.259	6.272	-6.030	H
HETATM 269 N	0	10.633	7.396	-5.047	N
HETATM 270 C	0	11.838	7.676	-4.276	C
HETATM 271 H	0	12.144	8.694	-4.401	H
HETATM 272 H	0	12.597	7.027	-4.659	H
HETATM 273 H	0	11.687	7.474	-3.237	H
HETATM 274 H	0	10.082	8.175	-5.377	H
HETATM 275 C	0	14.083	4.174	-0.263	C
HETATM 276 H	0	14.039	4.799	-1.130	H
HETATM 277 H	0	14.722	3.338	-0.458	H
HETATM 278 H	0	14.471	4.734	0.562	H
HETATM 279 C	0	12.736	3.524	-0.045	C
HETATM 280 O	0	12.698	2.394	0.423	O
HETATM 281 N	0	11.657	4.142	-0.534	N
HETATM 282 C	0	10.396	3.431	-0.804	C
HETATM 283 C	0	10.618	2.228	-1.742	C
HETATM 284 O	0	10.225	1.126	-1.391	O
HETATM 285 C	0	9.337	4.382	-1.388	C
HETATM 286 C	0	8.179	3.626	-2.020	C
HETATM 287 C	0	7.147	3.099	-1.220	C
HETATM 288 C	0	8.220	3.316	-3.395	C
HETATM 289 C	0	6.188	2.245	-1.793	C
HETATM 290 C	0	7.273	2.445	-3.955	C
HETATM 291 C	0	6.262	1.903	-3.153	C
HETATM 292 H	0	11.768	5.080	-0.882	H
HETATM 293 H	0	10.011	3.029	0.135	H
HETATM 294 H	0	8.960	5.033	-0.597	H
HETATM 295 H	0	9.800	5.010	-2.151	H
HETATM 296 H	0	7.110	3.315	-0.161	H
HETATM 297 H	0	9.002	3.710	-4.025	H
HETATM 298 H	0	5.403	1.818	-1.191	H

HETATM 299 H	0	7.320	2.179	-4.999	H
HETATM 300 H	0	5.552	1.216	-3.587	H
HETATM 301 N	0	11.193	2.404	-2.943	N
HETATM 302 C	0	11.272	1.331	-3.939	C
HETATM 303 H	0	11.594	0.434	-3.452	H
HETATM 304 H	0	11.959	1.579	-4.720	H
HETATM 305 H	0	10.297	1.180	-4.354	H
HETATM 306 H	0	11.445	3.344	-3.215	H
HETATM 307 C	0	13.885	-0.751	-2.112	C
HETATM 308 H	0	13.565	-1.061	-3.085	H
HETATM 309 H	0	14.914	-1.012	-1.975	H
HETATM 310 H	0	13.771	0.308	-2.020	H
HETATM 311 C	0	12.959	-1.471	-1.129	C
HETATM 312 O	0	12.807	-2.679	-1.244	O
HETATM 313 N	0	12.276	-0.745	-0.233	N
HETATM 314 C	0	11.261	-1.246	0.740	C
HETATM 315 C	0	10.095	-2.003	0.110	C
HETATM 316 O	0	9.746	-3.078	0.585	O
HETATM 317 C	0	10.835	-0.085	1.674	C
HETATM 318 C	0	9.460	-0.205	2.334	C
HETATM 319 C	0	11.881	0.083	2.783	C
HETATM 320 H	0	12.455	0.252	-0.210	H
HETATM 321 H	0	11.760	-1.988	1.365	H
HETATM 322 H	0	10.807	0.837	1.100	H
HETATM 323 H	0	9.332	-1.188	2.782	H
HETATM 324 H	0	8.699	-0.026	1.577	H
HETATM 325 H	0	9.344	0.558	3.104	H
HETATM 326 H	0	11.897	-0.800	3.424	H
HETATM 327 H	0	11.649	0.962	3.384	H
HETATM 328 H	0	12.869	0.223	2.343	H
HETATM 329 N	0	9.515	-1.480	-0.966	N
HETATM 330 C	0	8.601	-2.169	-1.874	C
HETATM 331 C	0	9.207	-3.493	-2.340	C
HETATM 332 O	0	8.663	-4.551	-2.056	O
HETATM 333 C	0	8.294	-1.223	-3.046	C
HETATM 334 C	0	7.416	-1.813	-4.134	C
HETATM 335 C	0	6.019	-1.796	-3.985	C
HETATM 336 C	0	7.989	-2.363	-5.298	C
HETATM 337 C	0	5.191	-2.335	-4.987	C
HETATM 338 C	0	7.166	-2.905	-6.304	C
HETATM 339 C	0	5.764	-2.903	-6.144	C
HETATM 340 O	0	4.969	-3.402	-7.128	O
HETATM 341 H	0	9.837	-0.556	-1.224	H
HETATM 342 H	0	7.672	-2.394	-1.348	H
HETATM 343 H	0	7.805	-0.335	-2.647	H
HETATM 344 H	0	9.231	-0.895	-3.497	H
HETATM 345 H	0	5.584	-1.356	-3.098	H
HETATM 346 H	0	9.063	-2.380	-5.420	H
HETATM 347 H	0	4.119	-2.296	-4.873	H

HETATM 348 H	0	7.603	-3.335	-7.193	H
HETATM 349 H	0	5.367	-3.178	-7.987	H
HETATM 350 N	0	10.349	-3.448	-3.029	N
HETATM 351 C	0	11.041	-4.637	-3.498	C
HETATM 352 H	0	11.720	-4.962	-2.737	H
HETATM 353 H	0	11.586	-4.425	-4.394	H
HETATM 354 H	0	10.324	-5.407	-3.690	H
HETATM 355 H	0	10.807	-2.553	-3.096	H
HETATM 356 C	0	12.077	-6.033	-0.055	C
HETATM 357 H	0	11.934	-5.576	-1.013	H
HETATM 358 H	0	12.840	-6.779	-0.126	H
HETATM 359 H	0	12.370	-5.289	0.655	H
HETATM 360 C	0	10.775	-6.696	0.359	C
HETATM 361 O	0	10.723	-7.915	0.429	O
HETATM 362 N	0	9.724	-5.916	0.619	N
HETATM 363 C	0	8.405	-6.380	1.091	C
HETATM 364 C	0	7.702	-7.344	0.135	C
HETATM 365 O	0	7.165	-8.359	0.572	O
HETATM 366 C	0	7.546	-5.173	1.454	C
HETATM 367 C	0	6.147	-5.558	1.945	C
HETATM 368 C	0	5.160	-5.707	0.802	C
HETATM 369 O	0	4.917	-4.767	0.064	O
HETATM 370 N	0	4.544	-6.847	0.626	N
HETATM 371 H	0	9.846	-4.916	0.493	H
HETATM 372 H	0	8.576	-6.946	2.008	H
HETATM 373 H	0	8.043	-4.635	2.258	H
HETATM 374 H	0	7.472	-4.511	0.591	H
HETATM 375 H	0	5.775	-4.748	2.563	H
HETATM 376 H	0	6.186	-6.465	2.550	H
HETATM 377 H	0	3.866	-6.824	-0.139	H
HETATM 378 H	0	4.870	-7.709	1.031	H
HETATM 379 N	0	7.642	-6.981	-1.142	N
HETATM 380 C	0	7.051	-7.771	-2.225	C
HETATM 381 C	0	7.946	-8.972	-2.601	C
HETATM 382 O	0	7.443	-9.969	-3.112	O
HETATM 383 C	0	6.780	-6.872	-3.457	C
HETATM 384 C	0	6.090	-7.614	-4.612	C
HETATM 385 C	0	5.856	-5.694	-3.109	C
HETATM 386 H	0	8.059	-6.087	-1.380	H
HETATM 387 H	0	6.098	-8.177	-1.885	H
HETATM 388 H	0	7.727	-6.474	-3.824	H
HETATM 389 H	0	5.164	-8.071	-4.260	H
HETATM 390 H	0	6.744	-8.391	-5.006	H
HETATM 391 H	0	5.865	-6.921	-5.422	H
HETATM 392 H	0	5.665	-5.091	-3.995	H
HETATM 393 H	0	6.297	-5.056	-2.350	H
HETATM 394 H	0	4.922	-6.080	-2.718	H
HETATM 395 N	0	9.265	-8.896	-2.350	N
HETATM 396 C	0	10.221	-9.998	-2.504	C

HETATM 397 H	0	10.975	-9.921	-1.749	H
HETATM 398 H	0	10.681	-9.989	-3.470	H
HETATM 399 H	0	9.679	-10.912	-2.376	H
HETATM 400 H	0	9.564	-8.080	-1.837	H
HETATM 401 C	0	17.191	-7.840	4.125	C
HETATM 402 H	0	17.926	-7.663	4.883	H
HETATM 403 H	0	17.679	-8.005	3.187	H
HETATM 404 H	0	16.614	-8.703	4.384	H
HETATM 405 C	0	16.343	-6.597	4.037	C
HETATM 406 O	0	16.756	-5.622	3.431	O
HETATM 407 N	0	15.183	-6.615	4.691	N
HETATM 408 C	0	14.280	-5.459	4.784	C
HETATM 409 C	0	14.864	-4.271	5.583	C
HETATM 410 O	0	14.547	-3.121	5.293	O
HETATM 411 C	0	12.943	-5.931	5.379	C
HETATM 412 C	0	11.826	-4.903	5.326	C
HETATM 413 C	0	11.192	-4.622	4.101	C
HETATM 414 C	0	11.417	-4.225	6.492	C
HETATM 415 C	0	10.163	-3.668	4.043	C
HETATM 416 C	0	10.380	-3.275	6.433	C
HETATM 417 C	0	9.753	-2.995	5.206	C
HETATM 418 H	0	14.909	-7.479	5.126	H
HETATM 419 H	0	14.093	-5.090	3.774	H
HETATM 420 H	0	12.607	-6.810	4.827	H
HETATM 421 H	0	13.102	-6.237	6.414	H
HETATM 422 H	0	11.502	-5.128	3.198	H
HETATM 423 H	0	11.909	-4.421	7.433	H
HETATM 424 H	0	9.698	-3.442	3.097	H
HETATM 425 H	0	10.078	-2.748	7.326	H
HETATM 426 H	0	8.963	-2.258	5.151	H
HETATM 427 N	0	15.705	-4.547	6.593	N
HETATM 428 C	0	16.508	-3.564	7.328	C
HETATM 429 H	0	16.452	-2.619	6.830	H
HETATM 430 H	0	17.521	-3.909	7.326	H
HETATM 431 H	0	16.171	-3.456	8.338	H
HETATM 432 H	0	15.903	-5.524	6.731	H
HETATM 433 C	0	-2.158	-4.354	-11.852	C
HETATM 434 H	0	-2.474	-5.333	-12.146	H
HETATM 435 H	0	-1.441	-3.985	-12.556	H
HETATM 436 H	0	-3.003	-3.699	-11.827	H
HETATM 437 C	0	-1.575	-4.430	-10.465	C
HETATM 438 O	0	-1.382	-5.516	-9.936	O
HETATM 439 N	0	-1.337	-3.265	-9.855	N
HETATM 440 C	0	-0.858	-3.153	-8.469	C
HETATM 441 C	0	-1.795	-3.789	-7.437	C
HETATM 442 O	0	-1.310	-4.498	-6.567	O
HETATM 443 C	0	-0.508	-1.696	-8.121	C
HETATM 444 C	0	0.997	-1.349	-8.079	C
HETATM 445 C	0	1.957	-2.357	-7.411	C

HETATM 446 N	0	1.502	-2.824	-6.097	N
HETATM 447 C	0	1.856	-3.917	-5.447	C
HETATM 448 N	0	2.741	-4.781	-5.843	N
HETATM 449 N	0	1.348	-4.180	-4.298	N
HETATM 450 H	0	-1.509	-2.429	-10.392	H
HETATM 451 H	0	0.040	-3.764	-8.395	H
HETATM 452 H	0	-1.001	-1.015	-8.816	H
HETATM 453 H	0	-0.936	-1.480	-7.153	H
HETATM 454 H	0	1.099	-0.394	-7.562	H
HETATM 455 H	0	1.339	-1.200	-9.104	H
HETATM 456 H	0	2.917	-1.863	-7.273	H
HETATM 457 H	0	2.102	-3.210	-8.076	H
HETATM 458 H	0	0.793	-2.265	-5.620	H
HETATM 459 H	0	2.913	-5.562	-5.208	H
HETATM 460 H	0	3.386	-4.532	-6.576	H
HETATM 461 H	0	0.743	-3.487	-3.855	H
HETATM 462 H	0	1.608	-5.063	-3.864	H
HETATM 463 N	0	-3.110	-3.563	-7.524	N
HETATM 464 C	0	-4.099	-4.199	-6.650	C
HETATM 465 H	0	-3.801	-4.061	-5.632	H
HETATM 466 H	0	-4.130	-5.246	-6.873	H
HETATM 467 H	0	-5.069	-3.773	-6.800	H
HETATM 468 H	0	-3.411	-2.944	-8.258	H
HETATM 469 C	0	0.050	-7.863	-7.224	C
HETATM 470 H	0	-0.091	-8.877	-7.534	H
HETATM 471 H	0	1.009	-7.520	-7.550	H
HETATM 472 H	0	-0.714	-7.249	-7.655	H
HETATM 473 C	0	-0.162	-7.860	-5.720	C
HETATM 474 O	0	-0.016	-8.919	-5.135	O
HETATM 475 N	0	-0.620	-6.754	-5.112	N
HETATM 476 C	0	-0.935	-6.598	-3.672	C
HETATM 477 C	0	-1.743	-7.767	-3.090	C
HETATM 478 O	0	-1.379	-8.364	-2.077	O
HETATM 479 C	0	-1.647	-5.262	-3.389	C
HETATM 480 C	0	-1.672	-4.954	-1.892	C
HETATM 481 O	0	-2.332	-5.620	-1.113	O
HETATM 482 N	0	-0.979	-3.954	-1.425	N
HETATM 483 H	0	-0.732	-5.935	-5.698	H
HETATM 484 H	0	-0.003	-6.542	-3.129	H
HETATM 485 H	0	-2.670	-5.320	-3.750	H
HETATM 486 H	0	-1.167	-4.440	-3.911	H
HETATM 487 H	0	-1.069	-3.730	-0.433	H
HETATM 488 H	0	-0.676	-3.213	-2.055	H
HETATM 489 N	0	-2.878	-8.071	-3.718	N
HETATM 490 C	0	-3.730	-9.163	-3.295	C
HETATM 491 H	0	-3.425	-9.482	-2.320	H
HETATM 492 H	0	-3.618	-9.972	-3.986	H
HETATM 493 H	0	-4.756	-8.858	-3.266	H
HETATM 494 H	0	-3.067	-7.564	-4.568	H

HETATM 495 C	0	-1.268 -11.865 -4.606	C
HETATM 496 H	0	-1.699 -12.837 -4.722	H
HETATM 497 H	0	-1.013 -11.470 -5.567	H
HETATM 498 H	0	-1.973 -11.217 -4.129	H
HETATM 499 C	0	-0.154 -11.954 -3.539	C
HETATM 500 O	0	-0.021 -13.012 -2.942	O
HETATM 501 N	0	0.540 -10.862 -3.174	N
HETATM 502 C	0	1.550 -10.758 -2.064	C
HETATM 503 C	0	0.996 -10.949 -0.639	C
HETATM 504 O	0	1.650 -11.586 0.182	O
HETATM 505 C	0	2.479 -9.541 -2.211	C
HETATM 506 C	0	1.647 -8.278 -2.205	C
HETATM 507 C	0	2.413 -6.986 -2.391	C
HETATM 508 O	0	2.710 -6.358 -1.360	O
HETATM 509 O	0	2.547 -6.472 -3.528	O
HETATM 510 H	0	0.370 -10.032 -3.733	H
HETATM 511 H	0	2.207 -11.620 -2.191	H
HETATM 512 H	0	3.196 -9.517 -1.389	H
HETATM 513 H	0	3.022 -9.611 -3.155	H
HETATM 514 H	0	1.100 -8.223 -1.267	H
HETATM 515 H	0	0.948 -8.360 -3.018	H
HETATM 516 N	0	-0.204 -10.449 -0.326	N
HETATM 517 C	0	-0.901 -10.772 0.934	C
HETATM 518 C	0	-1.596 -12.149 0.923	C
HETATM 519 O	0	-2.022 -12.621 1.977	O
HETATM 520 C	0	-1.975 -9.716 1.237	C
HETATM 521 C	0	-1.514 -8.424 1.884	C
HETATM 522 C	0	-0.808 -7.476 1.124	C
HETATM 523 C	0	-1.958 -8.087 3.181	C
HETATM 524 C	0	-0.598 -6.180 1.620	C
HETATM 525 C	0	-1.755 -6.784 3.680	C
HETATM 526 C	0	-1.102 -5.818 2.885	C
HETATM 527 O	0	-1.004 -4.535 3.315	O
HETATM 528 H	0	-0.654 -9.861 -1.020	H
HETATM 529 H	0	-0.184 -10.784 1.757	H
HETATM 530 H	0	-2.500 -9.476 0.311	H
HETATM 531 H	0	-2.719 -10.156 1.902	H
HETATM 532 H	0	-0.478 -7.714 0.126	H
HETATM 533 H	0	-2.493 -8.814 3.781	H
HETATM 534 H	0	-0.089 -5.455 1.004	H
HETATM 535 H	0	-2.131 -6.495 4.650	H
HETATM 536 H	0	-0.866 -3.949 2.530	H
HETATM 537 N	0	-1.794 -12.761 -0.251	N
HETATM 538 C	0	-2.400 -14.080 -0.405	C
HETATM 539 H	0	-2.070 -14.689 0.410	H
HETATM 540 H	0	-2.037 -14.488 -1.325	H
HETATM 541 H	0	-3.469 -14.057 -0.423	H
HETATM 542 H	0	-1.309 -12.365 -1.046	H
HETATM 543 C	0	-12.879 -7.413 1.575	C

HETATM 544 H	0	-12.647	-6.738	2.373	H
HETATM 545 H	0	-12.738	-8.420	1.909	H
HETATM 546 H	0	-13.897	-7.276	1.276	H
HETATM 547 C	0	-11.979	-7.124	0.389	C
HETATM 548 O	0	-12.075	-6.051	-0.192	O
HETATM 549 N	0	-11.115	-8.071	-0.010	N
HETATM 550 C	0	-10.149	-7.898	-1.124	C
HETATM 551 C	0	-10.772	-7.620	-2.493	C
HETATM 552 O	0	-10.140	-6.914	-3.272	O
HETATM 553 C	0	-9.137	-9.059	-1.190	C
HETATM 554 C	0	-8.021	-8.967	-0.132	C
HETATM 555 C	0	-7.262	-7.632	-0.232	C
HETATM 556 N	0	-6.001	-7.611	0.525	N
HETATM 557 C	0	-4.973	-6.833	0.246	C
HETATM 558 N	0	-4.989	-5.981	-0.729	N
HETATM 559 N	0	-3.872	-6.877	0.920	N
HETATM 560 H	0	-11.105	-8.924	0.530	H
HETATM 561 H	0	-9.608	-6.991	-0.910	H
HETATM 562 H	0	-9.660	-10.011	-1.086	H
HETATM 563 H	0	-8.658	-9.053	-2.172	H
HETATM 564 H	0	-7.321	-9.787	-0.300	H
HETATM 565 H	0	-8.453	-9.081	0.860	H
HETATM 566 H	0	-7.887	-6.822	0.147	H
HETATM 567 H	0	-7.051	-7.446	-1.287	H
HETATM 568 H	0	-5.930	-8.137	1.381	H
HETATM 569 H	0	-4.112	-5.505	-0.916	H
HETATM 570 H	0	-5.821	-5.738	-1.230	H
HETATM 571 H	0	-3.714	-7.474	1.710	H
HETATM 572 H	0	-3.076	-6.370	0.537	H
HETATM 573 N	0	-11.971	-8.135	-2.788	N
HETATM 574 C	0	-12.727	-7.799	-3.997	C
HETATM 575 H	0	-13.175	-8.664	-4.440	H
HETATM 576 H	0	-12.054	-7.348	-4.697	H
HETATM 577 H	0	-13.489	-7.097	-3.732	H
HETATM 578 H	0	-12.405	-8.699	-2.075	H
HETATM 579 C	0	-13.990	-4.418	-2.689	C
HETATM 580 H	0	-13.919	-5.159	-1.920	H
HETATM 581 H	0	-14.058	-4.899	-3.642	H
HETATM 582 H	0	-14.862	-3.819	-2.529	H
HETATM 583 C	0	-12.756	-3.530	-2.719	C
HETATM 584 O	0	-12.775	-2.523	-3.413	O
HETATM 585 N	0	-11.665	-3.922	-2.048	N
HETATM 586 C	0	-10.331	-3.306	-2.208	C
HETATM 587 C	0	-9.925	-3.227	-3.684	C
HETATM 588 O	0	-9.522	-2.164	-4.137	O
HETATM 589 C	0	-9.266	-4.042	-1.389	C
HETATM 590 C	0	-7.836	-3.810	-1.852	C
HETATM 591 C	0	-7.154	-2.640	-1.474	C
HETATM 592 C	0	-7.209	-4.736	-2.711	C

HETATM 593 C	0	-5.819	-2.429	-1.869	C
HETATM 594 C	0	-5.894	-4.502	-3.156	C
HETATM 595 C	0	-5.185	-3.367	-2.706	C
HETATM 596 O	0	-3.904	-3.188	-3.104	O
HETATM 597 H	0	-11.765	-4.722	-1.434	H
HETATM 598 H	0	-10.383	-2.281	-1.842	H
HETATM 599 H	0	-9.363	-3.761	-0.340	H
HETATM 600 H	0	-9.466	-5.098	-1.466	H
HETATM 601 H	0	-7.670	-1.905	-0.879	H
HETATM 602 H	0	-7.752	-5.605	-3.062	H
HETATM 603 H	0	-5.262	-1.561	-1.544	H
HETATM 604 H	0	-5.399	-5.189	-3.826	H
HETATM 605 H	0	-3.412	-2.478	-2.612	H
HETATM 606 N	0	-9.992	-4.329	-4.435	N
HETATM 607 C	0	-9.640	-4.357	-5.846	C
HETATM 608 H	0	-9.775	-5.338	-6.252	H
HETATM 609 H	0	-8.619	-4.060	-5.961	H
HETATM 610 H	0	-10.273	-3.667	-6.364	H
HETATM 611 H	0	-10.280	-5.189	-3.980	H
HETATM 612 C	0	-12.034	0.437	-4.908	C
HETATM 613 H	0	-11.891	0.007	-3.939	H
HETATM 614 H	0	-12.364	-0.320	-5.589	H
HETATM 615 H	0	-12.772	1.210	-4.850	H
HETATM 616 C	0	-10.757	1.034	-5.443	C
HETATM 617 O	0	-10.794	2.100	-6.040	O
HETATM 618 N	0	-9.643	0.325	-5.262	N
HETATM 619 C	0	-8.288	0.695	-5.694	C
HETATM 620 C	0	-8.249	0.905	-7.227	C
HETATM 621 O	0	-7.576	1.810	-7.719	O
HETATM 622 C	0	-7.285	-0.354	-5.213	C
HETATM 623 C	0	-5.820	-0.023	-5.400	C
HETATM 624 C	0	-4.895	-1.070	-5.269	C
HETATM 625 C	0	-5.365	1.281	-5.685	C
HETATM 626 C	0	-3.522	-0.834	-5.435	C
HETATM 627 C	0	-3.999	1.512	-5.903	C
HETATM 628 C	0	-3.078	0.456	-5.778	C
HETATM 629 O	0	-1.767	0.701	-5.971	O
HETATM 630 H	0	-9.750	-0.553	-4.769	H
HETATM 631 H	0	-8.058	1.653	-5.228	H
HETATM 632 H	0	-7.441	-0.529	-4.151	H
HETATM 633 H	0	-7.494	-1.290	-5.733	H
HETATM 634 H	0	-5.246	-2.063	-5.035	H
HETATM 635 H	0	-6.040	2.118	-5.786	H
HETATM 636 H	0	-2.814	-1.639	-5.302	H
HETATM 637 H	0	-3.647	2.494	-6.162	H
HETATM 638 H	0	-1.226	-0.053	-5.638	H
HETATM 639 N	0	-8.999	0.083	-7.977	N
HETATM 640 C	0	-9.288	0.269	-9.397	C
HETATM 641 H	0	-9.597	-0.657	-9.836	H

HETATM 642 H	0	-8.409	0.623	-9.895	H
HETATM 643 H	0	-10.071	0.991	-9.499	H
HETATM 644 H	0	-9.531	-0.595	-7.455	H
HETATM 645 C	0	-9.687	5.745	-6.239	C
HETATM 646 H	0	-10.399	6.426	-5.821	H
HETATM 647 H	0	-10.203	4.947	-6.731	H
HETATM 648 H	0	-9.072	6.262	-6.946	H
HETATM 649 C	0	-8.899	5.191	-5.066	C
HETATM 650 O	0	-9.277	4.178	-4.488	O
HETATM 651 N	0	-7.874	5.920	-4.613	N
HETATM 652 C	0	-7.144	5.614	-3.370	C
HETATM 653 C	0	-8.080	5.442	-2.150	C
HETATM 654 O	0	-7.776	4.668	-1.253	O
HETATM 655 C	0	-6.070	6.675	-3.141	C
HETATM 656 H	0	-7.653	6.769	-5.107	H
HETATM 657 H	0	-6.641	4.655	-3.504	H
HETATM 658 H	0	-5.520	6.407	-2.242	H
HETATM 659 H	0	-6.525	7.656	-3.010	H
HETATM 660 H	0	-5.384	6.700	-3.988	H
HETATM 661 N	0	-9.211	6.156	-2.116	N
HETATM 662 C	0	-10.177	6.209	-1.014	C
HETATM 663 C	0	-11.212	5.083	-1.008	C
HETATM 664 O	0	-11.476	4.516	0.049	O
HETATM 665 C	0	-10.867	7.587	-1.012	C
HETATM 666 C	0	-9.941	8.755	-0.600	C
HETATM 667 C	0	-8.823	9.073	-1.594	C
HETATM 668 O	0	-8.949	8.903	-2.798	O
HETATM 669 N	0	-7.670	9.523	-1.150	N
HETATM 670 H	0	-9.308	6.837	-2.859	H
HETATM 671 H	0	-9.626	6.149	-0.083	H
HETATM 672 H	0	-11.299	7.787	-1.994	H
HETATM 673 H	0	-11.685	7.554	-0.292	H
HETATM 674 H	0	-9.503	8.531	0.374	H
HETATM 675 H	0	-10.551	9.652	-0.493	H
HETATM 676 H	0	-7.012	9.735	-1.875	H
HETATM 677 H	0	-7.459	9.695	-0.171	H
HETATM 678 N	0	-11.807	4.757	-2.162	N
HETATM 679 C	0	-12.826	3.700	-2.283	C
HETATM 680 H	0	-13.067	3.544	-3.334	H
HETATM 681 C	0	-12.365	2.366	-1.692	C
HETATM 682 O	0	-13.140	1.656	-1.059	O
HETATM 683 H	0	-11.495	5.226	-2.999	H
HETATM 684 H	0	-13.731	4.009	-1.760	H
HETATM 685 N	0	-11.082	2.042	-1.886	N
HETATM 686 C	0	-10.433	0.827	-1.375	C
HETATM 687 C	0	-10.345	0.774	0.152	C
HETATM 688 O	0	-10.352	-0.332	0.680	O
HETATM 689 C	0	-9.042	0.666	-2.011	C
HETATM 690 C	0	-7.896	1.249	-1.191	C

HETATM 691 C	0	-6.603	1.329	-1.972	C
HETATM 692 N	0	-5.601	1.943	-1.133	N
HETATM 693 C	0	-4.340	2.124	-1.506	C
HETATM 694 N	0	-3.912	1.678	-2.704	N
HETATM 695 N	0	-3.529	2.799	-0.693	N
HETATM 696 H	0	-10.545	2.686	-2.454	H
HETATM 697 H	0	-11.081	-0.010	-1.662	H
HETATM 698 H	0	-8.843	-0.395	-2.196	H
HETATM 699 H	0	-9.024	1.160	-2.985	H
HETATM 700 H	0	-7.720	0.658	-0.283	H
HETATM 701 H	0	-8.150	2.260	-0.863	H
HETATM 702 H	0	-6.755	1.932	-2.879	H
HETATM 703 H	0	-6.298	0.322	-2.288	H
HETATM 704 H	0	-5.789	2.092	-0.128	H
HETATM 705 H	0	-2.926	1.438	-2.768	H
HETATM 706 H	0	-4.535	1.106	-3.261	H
HETATM 707 H	0	-3.908	2.855	0.272	H
HETATM 708 H	0	-2.512	2.679	-0.709	H
HETATM 709 N	0	-10.099	1.909	0.830	N
HETATM 710 C	0	-9.448	1.986	2.156	C
HETATM 711 C	0	-10.158	1.078	3.158	C
HETATM 712 O	0	-9.575	0.150	3.703	O
HETATM 713 C	0	-9.486	3.428	2.715	C
HETATM 714 C	0	-8.744	4.505	1.923	C
HETATM 715 C	0	-9.056	5.884	2.511	C
HETATM 716 C	0	-7.240	4.327	1.927	C
HETATM 717 H	0	-10.210	2.767	0.308	H
HETATM 718 H	0	-8.409	1.654	2.083	H
HETATM 719 H	0	-10.529	3.742	2.783	H
HETATM 720 H	0	-9.081	3.413	3.728	H
HETATM 721 H	0	-9.082	4.457	0.899	H
HETATM 722 H	0	-8.752	5.926	3.556	H
HETATM 723 H	0	-10.127	6.076	2.441	H
HETATM 724 H	0	-8.527	6.655	1.952	H
HETATM 725 H	0	-6.877	4.199	2.944	H
HETATM 726 H	0	-6.751	5.164	1.430	H
HETATM 727 H	0	-7.017	3.431	1.353	H
HETATM 728 N	0	-11.437	1.356	3.409	N
HETATM 729 C	0	-12.266	0.569	4.295	C
HETATM 730 H	0	-11.938	0.665	5.310	H
HETATM 731 H	0	-12.188	-0.453	3.990	H
HETATM 732 H	0	-13.285	0.888	4.218	H
HETATM 733 H	0	-11.845	2.109	2.872	H
HETATM 734 C	0	-12.055	-2.803	2.421	C
HETATM 735 H	0	-12.674	-3.651	2.218	H
HETATM 736 H	0	-12.137	-2.101	1.616	H
HETATM 737 H	0	-12.372	-2.339	3.331	H
HETATM 738 C	0	-10.620	-3.288	2.580	C
HETATM 739 O	0	-10.461	-4.421	3.019	O

HETATM 740 N	0	-9.577	-2.484	2.313	N
HETATM 741 C	0	-8.176	-2.830	2.655	C
HETATM 742 C	0	-8.038	-3.027	4.165	C
HETATM 743 O	0	-7.655	-4.113	4.586	O
HETATM 744 C	0	-7.127	-1.814	2.163	C
HETATM 745 C	0	-5.680	-2.315	2.407	C
HETATM 746 C	0	-5.325	-3.613	1.678	C
HETATM 747 C	0	-4.655	-1.298	1.938	C
HETATM 748 H	0	-9.780	-1.556	1.953	H
HETATM 749 H	0	-7.969	-3.781	2.170	H
HETATM 750 H	0	-7.266	-1.621	1.109	H
HETATM 751 H	0	-7.264	-0.866	2.685	H
HETATM 752 H	0	-5.523	-2.474	3.473	H
HETATM 753 H	0	-5.551	-3.521	0.619	H
HETATM 754 H	0	-5.876	-4.443	2.102	H
HETATM 755 H	0	-4.262	-3.830	1.797	H
HETATM 756 H	0	-4.721	-1.148	0.861	H
HETATM 757 H	0	-3.658	-1.634	2.219	H
HETATM 758 H	0	-4.841	-0.360	2.440	H
HETATM 759 N	0	-8.407	-2.025	4.968	N
HETATM 760 C	0	-8.477	-2.089	6.430	C
HETATM 761 C	0	-9.270	-3.301	6.928	C
HETATM 762 O	0	-8.884	-3.916	7.914	O
HETATM 763 C	0	-9.035	-0.786	7.032	C
HETATM 764 C	0	-8.047	0.367	7.082	C
HETATM 765 C	0	-8.263	1.529	6.318	C
HETATM 766 C	0	-6.893	0.270	7.886	C
HETATM 767 C	0	-7.319	2.573	6.326	C
HETATM 768 C	0	-5.944	1.312	7.897	C
HETATM 769 C	0	-6.152	2.465	7.109	C
HETATM 770 O	0	-5.228	3.463	7.094	O
HETATM 771 H	0	-8.666	-1.158	4.508	H
HETATM 772 H	0	-7.461	-2.221	6.803	H
HETATM 773 H	0	-9.929	-0.489	6.482	H
HETATM 774 H	0	-9.342	-0.985	8.060	H
HETATM 775 H	0	-9.145	1.615	5.701	H
HETATM 776 H	0	-6.722	-0.617	8.484	H
HETATM 777 H	0	-7.460	3.437	5.696	H
HETATM 778 H	0	-5.052	1.221	8.498	H
HETATM 779 H	0	-4.349	3.078	7.262	H
HETATM 780 N	0	-10.347	-3.678	6.235	N
HETATM 781 C	0	-11.085	-4.913	6.506	C
HETATM 782 H	0	-12.011	-4.914	5.932	H
HETATM 783 C	0	-10.300	-6.185	6.152	C
HETATM 784 O	0	-10.287	-7.130	6.930	O
HETATM 785 H	0	-10.568	-3.139	5.413	H
HETATM 786 H	0	-11.340	-4.956	7.566	H
HETATM 787 N	0	-9.652	-6.225	4.982	N
HETATM 788 C	0	-8.766	-7.317	4.545	C

HETATM 789 C	0	-7.492	-7.475	5.388	C
HETATM 790 O	0	-6.925	-8.563	5.431	O
HETATM 791 C	0	-8.438	-7.216	3.063	C
HETATM 792 O	0	-7.535	-6.176	2.785	O
HETATM 793 H	0	-9.762	-5.423	4.371	H
HETATM 794 H	0	-9.321	-8.245	4.680	H
HETATM 795 H	0	-9.358	-7.064	2.497	H
HETATM 796 H	0	-7.983	-8.157	2.757	H
HETATM 797 H	0	-7.638	-5.474	3.455	H
HETATM 798 N	0	-7.042	-6.397	6.032	N
HETATM 799 C	0	-6.019	-6.379	7.068	C
HETATM 800 C	0	-6.577	-6.839	8.431	C
HETATM 801 O	0	-5.907	-7.586	9.142	O
HETATM 802 C	0	-5.429	-4.964	7.143	C
HETATM 803 H	0	-7.514	-5.524	5.840	H
HETATM 804 H	0	-5.223	-7.073	6.792	H
HETATM 805 H	0	-4.626	-4.945	7.881	H
HETATM 806 H	0	-6.198	-4.249	7.437	H
HETATM 807 H	0	-5.025	-4.678	6.171	H
HETATM 808 N	0	-7.785	-6.386	8.800	N
HETATM 809 C	0	-8.521	-6.822	9.981	C
HETATM 810 H	0	-8.229	-6.232	10.825	H
HETATM 811 H	0	-8.257	-7.844	10.152	H
HETATM 812 H	0	-9.580	-6.746	9.843	H
HETATM 813 H	0	-8.236	-5.709	8.198	H
HETATM 814 N	0	3.141	-3.763	-1.750	N
HETATM 815 C	0	2.288	-2.770	-1.046	C
HETATM 816 C	0	2.595	-1.320	-1.555	C
HETATM 817 O	0	3.185	-1.236	-2.660	O
HETATM 818 O	0	2.313	-0.299	-0.888	O
HETATM 819 C	0	2.429	-3.033	0.468	C
HETATM 820 C	0	1.575	-2.170	1.407	C
HETATM 821 C	0	0.115	-2.116	1.011	C
HETATM 822 O	0	-0.610	-3.076	1.223	O
HETATM 823 N	0	-0.275	-0.982	0.405	N
HETATM 824 C	0	-1.667	-0.606	0.235	C
HETATM 825 C	0	-1.903	-0.553	-1.277	C
HETATM 826 O	0	-2.540	-1.404	-1.865	O
HETATM 827 C	0	-1.940	0.665	1.052	C
HETATM 828 S	0	-0.760	2.033	0.711	S
HETATM 829 N	0	-1.260	0.507	-1.911	N
HETATM 830 C	0	-0.301	0.284	-3.010	C
HETATM 831 C	0	-0.188	-1.102	-3.668	C
HETATM 832 O	0	0.214	-2.096	-3.028	O
HETATM 833 O	0	-0.386	-1.177	-4.898	O
HETATM 834 H	0	4.019	-3.904	-1.255	H
HETATM 835 H	0	3.311	-3.442	-2.692	H
HETATM 836 H	0	2.749	-4.709	-1.726	H
HETATM 837 H	0	1.247	-2.950	-1.306	H

HETATM 838 H	0	2.161	-4.076	0.647	H
HETATM 839 H	0	3.467	-2.901	0.751	H
HETATM 840 H	0	1.977	-1.159	1.444	H
HETATM 841 H	0	1.624	-2.580	2.413	H
HETATM 842 H	0	0.378	-0.190	0.377	H
HETATM 843 H	0	-2.268	-1.437	0.599	H
HETATM 844 H	0	-2.978	0.984	0.919	H
HETATM 845 H	0	-1.852	0.371	2.102	H
HETATM 846 H	0	-0.805	1.140	-1.226	H
HETATM 847 H	0	-0.516	0.992	-3.800	H
HETATM 848 H	0	0.691	0.517	-2.639	H
HETATM 849 C	0	-5.051	2.133	2.769	C
HETATM 850 O	0	-6.031	1.694	3.372	O
HETATM 851 C	0	-3.827	2.560	3.601	C
HETATM 852 C	0	-3.091	3.747	3.003	C
HETATM 853 C	0	-1.716	3.982	3.606	C
HETATM 854 C	0	-0.986	5.156	3.017	C
HETATM 855 O	0	-4.901	2.203	1.499	O
HETATM 856 C	0	-1.234	5.654	1.665	C
HETATM 857 C	0	-0.223	6.345	0.837	C
HETATM 858 O	0	-1.748	6.364	2.799	O
HETATM 859 C	0	-0.155	7.672	0.703	C
HETATM 860 C	0	0.777	8.349	-0.197	C
HETATM 861 C	0	0.568	9.575	-0.692	C
HETATM 862 C	0	1.442	10.179	-1.568	C
HETATM 863 C	0	1.298	11.384	-2.178	C
HETATM 864 C	0	0.095	12.300	-2.055	C
HETATM 865 C	0	-0.575	12.451	-3.414	C
HETATM 866 C	0	-1.864	12.119	-3.695	C
HETATM 867 C	0	-2.835	11.542	-2.682	C
HETATM 868 C	0	-2.645	10.027	-2.557	C
HETATM 869 C	0	-3.448	9.464	-1.377	C
HETATM 870 C	0	-3.219	7.955	-1.269	C
HETATM 871 C	0	-4.005	7.365	-0.096	C
HETATM 872 H	0	-4.157	2.757	4.626	H
HETATM 873 H	0	-3.147	1.698	3.639	H
HETATM 874 H	0	-3.700	4.656	3.084	H
HETATM 875 H	0	-2.950	3.534	1.944	H
HETATM 876 H	0	-1.090	3.105	3.414	H
HETATM 877 H	0	-1.778	4.128	4.695	H
HETATM 878 H	0	0.006	5.351	3.440	H
HETATM 879 H	0	-1.995	5.128	1.093	H
HETATM 880 H	0	0.432	5.703	0.257	H
HETATM 881 H	0	-0.853	8.305	1.256	H
HETATM 882 H	0	1.662	7.778	-0.479	H
HETATM 883 H	0	-0.338	10.086	-0.379	H
HETATM 884 H	0	2.352	9.639	-1.793	H
HETATM 885 H	0	2.106	11.713	-2.831	H
HETATM 886 H	0	0.449	13.282	-1.739	H

HETATM	887	H	0	-0.596	11.959	-1.293	H
HETATM	888	H	0	0.029	12.865	-4.221	H
HETATM	889	H	0	-2.224	12.283	-4.711	H
HETATM	890	H	0	-2.710	12.028	-1.714	H
HETATM	891	H	0	-3.854	11.745	-3.016	H
HETATM	892	H	0	-2.965	9.552	-3.486	H
HETATM	893	H	0	-1.588	9.811	-2.408	H
HETATM	894	H	0	-3.121	9.944	-0.452	H
HETATM	895	H	0	-4.510	9.666	-1.524	H
HETATM	896	H	0	-2.157	7.759	-1.117	H
HETATM	897	H	0	-3.528	7.478	-2.196	H
HETATM	898	H	0	-5.067	7.593	-0.193	H
HETATM	899	H	0	-3.872	6.282	-0.070	H
HETATM	900	H	0	-3.632	7.789	0.833	H
HETATM	901	O	0	6.733	3.586	10.559	O
HETATM	902	H	0	7.463	3.915	11.090	H
HETATM	903	H	0	6.564	2.710	10.916	H
HETATM	904	O	0	-4.019	10.712	2.590	O
HETATM	905	H	0	-3.891	9.766	2.815	H
HETATM	906	H	0	-3.713	11.147	3.416	H
HETATM	907	O	0	-5.847	6.619	3.794	O
HETATM	908	H	0	-6.061	5.790	3.347	H
HETATM	909	H	0	-5.948	6.393	4.740	H
HETATM	910	O	0	-6.478	10.469	1.400	O
HETATM	911	H	0	-6.768	11.383	1.476	H
HETATM	912	H	0	-5.553	10.517	1.719	H
HETATM	913	O	0	-3.693	8.172	3.383	O
HETATM	914	H	0	-4.495	7.618	3.487	H
HETATM	915	H	0	-3.044	7.540	3.026	H
HETATM	916	O	0	-0.156	11.613	5.347	O
HETATM	917	H	0	0.786	11.871	5.270	H
HETATM	918	H	0	-0.177	11.107	6.175	H
HETATM	919	O	0	-7.374	8.920	3.516	O
HETATM	920	H	0	-6.852	8.099	3.487	H
HETATM	921	H	0	-7.096	9.390	2.710	H
HETATM	922	O	0	-1.791	11.739	1.334	O
HETATM	923	H	0	-2.596	11.317	1.686	H
HETATM	924	H	0	-1.997	12.675	1.379	H
HETATM	925	O	0	-3.625	-1.506	5.843	O
HETATM	926	H	0	-4.438	-1.042	5.537	H
HETATM	927	H	0	-3.401	-2.056	5.088	H
HETATM	928	O	0	-5.192	8.623	6.973	O
HETATM	929	H	0	-6.022	9.078	6.702	H
HETATM	930	H	0	-5.452	7.687	6.904	H
HETATM	931	O	0	-5.788	-0.194	5.043	O
HETATM	932	H	0	-6.400	0.144	5.705	H
HETATM	933	H	0	-5.887	0.488	4.323	H
HETATM	934	O	0	-2.587	-0.140	7.888	O
HETATM	935	H	0	-2.985	-0.633	7.134	H

HETATM	936	H	0	-2.210	-0.847	8.418	H
HETATM	937	O	0	1.264	8.717	8.544	O
HETATM	938	H	0	1.791	9.391	8.982	H
HETATM	939	H	0	0.475	9.209	8.243	H
HETATM	940	O	0	6.295	-1.862	10.096	O
HETATM	941	H	0	6.115	-2.460	9.354	H
HETATM	942	H	0	7.234	-1.963	10.247	H
HETATM	943	O	0	-3.649	10.873	7.539	O
HETATM	944	H	0	-4.225	10.093	7.422	H
HETATM	945	H	0	-4.182	11.457	8.087	H
HETATM	946	O	0	-1.014	9.873	7.431	O
HETATM	947	H	0	-1.766	10.407	7.739	H
HETATM	948	H	0	-1.462	9.245	6.834	H
HETATM	949	O	0	-6.129	6.010	6.466	O
HETATM	950	H	0	-5.736	5.139	6.668	H
HETATM	951	H	0	-6.974	5.972	6.927	H
HETATM	952	O	0	-2.694	2.447	7.270	O
HETATM	953	H	0	-2.402	2.348	6.355	H
HETATM	954	H	0	-2.651	1.516	7.595	H
HETATM	955	O	0	-2.886	11.537	4.896	O
HETATM	956	H	0	-3.168	11.388	5.813	H
HETATM	957	H	0	-1.927	11.688	4.989	H
HETATM	958	O	0	0.558	11.146	2.687	O
HETATM	959	H	0	-0.148	11.286	2.033	H
HETATM	960	H	0	0.106	11.305	3.530	H
HETATM	961	O	0	-7.500	9.642	6.091	O
HETATM	962	H	0	-7.494	9.405	5.138	H
HETATM	963	H	0	-8.330	10.113	6.189	H
HETATM	964	O	0	2.495	11.909	4.560	O
HETATM	965	H	0	3.429	11.667	4.452	H
HETATM	966	H	0	2.115	11.707	3.687	H
HETATM	967	O	0	-1.891	4.564	8.766	O
HETATM	968	H	0	-2.291	4.424	9.630	H
HETATM	969	H	0	-2.118	3.739	8.286	H
HETATM	970	O	0	-2.730	8.313	5.899	O
HETATM	971	H	0	-2.989	8.452	4.967	H
HETATM	972	H	0	-3.581	8.447	6.362	H

TS (Tail-to-head orientation)

E = -2159.359872309970 hartrees

HETATM	1	C	0	5.435	-5.297	9.533	C
HETATM	2	H	0	5.735	-4.706	10.373	H
HETATM	3	H	0	5.795	-6.298	9.654	H
HETATM	4	H	0	4.367	-5.309	9.469	H
HETATM	5	C	0	6.021	-4.682	8.286	C
HETATM	6	O	0	6.016	-3.463	8.177	O
HETATM	7	N	0	6.504	-5.494	7.340	N

HETATM	8	C	0	6.994	-5.027	6.030	C
HETATM	9	H	0	7.265	-5.879	5.406	H
HETATM	10	C	0	5.931	-4.202	5.304	C
HETATM	11	O	0	6.183	-3.053	4.966	O
HETATM	12	H	0	6.501	-6.484	7.531	H
HETATM	13	H	0	7.879	-4.407	6.174	H
HETATM	14	N	0	4.730	-4.759	5.107	N
HETATM	15	C	0	3.553	-4.079	4.531	C
HETATM	16	C	0	3.257	-2.741	5.198	C
HETATM	17	O	0	3.147	-1.725	4.520	O
HETATM	18	C	0	2.329	-4.998	4.589	C
HETATM	19	O	0	2.183	-5.549	5.888	O
HETATM	20	H	0	4.574	-5.692	5.459	H
HETATM	21	H	0	3.755	-3.867	3.480	H
HETATM	22	H	0	2.453	-5.808	3.867	H
HETATM	23	H	0	1.440	-4.426	4.328	H
HETATM	24	H	0	1.391	-6.101	5.881	H
HETATM	25	N	0	3.167	-2.730	6.526	N
HETATM	26	C	0	2.981	-1.530	7.342	C
HETATM	27	C	0	4.099	-0.494	7.191	C
HETATM	28	O	0	3.842	0.708	7.176	O
HETATM	29	C	0	2.815	-1.932	8.821	C
HETATM	30	C	0	1.616	-2.853	9.122	C
HETATM	31	C	0	1.626	-3.228	10.604	C
HETATM	32	C	0	0.270	-2.194	8.808	C
HETATM	33	H	0	3.222	-3.635	6.971	H
HETATM	34	H	0	2.060	-1.045	7.030	H
HETATM	35	H	0	3.726	-2.430	9.150	H
HETATM	36	H	0	2.709	-1.022	9.414	H
HETATM	37	H	0	1.705	-3.770	8.540	H
HETATM	38	H	0	1.515	-2.335	11.219	H
HETATM	39	H	0	2.566	-3.720	10.855	H
HETATM	40	H	0	0.806	-3.915	10.817	H
HETATM	41	H	0	0.185	-1.247	9.341	H
HETATM	42	H	0	-0.540	-2.857	9.113	H
HETATM	43	H	0	0.181	-2.019	7.737	H
HETATM	44	N	0	5.338	-0.956	7.065	N
HETATM	45	C	0	6.490	-0.127	6.754	C
HETATM	46	H	0	7.396	-0.729	6.817	H
HETATM	47	C	0	6.405	0.469	5.356	C
HETATM	48	O	0	6.632	1.662	5.232	O
HETATM	49	H	0	5.471	-1.959	7.127	H
HETATM	50	H	0	6.560	0.685	7.479	H
HETATM	51	N	0	6.045	-0.310	4.325	N
HETATM	52	C	0	5.703	0.220	2.990	C
HETATM	53	C	0	4.604	1.271	3.122	C
HETATM	54	O	0	4.816	2.379	2.668	O
HETATM	55	C	0	5.366	-0.850	1.950	C
HETATM	56	C	0	5.175	-0.204	0.576	C

HETATM	57	C	0	6.497	-1.856	1.755	C
HETATM	58	H	0	5.911	-1.298	4.513	H
HETATM	59	H	0	6.583	0.747	2.624	H
HETATM	60	H	0	4.462	-1.375	2.249	H
HETATM	61	H	0	6.070	0.358	0.309	H
HETATM	62	H	0	4.320	0.470	0.590	H
HETATM	63	H	0	5.010	-0.969	-0.180	H
HETATM	64	H	0	7.368	-1.383	1.314	H
HETATM	65	H	0	6.162	-2.622	1.066	H
HETATM	66	H	0	6.783	-2.314	2.695	H
HETATM	67	N	0	3.485	0.981	3.791	N
HETATM	68	C	0	2.378	1.907	4.111	C
HETATM	69	C	0	2.845	3.244	4.709	C
HETATM	70	O	0	2.504	4.309	4.194	O
HETATM	71	C	0	1.341	1.166	4.994	C
HETATM	72	C	0	0.452	0.291	4.092	C
HETATM	73	C	0	0.499	2.091	5.890	C
HETATM	74	C	0	-0.308	-0.829	4.810	C
HETATM	75	H	0	3.409	0.027	4.126	H
HETATM	76	H	0	1.877	2.170	3.178	H
HETATM	77	H	0	1.883	0.503	5.654	H
HETATM	78	H	0	-0.255	0.921	3.565	H
HETATM	79	H	0	1.082	-0.180	3.347	H
HETATM	80	H	0	0.088	2.904	5.299	H
HETATM	81	H	0	1.123	2.507	6.681	H
HETATM	82	H	0	-0.306	1.534	6.365	H
HETATM	83	H	0	-1.007	-0.415	5.534	H
HETATM	84	H	0	0.394	-1.491	5.314	H
HETATM	85	H	0	-0.870	-1.407	4.075	H
HETATM	86	N	0	3.607	3.204	5.802	N
HETATM	87	C	0	4.224	4.380	6.429	C
HETATM	88	C	0	5.161	5.081	5.439	C
HETATM	89	O	0	4.980	6.260	5.159	O
HETATM	90	C	0	4.973	3.928	7.685	C
HETATM	91	O	0	5.459	5.041	8.399	O
HETATM	92	H	0	3.809	2.285	6.183	H
HETATM	93	H	0	3.446	5.085	6.721	H
HETATM	94	H	0	5.805	3.278	7.408	H
HETATM	95	H	0	4.292	3.368	8.327	H
HETATM	96	H	0	5.922	4.702	9.193	H
HETATM	97	N	0	6.117	4.358	4.845	N
HETATM	98	C	0	7.087	4.839	3.859	C
HETATM	99	C	0	6.468	5.438	2.585	C
HETATM	100	O	0	7.049	6.359	2.011	O
HETATM	101	C	0	8.075	3.720	3.504	C
HETATM	102	H	0	6.175	3.376	5.085	H
HETATM	103	H	0	7.658	5.641	4.329	H
HETATM	104	H	0	8.840	4.108	2.831	H
HETATM	105	H	0	7.551	2.902	3.010	H

HETATM 106 H	0	8.559	3.350	4.409	H
HETATM 107 N	0	5.292	4.961	2.149	N
HETATM 108 C	0	4.476	5.587	1.104	C
HETATM 109 C	0	4.231	7.056	1.482	C
HETATM 110 O	0	4.313	7.918	0.623	O
HETATM 111 C	0	3.116	4.913	0.876	C
HETATM 112 C	0	3.108	3.449	0.428	C
HETATM 113 C	0	2.041	3.222	-0.644	C
HETATM 114 N	0	2.502	3.644	-1.971	N
HETATM 115 C	0	2.962	2.885	-2.939	C
HETATM 116 N	0	3.068	1.600	-2.826	N
HETATM 117 N	0	3.323	3.427	-4.057	N
HETATM 118 H	0	4.930	4.144	2.631	H
HETATM 119 H	0	5.034	5.588	0.169	H
HETATM 120 H	0	2.503	5.001	1.771	H
HETATM 121 H	0	2.631	5.496	0.098	H
HETATM 122 H	0	2.847	2.826	1.278	H
HETATM 123 H	0	4.086	3.158	0.053	H
HETATM 124 H	0	1.165	3.813	-0.385	H
HETATM 125 H	0	1.746	2.173	-0.647	H
HETATM 126 H	0	2.530	4.642	-2.139	H
HETATM 127 H	0	3.355	0.999	-3.575	H
HETATM 128 H	0	2.789	1.127	-1.963	H
HETATM 129 H	0	3.072	4.383	-4.249	H
HETATM 130 H	0	3.757	2.858	-4.772	H
HETATM 131 N	0	3.904	7.368	2.742	N
HETATM 132 C	0	3.642	8.748	3.238	C
HETATM 133 C	0	4.889	9.475	3.756	C
HETATM 134 O	0	4.951	10.694	3.615	O
HETATM 135 C	0	2.508	8.765	4.264	C
HETATM 136 C	0	1.183	8.298	3.655	C
HETATM 137 C	0	-0.050	8.813	4.378	C
HETATM 138 N	0	-0.044	8.475	5.798	N
HETATM 139 C	0	-0.351	7.283	6.304	C
HETATM 140 N	0	-0.866	6.311	5.577	N
HETATM 141 N	0	-0.073	7.061	7.622	N
HETATM 142 H	0	3.896	6.599	3.403	H
HETATM 143 H	0	3.318	9.348	2.378	H
HETATM 144 H	0	2.763	8.157	5.141	H
HETATM 145 H	0	2.394	9.796	4.631	H
HETATM 146 H	0	1.141	7.203	3.625	H
HETATM 147 H	0	1.106	8.648	2.619	H
HETATM 148 H	0	-0.956	8.413	3.919	H
HETATM 149 H	0	-0.099	9.902	4.332	H
HETATM 150 H	0	0.429	9.107	6.436	H
HETATM 151 H	0	-1.107	5.484	6.119	H
HETATM 152 H	0	-1.147	6.361	4.546	H
HETATM 153 H	0	0.021	7.910	8.183	H
HETATM 154 H	0	-0.613	6.323	8.058	H

HETATM 155	N	0	5.860	8.759	4.334	N
HETATM 156	C	0	7.155	9.257	4.800	C
HETATM 157	H	0	7.302	10.230	4.378	H
HETATM 158	H	0	7.939	8.605	4.474	H
HETATM 159	H	0	7.168	9.325	5.867	H
HETATM 160	H	0	5.649	7.776	4.454	H
HETATM 161	C	0	5.297	10.970	-0.652	C
HETATM 162	H	0	5.236	12.024	-0.828	H
HETATM 163	H	0	6.283	10.721	-0.318	H
HETATM 164	H	0	4.586	10.692	0.097	H
HETATM 165	C	0	5.045	10.205	-1.952	C
HETATM 166	O	0	5.249	10.747	-3.031	O
HETATM 167	N	0	4.623	8.939	-1.863	N
HETATM 168	C	0	4.534	7.932	-2.944	C
HETATM 169	C	0	3.125	7.362	-3.089	C
HETATM 170	O	0	2.768	6.372	-2.457	O
HETATM 171	C	0	5.626	6.851	-2.820	C
HETATM 172	C	0	5.708	6.087	-4.142	C
HETATM 173	C	0	7.016	7.449	-2.558	C
HETATM 174	H	0	4.506	8.605	-0.916	H
HETATM 175	H	0	4.746	8.458	-3.875	H
HETATM 176	H	0	5.384	6.157	-2.016	H
HETATM 177	H	0	5.976	6.756	-4.959	H
HETATM 178	H	0	4.753	5.623	-4.352	H
HETATM 179	H	0	6.452	5.300	-4.071	H
HETATM 180	H	0	7.228	8.239	-3.279	H
HETATM 181	H	0	7.775	6.674	-2.640	H
HETATM 182	H	0	7.056	7.859	-1.549	H
HETATM 183	N	0	2.320	7.975	-3.961	N
HETATM 184	C	0	0.933	7.587	-4.270	C
HETATM 185	C	0	0.802	6.091	-4.652	C
HETATM 186	O	0	1.738	5.523	-5.220	O
HETATM 187	C	0	0.406	8.461	-5.409	C
HETATM 188	O	0	0.618	9.824	-5.107	O
HETATM 189	H	0	2.665	8.815	-4.407	H
HETATM 190	H	0	0.337	7.780	-3.380	H
HETATM 191	H	0	-0.660	8.282	-5.554	H
HETATM 192	H	0	0.936	8.215	-6.331	H
HETATM 193	H	0	0.182	10.035	-4.269	H
HETATM 194	N	0	-0.327	5.417	-4.356	N
HETATM 195	C	0	-0.397	3.948	-4.302	C
HETATM 196	C	0	0.015	3.137	-5.551	C
HETATM 197	O	0	0.876	2.273	-5.399	O
HETATM 198	C	0	-1.773	3.599	-3.745	C
HETATM 199	C	0	-2.563	4.904	-3.668	C
HETATM 200	C	0	-1.506	6.002	-3.731	C
HETATM 201	H	0	0.310	3.649	-3.530	H
HETATM 202	H	0	-2.278	2.875	-4.377	H
HETATM 203	H	0	-1.644	3.200	-2.739	H

HETATM 204 H	0	-3.139	4.962	-2.746	H
HETATM 205 H	0	-3.234	4.989	-4.522	H
HETATM 206 H	0	-1.257	6.324	-2.721	H
HETATM 207 H	0	-1.884	6.847	-4.307	H
HETATM 208 N	0	-0.525	3.360	-6.771	N
HETATM 209 C	0	-0.145	2.595	-7.977	C
HETATM 210 C	0	1.336	2.615	-8.329	C
HETATM 211 O	0	1.771	1.859	-9.199	O
HETATM 212 C	0	-0.946	3.217	-9.128	C
HETATM 213 C	0	-2.145	3.858	-8.441	C
HETATM 214 C	0	-1.572	4.315	-7.102	C
HETATM 215 H	0	-0.450	1.558	-7.857	H
HETATM 216 H	0	-0.360	3.997	-9.618	H
HETATM 217 H	0	-1.254	2.464	-9.855	H
HETATM 218 H	0	-2.916	3.104	-8.279	H
HETATM 219 H	0	-2.544	4.694	-9.017	H
HETATM 220 H	0	-2.363	4.320	-6.359	H
HETATM 221 H	0	-1.137	5.310	-7.203	H
HETATM 222 N	0	2.107	3.505	-7.701	N
HETATM 223 C	0	3.536	3.590	-7.888	C
HETATM 224 C	0	4.233	2.324	-7.354	C
HETATM 225 O	0	4.697	2.262	-6.218	O
HETATM 226 C	0	4.077	4.932	-7.373	C
HETATM 227 C	0	3.373	6.191	-7.922	C
HETATM 228 C	0	3.970	7.438	-7.272	C
HETATM 229 C	0	3.531	6.329	-9.438	C
HETATM 230 H	0	1.696	4.049	-6.955	H
HETATM 231 H	0	3.717	3.591	-8.964	H
HETATM 232 H	0	4.020	4.935	-6.290	H
HETATM 233 H	0	5.119	5.002	-7.664	H
HETATM 234 H	0	2.309	6.162	-7.689	H
HETATM 235 H	0	5.031	7.514	-7.508	H
HETATM 236 H	0	3.847	7.375	-6.193	H
HETATM 237 H	0	3.454	8.329	-7.631	H
HETATM 238 H	0	4.587	6.329	-9.708	H
HETATM 239 H	0	3.077	7.263	-9.771	H
HETATM 240 H	0	3.025	5.507	-9.944	H
HETATM 241 N	0	4.360	1.320	-8.228	N
HETATM 242 C	0	5.354	0.227	-8.196	C
HETATM 243 C	0	6.784	0.802	-8.435	C
HETATM 244 O	0	7.584	0.246	-9.186	O
HETATM 245 C	0	4.976	-0.845	-9.244	C
HETATM 246 O	0	5.915	-1.895	-9.245	O
HETATM 247 C	0	4.845	-0.337	-10.683	C
HETATM 248 H	0	3.780	1.422	-9.053	H
HETATM 249 H	0	5.345	-0.239	-7.211	H
HETATM 250 H	0	4.012	-1.264	-8.968	H
HETATM 251 H	0	5.779	0.108	-11.027	H
HETATM 252 H	0	4.045	0.399	-10.753	H

HETATM 253	H	0	4.597	-1.175	-11.336	H
HETATM 254	H	0	6.759	-1.479	-9.490	H
HETATM 255	N	0	7.101	1.954	-7.832	N
HETATM 256	C	0	8.216	2.865	-8.132	C
HETATM 257	H	0	8.184	3.149	-9.184	H
HETATM 258	C	0	8.122	4.129	-7.269	C
HETATM 259	O	0	7.124	4.327	-6.586	O
HETATM 260	H	0	6.436	2.306	-7.150	H
HETATM 261	H	0	9.160	2.360	-7.925	H
HETATM 262	N	0	9.133	4.997	-7.291	N
HETATM 263	C	0	9.118	6.268	-6.550	C
HETATM 264	C	0	10.227	6.380	-5.503	C
HETATM 265	O	0	10.834	5.383	-5.106	O
HETATM 266	H	0	9.961	4.754	-7.811	H
HETATM 267	H	0	9.234	7.084	-7.263	H
HETATM 268	H	0	8.166	6.407	-6.038	H
HETATM 269	N	0	10.509	7.616	-5.076	N
HETATM 270	C	0	11.704	7.936	-4.305	C
HETATM 271	H	0	11.983	8.960	-4.440	H
HETATM 272	H	0	12.481	7.303	-4.678	H
HETATM 273	H	0	11.553	7.742	-3.264	H
HETATM 274	H	0	9.936	8.375	-5.412	H
HETATM 275	C	0	14.020	4.537	-0.244	C
HETATM 276	H	0	13.964	5.152	-1.118	H
HETATM 277	H	0	14.682	3.717	-0.427	H
HETATM 278	H	0	14.389	5.117	0.576	H
HETATM 279	C	0	12.690	3.854	-0.025	C
HETATM 280	O	0	12.680	2.727	0.453	O
HETATM 281	N	0	11.597	4.439	-0.523	N
HETATM 282	C	0	10.357	3.692	-0.793	C
HETATM 283	C	0	10.616	2.485	-1.716	C
HETATM 284	O	0	10.252	1.377	-1.355	O
HETATM 285	C	0	9.277	4.609	-1.394	C
HETATM 286	C	0	8.145	3.814	-2.024	C
HETATM 287	C	0	7.125	3.266	-1.223	C
HETATM 288	C	0	8.202	3.491	-3.395	C
HETATM 289	C	0	6.195	2.377	-1.791	C
HETATM 290	C	0	7.284	2.586	-3.950	C
HETATM 291	C	0	6.286	2.023	-3.147	C
HETATM 292	H	0	11.684	5.377	-0.878	H
HETATM 293	H	0	9.976	3.291	0.148	H
HETATM 294	H	0	8.878	5.258	-0.612	H
HETATM 295	H	0	9.728	5.241	-2.161	H
HETATM 296	H	0	7.075	3.495	-0.168	H
HETATM 297	H	0	8.976	3.901	-4.025	H
HETATM 298	H	0	5.420	1.935	-1.187	H
HETATM 299	H	0	7.345	2.311	-4.991	H
HETATM 300	H	0	5.599	1.310	-3.577	H
HETATM 301	N	0	11.191	2.664	-2.917	N

HETATM 302 C	0	11.302	1.582	-3.901	C
HETATM 303 H	0	11.646	0.700	-3.403	H
HETATM 304 H	0	11.986	1.840	-4.682	H
HETATM 305 H	0	10.334	1.402	-4.319	H
HETATM 306 H	0	11.419	3.607	-3.198	H
HETATM 307 C	0	13.961	-0.411	-2.040	C
HETATM 308 H	0	13.653	-0.740	-3.011	H
HETATM 309 H	0	14.995	-0.643	-1.895	H
HETATM 310 H	0	13.818	0.646	-1.960	H
HETATM 311 C	0	13.049	-1.144	-1.053	C
HETATM 312 O	0	12.930	-2.357	-1.156	O
HETATM 313 N	0	12.342	-0.427	-0.168	N
HETATM 314 C	0	11.337	-0.944	0.806	C
HETATM 315 C	0	10.193	-1.737	0.179	C
HETATM 316 O	0	9.868	-2.814	0.666	O
HETATM 317 C	0	10.879	0.216	1.726	C
HETATM 318 C	0	9.505	0.070	2.383	C
HETATM 319 C	0	11.917	0.422	2.836	C
HETATM 320 H	0	12.495	0.575	-0.157	H
HETATM 321 H	0	11.852	-1.666	1.440	H
HETATM 322 H	0	10.830	1.131	1.142	H
HETATM 323 H	0	9.400	-0.912	2.839	H
HETATM 324 H	0	8.743	0.225	1.623	H
HETATM 325 H	0	9.370	0.836	3.146	H
HETATM 326 H	0	11.953	-0.453	3.487	H
HETATM 327 H	0	11.662	1.302	3.426	H
HETATM 328 H	0	12.902	0.582	2.397	H
HETATM 329 N	0	9.607	-1.242	-0.906	N
HETATM 330 C	0	8.714	-1.964	-1.810	C
HETATM 331 C	0	9.356	-3.276	-2.260	C
HETATM 332 O	0	8.838	-4.346	-1.968	O
HETATM 333 C	0	8.385	-1.037	-2.991	C
HETATM 334 C	0	7.521	-1.658	-4.071	C
HETATM 335 C	0	6.125	-1.682	-3.916	C
HETATM 336 C	0	8.106	-2.200	-5.234	C
HETATM 337 C	0	5.309	-2.251	-4.912	C
HETATM 338 C	0	7.295	-2.771	-6.233	C
HETATM 339 C	0	5.894	-2.809	-6.068	C
HETATM 340 O	0	5.112	-3.337	-7.046	O
HETATM 341 H	0	9.907	-0.314	-1.174	H
HETATM 342 H	0	7.790	-2.208	-1.284	H
HETATM 343 H	0	7.876	-0.157	-2.600	H
HETATM 344 H	0	9.315	-0.692	-3.445	H
HETATM 345 H	0	5.678	-1.252	-3.029	H
HETATM 346 H	0	9.179	-2.186	-5.359	H
HETATM 347 H	0	4.238	-2.244	-4.791	H
HETATM 348 H	0	7.742	-3.194	-7.120	H
HETATM 349 H	0	5.514	-3.124	-7.906	H
HETATM 350 N	0	10.500	-3.209	-2.944	N

HETATM 351 C	0	11.226	-4.384	-3.396	C
HETATM 352 H	0	11.909	-4.684	-2.628	H
HETATM 353 H	0	11.769	-4.168	-4.292	H
HETATM 354 H	0	10.531	-5.175	-3.583	H
HETATM 355 H	0	10.934	-2.304	-3.018	H
HETATM 356 C	0	12.281	-5.716	0.066	C
HETATM 357 H	0	12.132	-5.273	-0.896	H
HETATM 358 H	0	13.065	-6.442	0.007	H
HETATM 359 H	0	12.552	-4.956	0.770	H
HETATM 360 C	0	10.995	-6.408	0.480	C
HETATM 361 O	0	10.972	-7.628	0.558	O
HETATM 362 N	0	9.924	-5.653	0.730	N
HETATM 363 C	0	8.615	-6.146	1.200	C
HETATM 364 C	0	7.944	-7.141	0.253	C
HETATM 365 O	0	7.424	-8.162	0.699	O
HETATM 366 C	0	7.717	-4.959	1.532	C
HETATM 367 C	0	6.336	-5.377	2.047	C
HETATM 368 C	0	5.333	-5.555	0.923	C
HETATM 369 O	0	4.992	-4.605	0.240	O
HETATM 370 N	0	4.806	-6.732	0.706	N
HETATM 371 H	0	10.021	-4.651	0.596	H
HETATM 372 H	0	8.794	-6.692	2.127	H
HETATM 373 H	0	8.201	-4.381	2.316	H
HETATM 374 H	0	7.614	-4.327	0.650	H
HETATM 375 H	0	5.956	-4.572	2.665	H
HETATM 376 H	0	6.406	-6.278	2.658	H
HETATM 377 H	0	4.107	-6.730	-0.040	H
HETATM 378 H	0	5.211	-7.583	1.065	H
HETATM 379 N	0	7.885	-6.796	-1.029	N
HETATM 380 C	0	7.313	-7.608	-2.106	C
HETATM 381 C	0	8.246	-8.779	-2.486	C
HETATM 382 O	0	7.779	-9.783	-3.019	O
HETATM 383 C	0	6.997	-6.718	-3.334	C
HETATM 384 C	0	6.312	-7.478	-4.479	C
HETATM 385 C	0	6.044	-5.568	-2.968	C
HETATM 386 H	0	8.286	-5.897	-1.276	H
HETATM 387 H	0	6.378	-8.047	-1.757	H
HETATM 388 H	0	7.926	-6.291	-3.715	H
HETATM 389 H	0	5.406	-7.963	-4.113	H
HETATM 390 H	0	6.983	-8.234	-4.885	H
HETATM 391 H	0	6.053	-6.792	-5.284	H
HETATM 392 H	0	5.815	-4.972	-3.851	H
HETATM 393 H	0	6.479	-4.913	-2.219	H
HETATM 394 H	0	5.130	-5.981	-2.556	H
HETATM 395 N	0	9.558	-8.675	-2.208	N
HETATM 396 C	0	10.542	-9.754	-2.347	C
HETATM 397 H	0	11.290	-9.649	-1.590	H
HETATM 398 H	0	11.007	-9.744	-3.311	H
HETATM 399 H	0	10.024	-10.680	-2.211	H

HETATM 400 H	0	9.828	-7.858	-1.681	H
HETATM 401 C	0	17.422	-7.343	4.289	C
HETATM 402 H	0	18.148	-7.137	5.048	H
HETATM 403 H	0	17.918	-7.505	3.355	H
HETATM 404 H	0	16.866	-8.218	4.555	H
HETATM 405 C	0	16.541	-6.124	4.183	C
HETATM 406 O	0	16.931	-5.145	3.567	O
HETATM 407 N	0	15.380	-6.164	4.833	N
HETATM 408 C	0	14.446	-5.032	4.909	C
HETATM 409 C	0	14.995	-3.820	5.698	C
HETATM 410 O	0	14.647	-2.682	5.396	O
HETATM 411 C	0	13.119	-5.533	5.503	C
HETATM 412 C	0	11.976	-4.535	5.434	C
HETATM 413 C	0	11.340	-4.284	4.203	C
HETATM 414 C	0	11.544	-3.857	6.591	C
HETATM 415 C	0	10.285	-3.359	4.131	C
HETATM 416 C	0	10.482	-2.936	6.517	C
HETATM 417 C	0	9.853	-2.685	5.285	C
HETATM 418 H	0	15.127	-7.030	5.278	H
HETATM 419 H	0	14.255	-4.679	3.894	H
HETATM 420 H	0	12.809	-6.427	4.958	H
HETATM 421 H	0	13.281	-5.824	6.542	H
HETATM 422 H	0	11.667	-4.791	3.307	H
HETATM 423 H	0	12.036	-4.030	7.536	H
HETATM 424 H	0	9.819	-3.155	3.180	H
HETATM 425 H	0	10.162	-2.408	7.404	H
HETATM 426 H	0	9.044	-1.970	5.219	H
HETATM 427 N	0	15.839	-4.063	6.714	N
HETATM 428 C	0	16.612	-3.051	7.442	C
HETATM 429 H	0	16.533	-2.113	6.934	H
HETATM 430 H	0	17.634	-3.370	7.448	H
HETATM 431 H	0	16.267	-2.941	8.449	H
HETATM 432 H	0	16.063	-5.032	6.863	H
HETATM 433 C	0	-1.936	-4.539	-11.811	C
HETATM 434 H	0	-2.225	-5.529	-12.095	H
HETATM 435 H	0	-1.226	-4.159	-12.516	H
HETATM 436 H	0	-2.798	-3.906	-11.797	H
HETATM 437 C	0	-1.357	-4.583	-10.421	C
HETATM 438 O	0	-1.141	-5.657	-9.878	O
HETATM 439 N	0	-1.151	-3.405	-9.824	N
HETATM 440 C	0	-0.684	-3.267	-8.435	C
HETATM 441 C	0	-1.609	-3.924	-7.406	C
HETATM 442 O	0	-1.111	-4.618	-6.531	O
HETATM 443 C	0	-0.387	-1.798	-8.090	C
HETATM 444 C	0	1.104	-1.399	-8.041	C
HETATM 445 C	0	2.086	-2.362	-7.342	C
HETATM 446 N	0	1.633	-2.817	-6.021	N
HETATM 447 C	0	2.012	-3.891	-5.353	C
HETATM 448 N	0	2.917	-4.740	-5.736	N

HETATM 449 N	0	1.513	-4.146	-4.198	N
HETATM 450 H	0	-1.339	-2.579	-10.371	H
HETATM 451 H	0	0.233	-3.848	-8.350	H
HETATM 452 H	0	-0.902	-1.136	-8.788	H
HETATM 453 H	0	-0.823	-1.596	-7.122	H
HETATM 454 H	0	1.169	-0.432	-7.541	H
HETATM 455 H	0	1.452	-1.259	-9.065	H
HETATM 456 H	0	3.029	-1.835	-7.204	H
HETATM 457 H	0	2.266	-3.223	-7.987	H
HETATM 458 H	0	0.908	-2.268	-5.557	H
HETATM 459 H	0	3.108	-5.507	-5.089	H
HETATM 460 H	0	3.556	-4.488	-6.473	H
HETATM 461 H	0	0.891	-3.461	-3.766	H
HETATM 462 H	0	1.794	-5.017	-3.753	H
HETATM 463 N	0	-2.929	-3.728	-7.497	N
HETATM 464 C	0	-3.905	-4.379	-6.620	C
HETATM 465 H	0	-3.616	-4.222	-5.602	H
HETATM 466 H	0	-3.908	-5.428	-6.832	H
HETATM 467 H	0	-4.885	-3.980	-6.779	H
HETATM 468 H	0	-3.242	-3.119	-8.234	H
HETATM 469 C	0	0.341	-7.938	-7.135	C
HETATM 470 H	0	0.229	-8.959	-7.434	H
HETATM 471 H	0	1.293	-7.574	-7.461	H
HETATM 472 H	0	-0.436	-7.350	-7.577	H
HETATM 473 C	0	0.124	-7.927	-5.632	C
HETATM 474 O	0	0.289	-8.979	-5.038	O
HETATM 475 N	0	-0.358	-6.825	-5.036	N
HETATM 476 C	0	-0.694	-6.662	-3.602	C
HETATM 477 C	0	-1.473	-7.849	-3.017	C
HETATM 478 O	0	-1.093	-8.437	-2.007	O
HETATM 479 C	0	-1.454	-5.342	-3.352	C
HETATM 480 C	0	-1.516	-5.008	-1.863	C
HETATM 481 O	0	-2.160	-5.687	-1.082	O
HETATM 482 N	0	-0.878	-3.965	-1.411	N
HETATM 483 H	0	-0.484	-6.015	-5.632	H
HETATM 484 H	0	0.229	-6.569	-3.046	H
HETATM 485 H	0	-2.471	-5.428	-3.727	H
HETATM 486 H	0	-0.988	-4.515	-3.879	H
HETATM 487 H	0	-1.030	-3.674	-0.443	H
HETATM 488 H	0	-0.594	-3.228	-2.054	H
HETATM 489 N	0	-2.601	-8.184	-3.642	N
HETATM 490 C	0	-3.422	-9.295	-3.209	C
HETATM 491 H	0	-3.114	-9.595	-2.230	H
HETATM 492 H	0	-3.285	-10.108	-3.891	H
HETATM 493 H	0	-4.455	-9.017	-3.188	H
HETATM 494 H	0	-2.806	-7.685	-4.493	H
HETATM 495 C	0	-0.883	-11.945	-4.479	C
HETATM 496 H	0	-1.288	-12.930	-4.587	H
HETATM 497 H	0	-0.635	-11.554	-5.443	H

HETATM 498 H	0	-1.608 -11.311 -4.013	H
HETATM 499 C	0	0.225 -11.992 -3.405	C
HETATM 500 O	0	0.378 -13.037 -2.789	O
HETATM 501 N	0	0.892 -10.879 -3.051	N
HETATM 502 C	0	1.892 -10.737 -1.937	C
HETATM 503 C	0	1.337 -10.933 -0.514	C
HETATM 504 O	0	2.002 -11.547 0.315	O
HETATM 505 C	0	2.789 -9.495 -2.090	C
HETATM 506 C	0	1.921 -8.255 -2.109	C
HETATM 507 C	0	2.645 -6.936 -2.277	C
HETATM 508 O	0	2.906 -6.303 -1.238	O
HETATM 509 O	0	2.767 -6.407 -3.409	O
HETATM 510 H	0	0.703 -10.061 -3.622	H
HETATM 511 H	0	2.574 -11.581 -2.054	H
HETATM 512 H	0	3.496 -9.441 -1.261	H
HETATM 513 H	0	3.344 -9.560 -3.027	H
HETATM 514 H	0	1.355 -8.218 -1.183	H
HETATM 515 H	0	1.243 -8.361 -2.936	H
HETATM 516 N	0	0.123 -10.461 -0.212	N
HETATM 517 C	0	-0.572 -10.784 1.050	C
HETATM 518 C	0	-1.286 -12.152 1.038	C
HETATM 519 O	0	-1.785 -12.584 2.077	O
HETATM 520 C	0	-1.623 -9.700 1.362	C
HETATM 521 C	0	-1.161 -8.368 1.942	C
HETATM 522 C	0	-0.544 -7.411 1.115	C
HETATM 523 C	0	-1.563 -7.992 3.243	C
HETATM 524 C	0	-0.389 -6.080 1.542	C
HETATM 525 C	0	-1.410 -6.657 3.676	C
HETATM 526 C	0	-0.853 -5.689 2.813	C
HETATM 527 O	0	-0.806 -4.383 3.185	O
HETATM 528 H	0	-0.339 -9.895 -0.916	H
HETATM 529 H	0	0.149 -10.808 1.869	H
HETATM 530 H	0	-2.185 -9.499 0.449	H
HETATM 531 H	0	-2.342 -10.115 2.069	H
HETATM 532 H	0	-0.249 -7.672 0.114	H
HETATM 533 H	0	-2.038 -8.715 3.895	H
HETATM 534 H	0	0.040 -5.347 0.875	H
HETATM 535 H	0	-1.760 -6.347 4.650	H
HETATM 536 H	0	-0.750 -3.798 2.391	H
HETATM 537 N	0	-1.403 -12.809 -0.121	N
HETATM 538 C	0	-1.977 -14.144 -0.260	C
HETATM 539 H	0	-1.635 -14.735 0.564	H
HETATM 540 H	0	-1.599 -14.552 -1.174	H
HETATM 541 H	0	-3.047 -14.148 -0.283	H
HETATM 542 H	0	-0.871 -12.441 -0.900	H
HETATM 543 C	0	-12.637 -7.734 1.601	C
HETATM 544 H	0	-12.427 -7.044 2.392	H
HETATM 545 H	0	-12.471 -8.733 1.946	H
HETATM 546 H	0	-13.656 -7.626 1.296	H

HETATM 547 C	0	-11.739	-7.433	0.415	C
HETATM 548 O	0	-11.861	-6.370	-0.177	O
HETATM 549 N	0	-10.849	-8.362	0.030	N
HETATM 550 C	0	-9.883	-8.175	-1.081	C
HETATM 551 C	0	-10.506	-7.929	-2.456	C
HETATM 552 O	0	-9.888	-7.216	-3.240	O
HETATM 553 C	0	-8.846	-9.315	-1.132	C
HETATM 554 C	0	-7.739	-9.193	-0.068	C
HETATM 555 C	0	-7.010	-7.843	-0.174	C
HETATM 556 N	0	-5.750	-7.793	0.581	N
HETATM 557 C	0	-4.749	-6.978	0.307	C
HETATM 558 N	0	-4.801	-6.107	-0.651	N
HETATM 559 N	0	-3.639	-7.006	0.968	N
HETATM 560 H	0	-10.819	-9.208	0.580	H
HETATM 561 H	0	-9.364	-7.252	-0.875	H
HETATM 562 H	0	-9.350	-10.277	-1.024	H
HETATM 563 H	0	-8.361	-9.307	-2.110	H
HETATM 564 H	0	-7.021	-9.999	-0.227	H
HETATM 565 H	0	-8.174	-9.309	0.923	H
HETATM 566 H	0	-7.653	-7.045	0.202	H
HETATM 567 H	0	-6.804	-7.656	-1.230	H
HETATM 568 H	0	-5.653	-8.341	1.419	H
HETATM 569 H	0	-3.940	-5.601	-0.838	H
HETATM 570 H	0	-5.645	-5.878	-1.137	H
HETATM 571 H	0	-3.461	-7.613	1.746	H
HETATM 572 H	0	-2.862	-6.470	0.588	H
HETATM 573 N	0	-11.690	-8.478	-2.749	N
HETATM 574 C	0	-12.448	-8.176	-3.966	C
HETATM 575 H	0	-12.872	-9.056	-4.402	H
HETATM 576 H	0	-11.784	-7.715	-4.668	H
HETATM 577 H	0	-13.230	-7.491	-3.712	H
HETATM 578 H	0	-12.112	-9.044	-2.032	H
HETATM 579 C	0	-13.805	-4.815	-2.701	C
HETATM 580 H	0	-13.719	-5.545	-1.923	H
HETATM 581 H	0	-13.856	-5.308	-3.649	H
HETATM 582 H	0	-14.694	-4.238	-2.551	H
HETATM 583 C	0	-12.595	-3.895	-2.730	C
HETATM 584 O	0	-12.638	-2.891	-3.427	O
HETATM 585 N	0	-11.495	-4.255	-2.054	N
HETATM 586 C	0	-10.179	-3.602	-2.216	C
HETATM 587 C	0	-9.773	-3.526	-3.691	C
HETATM 588 O	0	-9.402	-2.458	-4.156	O
HETATM 589 C	0	-9.087	-4.304	-1.400	C
HETATM 590 C	0	-7.660	-3.995	-1.835	C
HETATM 591 C	0	-7.038	-2.806	-1.419	C
HETATM 592 C	0	-6.966	-4.878	-2.688	C
HETATM 593 C	0	-5.699	-2.532	-1.767	C
HETATM 594 C	0	-5.646	-4.583	-3.084	C
HETATM 595 C	0	-4.995	-3.428	-2.594	C

HETATM 596 O	0	-3.708	-3.190	-2.946	O
HETATM 597 H	0	-11.575	-5.054	-1.436	H
HETATM 598 H	0	-10.261	-2.577	-1.855	H
HETATM 599 H	0	-9.211	-4.055	-0.346	H
HETATM 600 H	0	-9.233	-5.368	-1.505	H
HETATM 601 H	0	-7.604	-2.106	-0.828	H
HETATM 602 H	0	-7.459	-5.765	-3.066	H
HETATM 603 H	0	-5.189	-1.650	-1.406	H
HETATM 604 H	0	-5.101	-5.240	-3.744	H
HETATM 605 H	0	-3.246	-2.492	-2.413	H
HETATM 606 N	0	-9.802	-4.640	-4.429	N
HETATM 607 C	0	-9.444	-4.674	-5.839	C
HETATM 608 H	0	-9.551	-5.662	-6.234	H
HETATM 609 H	0	-8.431	-4.352	-5.953	H
HETATM 610 H	0	-10.093	-4.006	-6.367	H
HETATM 611 H	0	-10.065	-5.502	-3.965	H
HETATM 612 C	0	-11.968	0.066	-4.964	C
HETATM 613 H	0	-11.818	-0.350	-3.989	H
HETATM 614 H	0	-12.274	-0.707	-5.638	H
HETATM 615 H	0	-12.726	0.819	-4.917	H
HETATM 616 C	0	-10.705	0.690	-5.502	C
HETATM 617 O	0	-10.766	1.753	-6.103	O
HETATM 618 N	0	-9.575	0.009	-5.317	N
HETATM 619 C	0	-8.225	0.414	-5.736	C
HETATM 620 C	0	-8.182	0.607	-7.271	C
HETATM 621 O	0	-7.531	1.525	-7.770	O
HETATM 622 C	0	-7.202	-0.604	-5.234	C
HETATM 623 C	0	-5.747	-0.237	-5.415	C
HETATM 624 C	0	-4.794	-1.255	-5.262	C
HETATM 625 C	0	-5.327	1.075	-5.722	C
HETATM 626 C	0	-3.429	-0.983	-5.435	C
HETATM 627 C	0	-3.969	1.341	-5.942	C
HETATM 628 C	0	-3.021	0.313	-5.800	C
HETATM 629 O	0	-1.717	0.592	-5.997	O
HETATM 630 H	0	-9.663	-0.868	-4.820	H
HETATM 631 H	0	-8.028	1.382	-5.277	H
HETATM 632 H	0	-7.364	-0.771	-4.171	H
HETATM 633 H	0	-7.382	-1.552	-5.745	H
HETATM 634 H	0	-5.115	-2.253	-5.006	H
HETATM 635 H	0	-6.024	1.893	-5.838	H
HETATM 636 H	0	-2.701	-1.768	-5.290	H
HETATM 637 H	0	-3.643	2.329	-6.217	H
HETATM 638 H	0	-1.161	-0.138	-5.636	H
HETATM 639 N	0	-8.907	-0.242	-8.016	N
HETATM 640 C	0	-9.196	-0.079	-9.439	C
HETATM 641 H	0	-9.479	-1.017	-9.869	H
HETATM 642 H	0	-8.325	0.293	-9.936	H
HETATM 643 H	0	-9.998	0.621	-9.552	H
HETATM 644 H	0	-9.424	-0.928	-7.489	H

HETATM 645 C	0	-9.755	5.419	-6.342	C
HETATM 646 H	0	-10.486	6.085	-5.935	H
HETATM 647 H	0	-10.247	4.602	-6.828	H
HETATM 648 H	0	-9.150	5.944	-7.052	H
HETATM 649 C	0	-8.968	4.899	-5.153	C
HETATM 650 O	0	-9.328	3.888	-4.560	O
HETATM 651 N	0	-7.965	5.657	-4.703	N
HETATM 652 C	0	-7.222	5.386	-3.460	C
HETATM 653 C	0	-8.136	5.227	-2.223	C
HETATM 654 O	0	-7.788	4.512	-1.292	O
HETATM 655 C	0	-6.160	6.469	-3.288	C
HETATM 656 H	0	-7.766	6.504	-5.210	H
HETATM 657 H	0	-6.706	4.432	-3.582	H
HETATM 658 H	0	-5.547	6.220	-2.425	H
HETATM 659 H	0	-6.635	7.438	-3.136	H
HETATM 660 H	0	-5.522	6.511	-4.171	H
HETATM 661 N	0	-9.300	5.886	-2.214	N
HETATM 662 C	0	-10.281	5.926	-1.125	C
HETATM 663 C	0	-11.268	4.757	-1.111	C
HETATM 664 O	0	-11.513	4.190	-0.050	O
HETATM 665 C	0	-11.045	7.263	-1.180	C
HETATM 666 C	0	-10.185	8.499	-0.841	C
HETATM 667 C	0	-9.120	8.849	-1.882	C
HETATM 668 O	0	-9.250	8.594	-3.071	O
HETATM 669 N	0	-8.008	9.423	-1.487	N
HETATM 670 H	0	-9.435	6.523	-2.990	H
HETATM 671 H	0	-9.744	5.916	-0.184	H
HETATM 672 H	0	-11.500	7.391	-2.164	H
HETATM 673 H	0	-11.852	7.220	-0.447	H
HETATM 674 H	0	-9.704	8.340	0.125	H
HETATM 675 H	0	-10.847	9.360	-0.747	H
HETATM 676 H	0	-7.379	9.664	-2.228	H
HETATM 677 H	0	-7.805	9.630	-0.512	H
HETATM 678 N	0	-11.851	4.404	-2.264	N
HETATM 679 C	0	-12.857	3.335	-2.378	C
HETATM 680 H	0	-13.080	3.155	-3.430	H
HETATM 681 C	0	-12.398	2.019	-1.754	C
HETATM 682 O	0	-13.170	1.322	-1.104	O
HETATM 683 H	0	-11.552	4.877	-3.104	H
HETATM 684 H	0	-13.773	3.647	-1.877	H
HETATM 685 N	0	-11.115	1.698	-1.941	N
HETATM 686 C	0	-10.458	0.501	-1.404	C
HETATM 687 C	0	-10.359	0.487	0.123	C
HETATM 688 O	0	-10.354	-0.607	0.673	O
HETATM 689 C	0	-9.067	0.345	-2.037	C
HETATM 690 C	0	-7.951	1.021	-1.254	C
HETATM 691 C	0	-6.655	1.103	-2.024	C
HETATM 692 N	0	-5.700	1.798	-1.194	N
HETATM 693 C	0	-4.481	2.122	-1.592	C

HETATM 694 N	0	-4.008	1.683	-2.776	N
HETATM 695 N	0	-3.757	2.929	-0.816	N
HETATM 696 H	0	-10.584	2.333	-2.524	H
HETATM 697 H	0	-11.098	-0.349	-1.671	H
HETATM 698 H	0	-8.830	-0.715	-2.164	H
HETATM 699 H	0	-9.068	0.786	-3.035	H
HETATM 700 H	0	-7.757	0.498	-0.308	H
HETATM 701 H	0	-8.245	2.044	-0.999	H
HETATM 702 H	0	-6.812	1.661	-2.958	H
HETATM 703 H	0	-6.303	0.096	-2.288	H
HETATM 704 H	0	-5.887	1.938	-0.186	H
HETATM 705 H	0	-3.006	1.542	-2.847	H
HETATM 706 H	0	-4.566	1.021	-3.302	H
HETATM 707 H	0	-4.133	2.972	0.147	H
HETATM 708 H	0	-2.733	2.924	-0.849	H
HETATM 709 N	0	-10.113	1.639	0.773	N
HETATM 710 C	0	-9.456	1.758	2.094	C
HETATM 711 C	0	-10.140	0.840	3.106	C
HETATM 712 O	0	-9.533	-0.063	3.667	O
HETATM 713 C	0	-9.584	3.200	2.641	C
HETATM 714 C	0	-8.861	4.304	1.875	C
HETATM 715 C	0	-9.256	5.670	2.439	C
HETATM 716 C	0	-7.357	4.173	1.962	C
HETATM 717 H	0	-10.241	2.485	0.234	H
HETATM 718 H	0	-8.404	1.473	2.027	H
HETATM 719 H	0	-10.641	3.469	2.661	H
HETATM 720 H	0	-9.223	3.211	3.670	H
HETATM 721 H	0	-9.145	4.239	0.835	H
HETATM 722 H	0	-8.984	5.738	3.492	H
HETATM 723 H	0	-10.332	5.810	2.335	H
HETATM 724 H	0	-8.749	6.459	1.884	H
HETATM 725 H	0	-7.044	4.009	2.991	H
HETATM 726 H	0	-6.884	5.050	1.535	H
HETATM 727 H	0	-7.075	3.318	1.353	H
HETATM 728 N	0	-11.430	1.083	3.345	N
HETATM 729 C	0	-12.246	0.291	4.236	C
HETATM 730 H	0	-11.926	0.407	5.251	H
HETATM 731 H	0	-12.140	-0.732	3.943	H
HETATM 732 H	0	-13.272	0.582	4.151	H
HETATM 733 H	0	-11.854	1.815	2.793	H
HETATM 734 C	0	-11.938	-3.094	2.400	C
HETATM 735 H	0	-12.534	-3.961	2.203	H
HETATM 736 H	0	-12.034	-2.404	1.588	H
HETATM 737 H	0	-12.271	-2.629	3.304	H
HETATM 738 C	0	-10.490	-3.537	2.567	C
HETATM 739 O	0	-10.302	-4.662	3.015	O
HETATM 740 N	0	-9.467	-2.706	2.298	N
HETATM 741 C	0	-8.061	-3.017	2.652	C
HETATM 742 C	0	-7.933	-3.200	4.164	C

HETATM 743 O	0	-7.529	-4.274	4.597	O
HETATM 744 C	0	-7.014	-1.985	2.180	C
HETATM 745 C	0	-5.564	-2.471	2.455	C
HETATM 746 C	0	-5.180	-3.754	1.713	C
HETATM 747 C	0	-4.523	-1.446	2.038	C
HETATM 748 H	0	-9.694	-1.784	1.935	H
HETATM 749 H	0	-7.831	-3.965	2.174	H
HETATM 750 H	0	-7.130	-1.786	1.126	H
HETATM 751 H	0	-7.174	-1.041	2.702	H
HETATM 752 H	0	-5.434	-2.649	3.522	H
HETATM 753 H	0	-5.350	-3.633	0.648	H
HETATM 754 H	0	-5.755	-4.592	2.085	H
HETATM 755 H	0	-4.126	-3.982	1.879	H
HETATM 756 H	0	-4.612	-1.216	0.977	H
HETATM 757 H	0	-3.528	-1.828	2.262	H
HETATM 758 H	0	-4.664	-0.542	2.614	H
HETATM 759 N	0	-8.324	-2.197	4.955	N
HETATM 760 C	0	-8.399	-2.243	6.417	C
HETATM 761 C	0	-9.156	-3.475	6.922	C
HETATM 762 O	0	-8.751	-4.074	7.910	O
HETATM 763 C	0	-9.017	-0.958	6.997	C
HETATM 764 C	0	-8.082	0.238	7.050	C
HETATM 765 C	0	-8.347	1.388	6.284	C
HETATM 766 C	0	-6.935	0.197	7.869	C
HETATM 767 C	0	-7.455	2.477	6.302	C
HETATM 768 C	0	-6.039	1.284	7.891	C
HETATM 769 C	0	-6.296	2.425	7.102	C
HETATM 770 O	0	-5.419	3.464	7.091	O
HETATM 771 H	0	-8.600	-1.340	4.483	H
HETATM 772 H	0	-7.382	-2.333	6.800	H
HETATM 773 H	0	-9.916	-0.705	6.433	H
HETATM 774 H	0	-9.329	-1.160	8.023	H
HETATM 775 H	0	-9.227	1.431	5.662	H
HETATM 776 H	0	-6.731	-0.679	8.472	H
HETATM 777 H	0	-7.637	3.337	5.678	H
HETATM 778 H	0	-5.152	1.240	8.505	H
HETATM 779 H	0	-4.522	3.112	7.237	H
HETATM 780 N	0	-10.226	-3.882	6.234	N
HETATM 781 C	0	-10.932	-5.133	6.512	C
HETATM 782 H	0	-11.854	-5.165	5.932	H
HETATM 783 C	0	-10.112	-6.388	6.175	C
HETATM 784 O	0	-10.074	-7.322	6.965	O
HETATM 785 H	0	-10.464	-3.352	5.411	H
HETATM 786 H	0	-11.192	-5.173	7.571	H
HETATM 787 N	0	-9.461	-6.425	5.007	N
HETATM 788 C	0	-8.541	-7.497	4.588	C
HETATM 789 C	0	-7.264	-7.609	5.432	C
HETATM 790 O	0	-6.661	-8.677	5.480	O
HETATM 791 C	0	-8.219	-7.413	3.104	C

HETATM 792 O	0	-7.356	-6.344	2.808	O
HETATM 793 H	0	-9.590	-5.634	4.386	H
HETATM 794 H	0	-9.070	-8.439	4.737	H
HETATM 795 H	0	-9.145	-7.303	2.537	H
HETATM 796 H	0	-7.730	-8.341	2.813	H
HETATM 797 H	0	-7.478	-5.642	3.474	H
HETATM 798 N	0	-6.851	-6.515	6.074	N
HETATM 799 C	0	-5.833	-6.460	7.113	C
HETATM 800 C	0	-6.383	-6.919	8.479	C
HETATM 801 O	0	-5.696	-7.638	9.201	O
HETATM 802 C	0	-5.278	-5.030	7.174	C
HETATM 803 H	0	-7.352	-5.659	5.877	H
HETATM 804 H	0	-5.019	-7.137	6.847	H
HETATM 805 H	0	-4.478	-4.984	7.914	H
HETATM 806 H	0	-6.064	-4.332	7.458	H
HETATM 807 H	0	-4.878	-4.745	6.200	H
HETATM 808 N	0	-7.606	-6.496	8.837	N
HETATM 809 C	0	-8.336	-6.937	10.020	C
HETATM 810 H	0	-8.063	-6.331	10.858	H
HETATM 811 H	0	-8.045	-7.950	10.202	H
HETATM 812 H	0	-9.395	-6.890	9.876	H
HETATM 813 H	0	-8.071	-5.840	8.223	H
HETATM 814 N	0	3.202	-3.685	-1.605	N
HETATM 815 C	0	2.328	-2.677	-0.948	C
HETATM 816 C	0	2.646	-1.238	-1.480	C
HETATM 817 O	0	3.271	-1.179	-2.567	O
HETATM 818 O	0	2.340	-0.201	-0.845	O
HETATM 819 C	0	2.425	-2.905	0.572	C
HETATM 820 C	0	1.588	-1.980	1.463	C
HETATM 821 C	0	0.138	-1.844	1.040	C
HETATM 822 O	0	-0.602	-2.813	1.110	O
HETATM 823 N	0	-0.236	-0.612	0.627	N
HETATM 824 C	0	-1.611	-0.231	0.355	C
HETATM 825 C	0	-1.817	-0.417	-1.162	C
HETATM 826 O	0	-2.369	-1.397	-1.617	O
HETATM 827 C	0	-1.935	1.126	0.998	C
HETATM 828 S	0	-0.907	2.546	0.422	S
HETATM 829 N	0	-1.238	0.581	-1.938	N
HETATM 830 C	0	-0.259	0.294	-3.006	C
HETATM 831 C	0	-0.138	-1.110	-3.624	C
HETATM 832 O	0	0.301	-2.077	-2.969	O
HETATM 833 O	0	-0.329	-1.224	-4.852	O
HETATM 834 H	0	4.076	-3.796	-1.095	H
HETATM 835 H	0	3.387	-3.391	-2.553	H
HETATM 836 H	0	2.830	-4.638	-1.561	H
HETATM 837 H	0	1.294	-2.867	-1.228	H
HETATM 838 H	0	2.116	-3.932	0.774	H
HETATM 839 H	0	3.461	-2.801	0.877	H
HETATM 840 H	0	2.051	-0.996	1.495	H

HETATM 841 H	0	1.591	-2.377	2.476	H
HETATM 842 H	0	0.470	0.120	0.545	H
HETATM 843 H	0	-2.235	-0.992	0.817	H
HETATM 844 H	0	-3.003	1.329	0.886	H
HETATM 845 H	0	-1.778	0.994	2.071	H
HETATM 846 H	0	-0.838	1.335	-1.363	H
HETATM 847 H	0	-0.454	0.974	-3.825	H
HETATM 848 H	0	0.727	0.536	-2.627	H
HETATM 849 C	0	-5.193	1.954	2.687	C
HETATM 850 O	0	-6.164	1.399	3.201	O
HETATM 851 C	0	-4.077	2.435	3.644	C
HETATM 852 C	0	-3.309	3.633	3.110	C
HETATM 853 C	0	-1.853	3.746	3.547	C
HETATM 854 C	0	-1.075	4.849	2.825	C
HETATM 855 O	0	-4.966	2.096	1.432	O
HETATM 856 C	0	-1.435	5.053	1.414	C
HETATM 857 C	0	-0.749	5.866	0.422	C
HETATM 858 O	0	-1.572	6.135	3.044	O
HETATM 859 C	0	0.285	6.665	0.711	C
HETATM 860 C	0	0.882	7.693	-0.150	C
HETATM 861 C	0	0.247	8.733	-0.708	C
HETATM 862 C	0	0.938	9.686	-1.428	C
HETATM 863 C	0	0.446	10.812	-2.013	C
HETATM 864 C	0	-0.998	11.280	-1.976	C
HETATM 865 C	0	-1.587	11.271	-3.381	C
HETATM 866 C	0	-2.838	10.840	-3.691	C
HETATM 867 C	0	-3.833	10.356	-2.654	C
HETATM 868 C	0	-3.555	8.910	-2.230	C
HETATM 869 C	0	-4.395	8.552	-0.998	C
HETATM 870 C	0	-3.901	7.259	-0.344	C
HETATM 871 C	0	-4.996	6.678	0.548	C
HETATM 872 H	0	-4.530	2.622	4.620	H
HETATM 873 H	0	-3.392	1.582	3.765	H
HETATM 874 H	0	-3.829	4.572	3.333	H
HETATM 875 H	0	-3.329	3.504	2.029	H
HETATM 876 H	0	-1.341	2.798	3.375	H
HETATM 877 H	0	-1.798	3.953	4.628	H
HETATM 878 H	0	0.012	4.746	3.004	H
HETATM 879 H	0	-2.475	4.874	1.187	H
HETATM 880 H	0	-1.204	5.896	-0.561	H
HETATM 881 H	0	0.717	6.592	1.706	H
HETATM 882 H	0	1.968	7.643	-0.230	H
HETATM 883 H	0	-0.819	8.829	-0.540	H
HETATM 884 H	0	2.011	9.540	-1.528	H
HETATM 885 H	0	1.160	11.462	-2.519	H
HETATM 886 H	0	-1.013	12.306	-1.606	H
HETATM 887 H	0	-1.582	10.692	-1.277	H
HETATM 888 H	0	-0.981	11.686	-4.186	H
HETATM 889 H	0	-3.166	10.907	-4.728	H

HETATM 890 H	0	-3.793	11.020	-1.788	H
HETATM 891 H	0	-4.839	10.420	-3.070	H
HETATM 892 H	0	-3.792	8.237	-3.054	H
HETATM 893 H	0	-2.500	8.793	-1.998	H
HETATM 894 H	0	-4.333	9.352	-0.258	H
HETATM 895 H	0	-5.437	8.448	-1.298	H
HETATM 896 H	0	-3.018	7.480	0.256	H
HETATM 897 H	0	-3.637	6.522	-1.102	H
HETATM 898 H	0	-5.849	6.376	-0.062	H
HETATM 899 H	0	-4.616	5.802	1.073	H
HETATM 900 H	0	-5.327	7.424	1.270	H
HETATM 901 O	0	6.704	3.942	10.543	O
HETATM 902 H	0	7.429	4.354	11.022	H
HETATM 903 H	0	6.547	3.124	11.022	H
HETATM 904 O	0	-4.669	10.277	2.382	O
HETATM 905 H	0	-4.292	9.427	2.690	H
HETATM 906 H	0	-4.550	10.846	3.178	H
HETATM 907 O	0	-5.988	6.475	3.838	O
HETATM 908 H	0	-6.247	5.650	3.408	H
HETATM 909 H	0	-6.177	6.298	4.783	H
HETATM 910 O	0	-7.084	10.182	1.182	O
HETATM 911 H	0	-7.391	11.057	1.441	H
HETATM 912 H	0	-6.158	10.178	1.509	H
HETATM 913 O	0	-3.739	7.924	3.404	O
HETATM 914 H	0	-4.538	7.367	3.521	H
HETATM 915 H	0	-3.101	7.309	3.012	H
HETATM 916 O	0	-1.445	12.128	5.017	O
HETATM 917 H	0	-0.490	12.330	4.970	H
HETATM 918 H	0	-1.533	11.710	5.893	H
HETATM 919 O	0	-7.740	8.609	3.385	O
HETATM 920 H	0	-7.088	7.888	3.422	H
HETATM 921 H	0	-7.552	9.041	2.536	H
HETATM 922 O	0	-2.902	11.740	0.891	O
HETATM 923 H	0	-3.538	11.157	1.348	H
HETATM 924 H	0	-3.353	12.587	0.872	H
HETATM 925 O	0	-3.576	-1.578	5.805	O
HETATM 926 H	0	-4.407	-1.129	5.522	H
HETATM 927 H	0	-3.367	-2.131	5.047	H
HETATM 928 O	0	-5.896	8.634	6.763	O
HETATM 929 H	0	-6.791	8.942	6.497	H
HETATM 930 H	0	-6.016	7.668	6.771	H
HETATM 931 O	0	-5.764	-0.272	5.066	O
HETATM 932 H	0	-6.405	0.065	5.702	H
HETATM 933 H	0	-5.937	0.316	4.281	H
HETATM 934 O	0	-2.621	-0.169	7.861	O
HETATM 935 H	0	-2.969	-0.710	7.114	H
HETATM 936 H	0	-2.303	-0.838	8.471	H
HETATM 937 O	0	0.066	9.775	8.474	O
HETATM 938 H	0	0.465	10.462	9.015	H

HETATM	939	H	0	-0.748	10.205	8.135	H
HETATM	940	O	0	6.273	-1.624	10.182	O
HETATM	941	H	0	6.146	-2.229	9.434	H
HETATM	942	H	0	7.222	-1.601	10.298	H
HETATM	943	O	0	-4.914	11.188	7.186	O
HETATM	944	H	0	-5.257	10.276	7.096	H
HETATM	945	H	0	-5.607	11.631	7.685	H
HETATM	946	O	0	-2.162	10.721	7.281	O
HETATM	947	H	0	-3.029	11.115	7.485	H
HETATM	948	H	0	-2.433	9.907	6.801	H
HETATM	949	O	0	-6.521	5.925	6.467	O
HETATM	950	H	0	-6.047	5.106	6.711	H
HETATM	951	H	0	-7.344	5.846	6.962	H
HETATM	952	O	0	-2.929	2.308	6.923	O
HETATM	953	H	0	-3.010	2.038	5.999	H
HETATM	954	H	0	-2.793	1.443	7.375	H
HETATM	955	O	0	-4.120	11.714	4.549	O
HETATM	956	H	0	-4.430	11.617	5.466	H
HETATM	957	H	0	-3.189	11.985	4.666	H
HETATM	958	O	0	-0.586	11.615	2.376	O
HETATM	959	H	0	-1.255	11.612	1.668	H
HETATM	960	H	0	-1.115	11.800	3.168	H
HETATM	961	O	0	-8.339	9.289	5.896	O
HETATM	962	H	0	-8.178	9.068	4.952	H
HETATM	963	H	0	-9.245	9.603	5.894	H
HETATM	964	O	0	1.226	12.243	4.345	O
HETATM	965	H	0	2.165	12.352	4.161	H
HETATM	966	H	0	0.845	12.047	3.469	H
HETATM	967	O	0	-1.292	4.351	7.641	O
HETATM	968	H	0	-0.613	3.825	8.072	H
HETATM	969	H	0	-1.971	3.679	7.425	H
HETATM	970	O	0	-3.277	8.659	5.996	O
HETATM	971	H	0	-3.362	8.469	5.043	H
HETATM	972	H	0	-4.203	8.618	6.301	H

PC (Tail-to-head orientation)

E = -2159.45034014 hartrees

HETATM	1	C	0	5.322	-5.657	9.417	C
HETATM	2	H	0	5.639	-5.091	10.268	H
HETATM	3	H	0	5.662	-6.667	9.514	H
HETATM	4	H	0	4.254	-5.644	9.357	H
HETATM	5	C	0	5.914	-5.026	8.179	C
HETATM	6	O	0	5.937	-3.805	8.096	O
HETATM	7	N	0	6.370	-5.827	7.212	N
HETATM	8	C	0	6.872	-5.342	5.913	C
HETATM	9	H	0	7.132	-6.186	5.274	H
HETATM	10	C	0	5.829	-4.483	5.195	C

HETATM	11	O	0	6.112	-3.343	4.849	O
HETATM	12	H	0	6.344	-6.821	7.380	H
HETATM	13	H	0	7.767	-4.741	6.073	H
HETATM	14	N	0	4.610	-5.004	5.007	N
HETATM	15	C	0	3.445	-4.287	4.452	C
HETATM	16	C	0	3.184	-2.960	5.155	C
HETATM	17	O	0	3.104	-1.924	4.504	O
HETATM	18	C	0	2.203	-5.182	4.499	C
HETATM	19	O	0	2.059	-5.763	5.785	O
HETATM	20	H	0	4.430	-5.933	5.360	H
HETATM	21	H	0	3.646	-4.055	3.405	H
HETATM	22	H	0	2.302	-5.975	3.756	H
HETATM	23	H	0	1.322	-4.586	4.263	H
HETATM	24	H	0	1.262	-6.309	5.770	H
HETATM	25	N	0	3.091	-2.978	6.482	N
HETATM	26	C	0	2.941	-1.790	7.322	C
HETATM	27	C	0	4.084	-0.778	7.184	C
HETATM	28	O	0	3.862	0.431	7.209	O
HETATM	29	C	0	2.780	-2.215	8.795	C
HETATM	30	C	0	1.544	-3.085	9.097	C
HETATM	31	C	0	1.581	-3.527	10.560	C
HETATM	32	C	0	0.227	-2.341	8.861	C
HETATM	33	H	0	3.117	-3.894	6.907	H
HETATM	34	H	0	2.031	-1.274	7.028	H
HETATM	35	H	0	3.673	-2.762	9.097	H
HETATM	36	H	0	2.726	-1.315	9.410	H
HETATM	37	H	0	1.563	-3.979	8.473	H
HETATM	38	H	0	1.543	-2.657	11.217	H
HETATM	39	H	0	2.498	-4.081	10.757	H
HETATM	40	H	0	0.730	-4.174	10.773	H
HETATM	41	H	0	0.211	-1.418	9.442	H
HETATM	42	H	0	-0.609	-2.973	9.161	H
HETATM	43	H	0	0.114	-2.108	7.804	H
HETATM	44	N	0	5.309	-1.267	7.026	N
HETATM	45	C	0	6.477	-0.449	6.749	C
HETATM	46	H	0	7.372	-1.065	6.822	H
HETATM	47	C	0	6.434	0.171	5.358	C
HETATM	48	O	0	6.725	1.352	5.255	O
HETATM	49	H	0	5.420	-2.273	7.061	H
HETATM	50	H	0	6.545	0.350	7.487	H
HETATM	51	N	0	6.039	-0.573	4.312	N
HETATM	52	C	0	5.681	-0.002	2.998	C
HETATM	53	C	0	4.628	1.078	3.205	C
HETATM	54	O	0	4.917	2.210	2.869	O
HETATM	55	C	0	5.271	-1.045	1.951	C
HETATM	56	C	0	4.949	-0.371	0.614	C
HETATM	57	C	0	6.406	-2.021	1.650	C
HETATM	58	H	0	5.866	-1.558	4.484	H
HETATM	59	H	0	6.566	0.504	2.612	H

HETATM	60	H	0	4.405	-1.601	2.301	H
HETATM	61	H	0	5.795	0.243	0.309	H
HETATM	62	H	0	4.060	0.252	0.701	H
HETATM	63	H	0	4.775	-1.121	-0.155	H
HETATM	64	H	0	7.227	-1.517	1.151	H
HETATM	65	H	0	6.039	-2.787	0.976	H
HETATM	66	H	0	6.773	-2.487	2.560	H
HETATM	67	N	0	3.475	0.783	3.813	N
HETATM	68	C	0	2.398	1.730	4.171	C
HETATM	69	C	0	2.916	3.046	4.777	C
HETATM	70	O	0	2.647	4.121	4.243	O
HETATM	71	C	0	1.353	1.027	5.075	C
HETATM	72	C	0	0.468	0.122	4.201	C
HETATM	73	C	0	0.501	2.001	5.909	C
HETATM	74	C	0	-0.313	-0.965	4.945	C
HETATM	75	H	0	3.355	-0.187	4.085	H
HETATM	76	H	0	1.882	2.019	3.255	H
HETATM	77	H	0	1.881	0.391	5.771	H
HETATM	78	H	0	-0.226	0.739	3.641	H
HETATM	79	H	0	1.106	-0.386	3.488	H
HETATM	80	H	0	0.138	2.810	5.280	H
HETATM	81	H	0	1.101	2.427	6.713	H
HETATM	82	H	0	-0.339	1.486	6.370	H
HETATM	83	H	0	-0.987	-0.523	5.674	H
HETATM	84	H	0	0.378	-1.642	5.445	H
HETATM	85	H	0	-0.901	-1.537	4.226	H
HETATM	86	N	0	3.651	2.969	5.887	N
HETATM	87	C	0	4.307	4.111	6.535	C
HETATM	88	C	0	5.270	4.804	5.564	C
HETATM	89	O	0	5.133	5.997	5.314	O
HETATM	90	C	0	5.039	3.605	7.780	C
HETATM	91	O	0	5.589	4.678	8.509	O
HETATM	92	H	0	3.798	2.042	6.273	H
HETATM	93	H	0	3.552	4.835	6.843	H
HETATM	94	H	0	5.833	2.916	7.489	H
HETATM	95	H	0	4.332	3.072	8.418	H
HETATM	96	H	0	6.012	4.298	9.307	H
HETATM	97	N	0	6.202	4.071	4.945	N
HETATM	98	C	0	7.168	4.566	3.962	C
HETATM	99	C	0	6.547	5.233	2.724	C
HETATM	100	O	0	7.122	6.179	2.185	O
HETATM	101	C	0	8.131	3.445	3.550	C
HETATM	102	H	0	6.234	3.079	5.148	H
HETATM	103	H	0	7.763	5.336	4.455	H
HETATM	104	H	0	8.891	3.844	2.878	H
HETATM	105	H	0	7.588	2.652	3.037	H
HETATM	106	H	0	8.625	3.036	4.432	H
HETATM	107	N	0	5.364	4.787	2.283	N
HETATM	108	C	0	4.562	5.431	1.237	C

HETATM 109 C	0	4.213	6.879	1.616	C
HETATM 110 O	0	3.956	7.695	0.738	O
HETATM 111 C	0	3.223	4.737	0.955	C
HETATM 112 C	0	3.329	3.253	0.628	C
HETATM 113 C	0	2.435	2.801	-0.513	C
HETATM 114 N	0	2.792	3.411	-1.798	N
HETATM 115 C	0	2.943	2.783	-2.941	C
HETATM 116 N	0	2.781	1.503	-3.089	N
HETATM 117 N	0	3.278	3.470	-3.984	N
HETATM 118 H	0	4.992	3.968	2.755	H
HETATM 119 H	0	5.144	5.472	0.317	H
HETATM 120 H	0	2.548	4.861	1.802	H
HETATM 121 H	0	2.774	5.253	0.111	H
HETATM 122 H	0	3.006	2.696	1.499	H
HETATM 123 H	0	4.360	2.997	0.399	H
HETATM 124 H	0	1.401	3.015	-0.282	H
HETATM 125 H	0	2.547	1.732	-0.562	H
HETATM 126 H	0	2.902	4.415	-1.834	H
HETATM 127 H	0	2.786	1.085	-3.999	H
HETATM 128 H	0	2.531	0.908	-2.296	H
HETATM 129 H	0	3.274	4.473	-3.941	H
HETATM 130 H	0	3.561	2.974	-4.818	H
HETATM 131 N	0	4.148	7.191	2.913	N
HETATM 132 C	0	3.791	8.503	3.500	C
HETATM 133 C	0	4.992	9.233	4.119	C
HETATM 134 O	0	4.969	10.462	4.165	O
HETATM 135 C	0	2.626	8.344	4.476	C
HETATM 136 C	0	1.353	7.788	3.812	C
HETATM 137 C	0	0.090	8.444	4.355	C
HETATM 138 N	0	-0.076	8.290	5.785	N
HETATM 139 C	0	-0.685	7.227	6.374	C
HETATM 140 N	0	-1.396	6.374	5.704	N
HETATM 141 N	0	-0.453	7.136	7.742	N
HETATM 142 H	0	4.328	6.423	3.552	H
HETATM 143 H	0	3.465	9.156	2.683	H
HETATM 144 H	0	2.916	7.717	5.328	H
HETATM 145 H	0	2.406	9.334	4.902	H
HETATM 146 H	0	1.281	6.702	3.941	H
HETATM 147 H	0	1.374	7.973	2.731	H
HETATM 148 H	0	-0.795	8.039	3.865	H
HETATM 149 H	0	0.127	9.519	4.153	H
HETATM 150 H	0	0.589	8.780	6.378	H
HETATM 151 H	0	-1.833	5.756	6.402	H
HETATM 152 H	0	-1.492	6.020	3.991	H
HETATM 153 H	0	-0.262	8.040	8.184	H
HETATM 154 H	0	-1.171	6.604	8.225	H
HETATM 155 N	0	6.028	8.497	4.540	N
HETATM 156 C	0	7.335	8.960	5.000	C
HETATM 157 H	0	7.502	9.938	4.600	H

HETATM 158 H	0	8.103	8.298	4.657	H
HETATM 159 H	0	7.354	9.003	6.069	H
HETATM 160 H	0	5.855	7.499	4.541	H
HETATM 161 C	0	5.491	10.833	-0.403	C
HETATM 162 H	0	5.452	11.892	-0.556	H
HETATM 163 H	0	6.473	10.556	-0.079	H
HETATM 164 H	0	4.777	10.553	0.343	H
HETATM 165 C	0	5.209	10.089	-1.707	C
HETATM 166 O	0	5.420	10.643	-2.777	O
HETATM 167 N	0	4.754	8.829	-1.636	N
HETATM 168 C	0	4.653	7.864	-2.758	C
HETATM 169 C	0	3.259	7.265	-2.958	C
HETATM 170 O	0	2.931	6.200	-2.434	O
HETATM 171 C	0	5.762	6.791	-2.687	C
HETATM 172 C	0	5.868	6.088	-4.041	C
HETATM 173 C	0	7.147	7.386	-2.387	C
HETATM 174 H	0	4.591	8.472	-0.701	H
HETATM 175 H	0	4.862	8.429	-3.667	H
HETATM 176 H	0	5.526	6.057	-1.916	H
HETATM 177 H	0	6.089	6.804	-4.831	H
HETATM 178 H	0	4.941	5.574	-4.264	H
HETATM 179 H	0	6.658	5.343	-4.012	H
HETATM 180 H	0	7.362	8.203	-3.076	H
HETATM 181 H	0	7.911	6.618	-2.490	H
HETATM 182 H	0	7.178	7.757	-1.363	H
HETATM 183 N	0	2.442	7.950	-3.766	N
HETATM 184 C	0	1.040	7.627	-4.074	C
HETATM 185 C	0	0.841	6.165	-4.552	C
HETATM 186 O	0	1.690	5.641	-5.272	O
HETATM 187 C	0	0.514	8.601	-5.133	C
HETATM 188 O	0	0.839	9.939	-4.803	O
HETATM 189 H	0	2.781	8.829	-4.134	H
HETATM 190 H	0	0.475	7.785	-3.158	H
HETATM 191 H	0	-0.568	8.498	-5.226	H
HETATM 192 H	0	0.972	8.361	-6.095	H
HETATM 193 H	0	0.359	10.229	-4.015	H
HETATM 194 N	0	-0.263	5.487	-4.182	N
HETATM 195 C	0	-0.369	4.018	-4.181	C
HETATM 196 C	0	0.018	3.220	-5.448	C
HETATM 197 O	0	0.854	2.326	-5.324	O
HETATM 198 C	0	-1.735	3.669	-3.598	C
HETATM 199 C	0	-2.454	5.007	-3.398	C
HETATM 200 C	0	-1.341	6.042	-3.382	C
HETATM 201 H	0	0.347	3.688	-3.427	H
HETATM 202 H	0	-2.293	3.021	-4.270	H
HETATM 203 H	0	-1.599	3.173	-2.635	H
HETATM 204 H	0	-3.013	5.033	-2.464	H
HETATM 205 H	0	-3.118	5.201	-4.240	H
HETATM 206 H	0	-0.992	6.178	-2.358	H

HETATM 207 H	0	-1.702	6.987	-3.788	H
HETATM 208 N	0	-0.519	3.488	-6.660	N
HETATM 209 C	0	-0.162	2.743	-7.886	C
HETATM 210 C	0	1.318	2.746	-8.245	C
HETATM 211 O	0	1.735	1.999	-9.132	O
HETATM 212 C	0	-0.955	3.413	-9.015	C
HETATM 213 C	0	-2.127	4.081	-8.306	C
HETATM 214 C	0	-1.535	4.485	-6.958	C
HETATM 215 H	0	-0.482	1.708	-7.799	H
HETATM 216 H	0	-0.348	4.184	-9.496	H
HETATM 217 H	0	-1.293	2.686	-9.754	H
HETATM 218 H	0	-2.924	3.352	-8.161	H
HETATM 219 H	0	-2.497	4.945	-8.860	H
HETATM 220 H	0	-2.319	4.502	-6.205	H
HETATM 221 H	0	-1.065	5.466	-7.039	H
HETATM 222 N	0	2.109	3.610	-7.607	N
HETATM 223 C	0	3.540	3.656	-7.793	C
HETATM 224 C	0	4.200	2.361	-7.288	C
HETATM 225 O	0	4.649	2.266	-6.150	O
HETATM 226 C	0	4.121	4.970	-7.249	C
HETATM 227 C	0	3.507	6.259	-7.834	C
HETATM 228 C	0	4.106	7.476	-7.130	C
HETATM 229 C	0	3.780	6.403	-9.333	C
HETATM 230 H	0	1.712	4.165	-6.859	H
HETATM 231 H	0	3.722	3.673	-8.868	H
HETATM 232 H	0	4.012	4.978	-6.170	H
HETATM 233 H	0	5.178	4.989	-7.488	H
HETATM 234 H	0	2.429	6.270	-7.679	H
HETATM 235 H	0	5.183	7.510	-7.288	H
HETATM 236 H	0	3.901	7.411	-6.064	H
HETATM 237 H	0	3.653	8.389	-7.516	H
HETATM 238 H	0	4.852	6.359	-9.527	H
HETATM 239 H	0	3.393	7.359	-9.686	H
HETATM 240 H	0	3.277	5.610	-9.884	H
HETATM 241 N	0	4.315	1.378	-8.187	N
HETATM 242 C	0	5.284	0.263	-8.185	C
HETATM 243 C	0	6.731	0.809	-8.390	C
HETATM 244 O	0	7.536	0.236	-9.123	O
HETATM 245 C	0	4.896	-0.756	-9.281	C
HETATM 246 O	0	5.800	-1.836	-9.304	O
HETATM 247 C	0	4.816	-0.189	-10.702	C
HETATM 248 H	0	3.738	1.513	-9.011	H
HETATM 249 H	0	5.253	-0.240	-7.218	H
HETATM 250 H	0	3.913	-1.152	-9.046	H
HETATM 251 H	0	5.772	0.233	-11.010	H
HETATM 252 H	0	4.045	0.579	-10.760	H
HETATM 253 H	0	4.551	-0.991	-11.392	H
HETATM 254 H	0	6.664	-1.437	-9.507	H
HETATM 255 N	0	7.060	1.957	-7.787	N

HETATM 256 C	0	8.203	2.837	-8.075	C
HETATM 257 H	0	8.172	3.143	-9.121	H
HETATM 258 C	0	8.166	4.085	-7.186	C
HETATM 259 O	0	7.196	4.295	-6.469	O
HETATM 260 H	0	6.399	2.320	-7.105	H
HETATM 261 H	0	9.130	2.294	-7.889	H
HETATM 262 N	0	9.196	4.932	-7.227	N
HETATM 263 C	0	9.226	6.198	-6.476	C
HETATM 264 C	0	10.305	6.251	-5.393	C
HETATM 265 O	0	10.870	5.228	-4.999	O
HETATM 266 H	0	10.000	4.680	-7.779	H
HETATM 267 H	0	9.407	7.009	-7.181	H
HETATM 268 H	0	8.265	6.385	-5.996	H
HETATM 269 N	0	10.615	7.469	-4.934	N
HETATM 270 C	0	11.815	7.745	-4.154	C
HETATM 271 H	0	12.116	8.766	-4.267	H
HETATM 272 H	0	12.577	7.103	-4.544	H
HETATM 273 H	0	11.665	7.530	-3.116	H
HETATM 274 H	0	10.072	8.250	-5.271	H
HETATM 275 C	0	14.076	4.207	-0.180	C
HETATM 276 H	0	14.029	4.842	-1.040	H
HETATM 277 H	0	14.719	3.377	-0.384	H
HETATM 278 H	0	14.461	4.760	0.651	H
HETATM 279 C	0	12.729	3.553	0.031	C
HETATM 280 O	0	12.694	2.420	0.492	O
HETATM 281 N	0	11.649	4.171	-0.456	N
HETATM 282 C	0	10.393	3.453	-0.730	C
HETATM 283 C	0	10.621	2.263	-1.682	C
HETATM 284 O	0	10.236	1.154	-1.342	O
HETATM 285 C	0	9.318	4.396	-1.302	C
HETATM 286 C	0	8.159	3.639	-1.937	C
HETATM 287 C	0	7.123	3.111	-1.142	C
HETATM 288 C	0	8.191	3.344	-3.316	C
HETATM 289 C	0	6.147	2.281	-1.727	C
HETATM 290 C	0	7.227	2.497	-3.886	C
HETATM 291 C	0	6.207	1.963	-3.091	C
HETATM 292 H	0	11.757	5.110	-0.801	H
HETATM 293 H	0	10.014	3.038	0.205	H
HETATM 294 H	0	8.940	5.038	-0.505	H
HETATM 295 H	0	9.771	5.035	-2.062	H
HETATM 296 H	0	7.091	3.314	-0.081	H
HETATM 297 H	0	8.976	3.737	-3.944	H
HETATM 298 H	0	5.353	1.854	-1.138	H
HETATM 299 H	0	7.265	2.248	-4.934	H
HETATM 300 H	0	5.474	1.301	-3.532	H
HETATM 301 N	0	11.193	2.456	-2.881	N
HETATM 302 C	0	11.279	1.394	-3.888	C
HETATM 303 H	0	11.605	0.493	-3.412	H
HETATM 304 H	0	11.965	1.654	-4.667	H

HETATM 305 H	0	10.305	1.243	-4.306	H
HETATM 306 H	0	11.436	3.401	-3.144	H
HETATM 307 C	0	13.902	-0.697	-2.085	C
HETATM 308 H	0	13.583	-0.998	-3.061	H
HETATM 309 H	0	14.931	-0.955	-1.951	H
HETATM 310 H	0	13.782	0.361	-1.981	H
HETATM 311 C	0	12.979	-1.431	-1.110	C
HETATM 312 O	0	12.835	-2.640	-1.237	O
HETATM 313 N	0	12.290	-0.719	-0.207	N
HETATM 314 C	0	11.280	-1.237	0.760	C
HETATM 315 C	0	10.116	-1.991	0.123	C
HETATM 316 O	0	9.771	-3.072	0.587	O
HETATM 317 C	0	10.848	-0.091	1.711	C
HETATM 318 C	0	9.478	-0.235	2.377	C
HETATM 319 C	0	11.899	0.073	2.816	C
HETATM 320 H	0	12.463	0.279	-0.175	H
HETATM 321 H	0	11.782	-1.985	1.375	H
HETATM 322 H	0	10.807	0.838	1.149	H
HETATM 323 H	0	9.363	-1.225	2.811	H
HETATM 324 H	0	8.712	-0.054	1.629	H
HETATM 325 H	0	9.359	0.515	3.159	H
HETATM 326 H	0	11.927	-0.817	3.446	H
HETATM 327 H	0	11.661	0.942	3.429	H
HETATM 328 H	0	12.882	0.228	2.372	H
HETATM 329 N	0	9.534	-1.459	-0.948	N
HETATM 330 C	0	8.624	-2.142	-1.865	C
HETATM 331 C	0	9.238	-3.458	-2.343	C
HETATM 332 O	0	8.703	-4.524	-2.065	O
HETATM 333 C	0	8.312	-1.184	-3.027	C
HETATM 334 C	0	7.442	-1.766	-4.125	C
HETATM 335 C	0	6.044	-1.739	-3.991	C
HETATM 336 C	0	8.023	-2.319	-5.284	C
HETATM 337 C	0	5.223	-2.274	-5.001	C
HETATM 338 C	0	7.206	-2.854	-6.299	C
HETATM 339 C	0	5.803	-2.844	-6.153	C
HETATM 340 O	0	5.016	-3.338	-7.145	O
HETATM 341 H	0	9.853	-0.532	-1.197	H
HETATM 342 H	0	7.696	-2.378	-1.343	H
HETATM 343 H	0	7.817	-0.303	-2.619	H
HETATM 344 H	0	9.249	-0.845	-3.471	H
HETATM 345 H	0	5.596	-1.296	-3.111	H
HETATM 346 H	0	9.098	-2.341	-5.396	H
HETATM 347 H	0	4.151	-2.228	-4.893	H
HETATM 348 H	0	7.650	-3.286	-7.184	H
HETATM 349 H	0	5.410	-3.091	-8.000	H
HETATM 350 N	0	10.378	-3.400	-3.035	N
HETATM 351 C	0	11.077	-4.580	-3.516	C
HETATM 352 H	0	11.756	-4.911	-2.759	H
HETATM 353 H	0	11.620	-4.355	-4.410	H

HETATM 354 H	0	10.363	-5.351	-3.717	H
HETATM 355 H	0	10.828	-2.501	-3.097	H
HETATM 356 C	0	12.117	-6.011	-0.089	C
HETATM 357 H	0	11.973	-5.544	-1.041	H
HETATM 358 H	0	12.885	-6.752	-0.168	H
HETATM 359 H	0	12.407	-5.273	0.630	H
HETATM 360 C	0	10.820	-6.685	0.316	C
HETATM 361 O	0	10.772	-7.906	0.369	O
HETATM 362 N	0	9.765	-5.913	0.587	N
HETATM 363 C	0	8.448	-6.388	1.052	C
HETATM 364 C	0	7.753	-7.349	0.088	C
HETATM 365 O	0	7.218	-8.370	0.514	O
HETATM 366 C	0	7.578	-5.183	1.405	C
HETATM 367 C	0	6.192	-5.572	1.928	C
HETATM 368 C	0	5.177	-5.727	0.812	C
HETATM 369 O	0	4.833	-4.765	0.147	O
HETATM 370 N	0	4.643	-6.898	0.583	N
HETATM 371 H	0	9.884	-4.911	0.473	H
HETATM 372 H	0	8.616	-6.953	1.969	H
HETATM 373 H	0	8.081	-4.625	2.190	H
HETATM 374 H	0	7.481	-4.537	0.532	H
HETATM 375 H	0	5.835	-4.757	2.548	H
HETATM 376 H	0	6.247	-6.474	2.538	H
HETATM 377 H	0	3.942	-6.883	-0.161	H
HETATM 378 H	0	5.052	-7.757	0.920	H
HETATM 379 N	0	7.694	-6.973	-1.186	N
HETATM 380 C	0	7.100	-7.747	-2.279	C
HETATM 381 C	0	8.006	-8.929	-2.690	C
HETATM 382 O	0	7.515	-9.910	-3.244	O
HETATM 383 C	0	6.803	-6.820	-3.485	C
HETATM 384 C	0	6.095	-7.537	-4.644	C
HETATM 385 C	0	5.881	-5.655	-3.090	C
HETATM 386 H	0	8.111	-6.076	-1.413	H
HETATM 387 H	0	6.156	-8.172	-1.938	H
HETATM 388 H	0	7.741	-6.409	-3.860	H
HETATM 389 H	0	5.178	-8.006	-4.287	H
HETATM 390 H	0	6.745	-8.300	-5.070	H
HETATM 391 H	0	5.852	-6.826	-5.433	H
HETATM 392 H	0	5.663	-5.034	-3.957	H
HETATM 393 H	0	6.335	-5.028	-2.328	H
HETATM 394 H	0	4.959	-6.053	-2.683	H
HETATM 395 N	0	9.321	-8.859	-2.416	N
HETATM 396 C	0	10.281	-9.956	-2.584	C
HETATM 397 H	0	11.035	-9.884	-1.828	H
HETATM 398 H	0	10.742	-9.934	-3.549	H
HETATM 399 H	0	9.744	-10.874	-2.466	H
HETATM 400 H	0	9.610	-8.061	-1.871	H
HETATM 401 C	0	17.240	-7.841	4.072	C
HETATM 402 H	0	17.974	-7.669	4.831	H

HETATM 403	H	0	17.728	-7.993	3.132	H
HETATM 404	H	0	16.667	-8.710	4.320	H
HETATM 405	C	0	16.385	-6.601	3.997	C
HETATM 406	O	0	16.794	-5.618	3.401	O
HETATM 407	N	0	15.226	-6.631	4.650	N
HETATM 408	C	0	14.317	-5.482	4.757	C
HETATM 409	C	0	14.897	-4.299	5.567	C
HETATM 410	O	0	14.577	-3.148	5.289	O
HETATM 411	C	0	12.984	-5.967	5.350	C
HETATM 412	C	0	11.862	-4.945	5.310	C
HETATM 413	C	0	11.223	-4.657	4.089	C
HETATM 414	C	0	11.454	-4.278	6.482	C
HETATM 415	C	0	10.188	-3.708	4.043	C
HETATM 416	C	0	10.412	-3.333	6.434	C
HETATM 417	C	0	9.779	-3.046	5.213	C
HETATM 418	H	0	14.957	-7.502	5.077	H
HETATM 419	H	0	14.126	-5.103	3.751	H
HETATM 420	H	0	12.652	-6.843	4.790	H
HETATM 421	H	0	13.147	-6.282	6.382	H
HETATM 422	H	0	11.532	-5.154	3.181	H
HETATM 423	H	0	11.950	-4.480	7.421	H
HETATM 424	H	0	9.720	-3.476	3.099	H
HETATM 425	H	0	10.111	-2.815	7.333	H
HETATM 426	H	0	8.986	-2.313	5.166	H
HETATM 427	N	0	15.738	-4.583	6.577	N
HETATM 428	C	0	16.536	-3.605	7.323	C
HETATM 429	H	0	16.476	-2.654	6.836	H
HETATM 430	H	0	17.551	-3.945	7.317	H
HETATM 431	H	0	16.198	-3.510	8.334	H
HETATM 432	H	0	15.938	-5.560	6.706	H
HETATM 433	C	0	-2.122	-4.264	-11.870	C
HETATM 434	H	0	-2.434	-5.242	-12.174	H
HETATM 435	H	0	-1.407	-3.884	-12.569	H
HETATM 436	H	0	-2.971	-3.613	-11.838	H
HETATM 437	C	0	-1.542	-4.351	-10.482	C
HETATM 438	O	0	-1.354	-5.441	-9.960	O
HETATM 439	N	0	-1.304	-3.192	-9.862	N
HETATM 440	C	0	-0.829	-3.095	-8.472	C
HETATM 441	C	0	-1.763	-3.749	-7.450	C
HETATM 442	O	0	-1.276	-4.462	-6.582	O
HETATM 443	C	0	-0.483	-1.645	-8.100	C
HETATM 444	C	0	1.021	-1.291	-8.095	C
HETATM 445	C	0	2.001	-2.294	-7.447	C
HETATM 446	N	0	1.577	-2.754	-6.120	N
HETATM 447	C	0	1.918	-3.860	-5.486	C
HETATM 448	N	0	2.787	-4.734	-5.897	N
HETATM 449	N	0	1.409	-4.130	-4.339	N
HETATM 450	H	0	-1.470	-2.350	-10.390	H
HETATM 451	H	0	0.071	-3.704	-8.405	H

HETATM 452 H	0	-1.003	-0.952	-8.764	H
HETATM 453 H	0	-0.886	-1.462	-7.114	H
HETATM 454 H	0	1.131	-0.335	-7.581	H
HETATM 455 H	0	1.339	-1.140	-9.127	H
HETATM 456 H	0	2.961	-1.796	-7.329	H
HETATM 457 H	0	2.135	-3.149	-8.111	H
HETATM 458 H	0	0.930	-2.149	-5.611	H
HETATM 459 H	0	2.967	-5.511	-5.263	H
HETATM 460 H	0	3.441	-4.468	-6.617	H
HETATM 461 H	0	0.797	-3.439	-3.905	H
HETATM 462 H	0	1.665	-5.016	-3.909	H
HETATM 463 N	0	-3.079	-3.528	-7.534	N
HETATM 464 C	0	-4.065	-4.178	-6.667	C
HETATM 465 H	0	-3.769	-4.049	-5.647	H
HETATM 466 H	0	-4.091	-5.222	-6.902	H
HETATM 467 H	0	-5.037	-3.755	-6.812	H
HETATM 468 H	0	-3.383	-2.907	-8.265	H
HETATM 469 C	0	0.101	-7.815	-7.281	C
HETATM 470 H	0	-0.035	-8.827	-7.602	H
HETATM 471 H	0	1.059	-7.464	-7.603	H
HETATM 472 H	0	-0.665	-7.200	-7.706	H
HETATM 473 C	0	-0.118	-7.840	-5.780	C
HETATM 474 O	0	-0.008	-8.917	-5.219	O
HETATM 475 N	0	-0.551	-6.736	-5.152	N
HETATM 476 C	0	-0.891	-6.596	-3.716	C
HETATM 477 C	0	-1.695	-7.778	-3.158	C
HETATM 478 O	0	-1.318	-8.406	-2.172	O
HETATM 479 C	0	-1.625	-5.256	-3.462	C
HETATM 480 C	0	-1.706	-4.912	-1.977	C
HETATM 481 O	0	-2.324	-5.612	-1.194	O
HETATM 482 N	0	-1.118	-3.833	-1.539	N
HETATM 483 H	0	-0.642	-5.906	-5.728	H
HETATM 484 H	0	0.030	-6.534	-3.151	H
HETATM 485 H	0	-2.637	-5.305	-3.854	H
HETATM 486 H	0	-1.122	-4.443	-3.977	H
HETATM 487 H	0	-1.216	-3.542	-0.563	H
HETATM 488 H	0	-0.773	-3.134	-2.191	H
HETATM 489 N	0	-2.836	-8.071	-3.780	N
HETATM 490 C	0	-3.674	-9.178	-3.368	C
HETATM 491 H	0	-3.368	-9.506	-2.397	H
HETATM 492 H	0	-3.557	-9.978	-4.069	H
HETATM 493 H	0	-4.700	-8.878	-3.336	H
HETATM 494 H	0	-3.040	-7.549	-4.617	H
HETATM 495 C	0	-1.198	-11.853	-4.709	C
HETATM 496 H	0	-1.624	-12.826	-4.837	H
HETATM 497 H	0	-0.945	-11.446	-5.666	H
HETATM 498 H	0	-1.907	-11.214	-4.225	H
HETATM 499 C	0	-0.086	-11.949	-3.641	C
HETATM 500 O	0	0.048	-13.011	-3.050	O

HETATM 501 N	0	0.604 -10.858 -3.265	N
HETATM 502 C	0	1.614 -10.762 -2.154	C
HETATM 503 C	0	1.064 -10.967 -0.730	C
HETATM 504 O	0	1.727 -11.600 0.087	O
HETATM 505 C	0	2.544 -9.547 -2.295	C
HETATM 506 C	0	1.703 -8.291 -2.320	C
HETATM 507 C	0	2.465 -6.994 -2.426	C
HETATM 508 O	0	2.754 -6.431 -1.355	O
HETATM 509 O	0	2.591 -6.410 -3.530	O
HETATM 510 H	0	0.425 -10.024 -3.815	H
HETATM 511 H	0	2.270 -11.623 -2.289	H
HETATM 512 H	0	3.243 -9.512 -1.458	H
HETATM 513 H	0	3.106 -9.622 -3.227	H
HETATM 514 H	0	1.112 -8.261 -1.410	H
HETATM 515 H	0	1.047 -8.356 -3.169	H
HETATM 516 N	0	-0.145 -10.489 -0.417	N
HETATM 517 C	0	-0.838 -10.822 0.843	C
HETATM 518 C	0	-1.606 -12.160 0.798	C
HETATM 519 O	0	-2.147 -12.586 1.818	O
HETATM 520 C	0	-1.837 -9.702 1.205	C
HETATM 521 C	0	-1.325 -8.376 1.766	C
HETATM 522 C	0	-0.700 -7.440 0.922	C
HETATM 523 C	0	-1.698 -7.971 3.068	C
HETATM 524 C	0	-0.508 -6.106 1.327	C
HETATM 525 C	0	-1.505 -6.635 3.483	C
HETATM 526 C	0	-0.939 -5.688 2.600	C
HETATM 527 O	0	-0.848 -4.380 2.959	O
HETATM 528 H	0	-0.604 -9.909 -1.112	H
HETATM 529 H	0	-0.109 -10.902 1.651	H
HETATM 530 H	0	-2.432 -9.485 0.316	H
HETATM 531 H	0	-2.537 -10.099 1.941	H
HETATM 532 H	0	-0.425 -7.718 -0.078	H
HETATM 533 H	0	-2.183 -8.673 3.735	H
HETATM 534 H	0	-0.075 -5.390 0.645	H
HETATM 535 H	0	-1.832 -6.305 4.457	H
HETATM 536 H	0	-0.800 -3.787 2.174	H
HETATM 537 N	0	-1.715 -12.803 -0.371	N
HETATM 538 C	0	-2.321 -14.121 -0.535	C
HETATM 539 H	0	-1.988 -14.738 0.274	H
HETATM 540 H	0	-1.955 -14.517 -1.459	H
HETATM 541 H	0	-3.390 -14.103 -0.553	H
HETATM 542 H	0	-1.156 -12.444 -1.135	H
HETATM 543 C	0	-12.831 -7.527 1.520	C
HETATM 544 H	0	-12.603 -6.860 2.325	H
HETATM 545 H	0	-12.686 -8.537 1.841	H
HETATM 546 H	0	-13.850 -7.391 1.221	H
HETATM 547 C	0	-11.934 -7.220 0.335	C
HETATM 548 O	0	-12.037 -6.144 -0.237	O
HETATM 549 N	0	-11.065 -8.159 -0.074	N

HETATM 550 C	0	-10.099	-7.968	-1.185	C
HETATM 551 C	0	-10.719	-7.689	-2.556	C
HETATM 552 O	0	-10.082	-6.993	-3.340	O
HETATM 553 C	0	-9.081	-9.123	-1.259	C
HETATM 554 C	0	-7.969	-9.038	-0.198	C
HETATM 555 C	0	-7.225	-7.694	-0.276	C
HETATM 556 N	0	-5.948	-7.690	0.453	N
HETATM 557 C	0	-4.926	-6.906	0.170	C
HETATM 558 N	0	-4.973	-6.009	-0.764	N
HETATM 559 N	0	-3.802	-6.991	0.801	N
HETATM 560 H	0	-11.049	-9.016	0.458	H
HETATM 561 H	0	-9.568	-7.054	-0.964	H
HETATM 562 H	0	-9.600	-10.079	-1.168	H
HETATM 563 H	0	-8.599	-9.105	-2.239	H
HETATM 564 H	0	-7.261	-9.848	-0.380	H
HETATM 565 H	0	-8.401	-9.173	0.791	H
HETATM 566 H	0	-7.850	-6.902	0.140	H
HETATM 567 H	0	-7.038	-7.474	-1.329	H
HETATM 568 H	0	-5.852	-8.253	1.282	H
HETATM 569 H	0	-4.108	-5.506	-0.936	H
HETATM 570 H	0	-5.829	-5.712	-1.189	H
HETATM 571 H	0	-3.630	-7.618	1.564	H
HETATM 572 H	0	-3.017	-6.464	0.422	H
HETATM 573 N	0	-11.922	-8.193	-2.849	N
HETATM 574 C	0	-12.676	-7.849	-4.057	C
HETATM 575 H	0	-13.121	-8.710	-4.510	H
HETATM 576 H	0	-12.006	-7.387	-4.751	H
HETATM 577 H	0	-13.442	-7.153	-3.784	H
HETATM 578 H	0	-12.362	-8.749	-2.134	H
HETATM 579 C	0	-13.956	-4.489	-2.711	C
HETATM 580 H	0	-13.882	-5.238	-1.950	H
HETATM 581 H	0	-14.021	-4.959	-3.670	H
HETATM 582 H	0	-14.831	-3.896	-2.544	H
HETATM 583 C	0	-12.728	-3.592	-2.726	C
HETATM 584 O	0	-12.755	-2.573	-3.402	O
HETATM 585 N	0	-11.634	-3.988	-2.063	N
HETATM 586 C	0	-10.302	-3.365	-2.216	C
HETATM 587 C	0	-9.909	-3.263	-3.694	C
HETATM 588 O	0	-9.530	-2.191	-4.144	O
HETATM 589 C	0	-9.228	-4.152	-1.459	C
HETATM 590 C	0	-7.801	-3.761	-1.810	C
HETATM 591 C	0	-7.260	-2.588	-1.265	C
HETATM 592 C	0	-7.028	-4.533	-2.702	C
HETATM 593 C	0	-5.923	-2.225	-1.520	C
HETATM 594 C	0	-5.705	-4.144	-3.002	C
HETATM 595 C	0	-5.136	-3.005	-2.386	C
HETATM 596 O	0	-3.846	-2.670	-2.639	O
HETATM 597 H	0	-11.730	-4.797	-1.461	H
HETATM 598 H	0	-10.343	-2.354	-1.813	H

HETATM	599	H	0	-9.385	-4.036	-0.386	H
HETATM	600	H	0	-9.345	-5.196	-1.703	H
HETATM	601	H	0	-7.897	-1.977	-0.646	H
HETATM	602	H	0	-7.461	-5.405	-3.177	H
HETATM	603	H	0	-5.473	-1.359	-1.050	H
HETATM	604	H	0	-5.097	-4.717	-3.685	H
HETATM	605	H	0	-3.526	-1.911	-2.087	H
HETATM	606	N	0	-9.954	-4.363	-4.453	N
HETATM	607	C	0	-9.606	-4.371	-5.866	C
HETATM	608	H	0	-9.736	-5.348	-6.283	H
HETATM	609	H	0	-8.586	-4.068	-5.977	H
HETATM	610	H	0	-10.242	-3.678	-6.376	H
HETATM	611	H	0	-10.222	-5.232	-4.005	H
HETATM	612	C	0	-12.023	0.400	-4.874	C
HETATM	613	H	0	-11.878	-0.040	-3.909	H
HETATM	614	H	0	-12.349	-0.350	-5.563	H
HETATM	615	H	0	-12.764	1.169	-4.807	H
HETATM	616	C	0	-10.748	1.011	-5.400	C
HETATM	617	O	0	-10.794	2.082	-5.989	O
HETATM	618	N	0	-9.629	0.310	-5.221	N
HETATM	619	C	0	-8.277	0.685	-5.656	C
HETATM	620	C	0	-8.256	0.928	-7.184	C
HETATM	621	O	0	-7.617	1.864	-7.664	O
HETATM	622	C	0	-7.265	-0.375	-5.211	C
HETATM	623	C	0	-5.800	-0.022	-5.383	C
HETATM	624	C	0	-4.849	-1.047	-5.235	C
HETATM	625	C	0	-5.372	1.289	-5.684	C
HETATM	626	C	0	-3.480	-0.786	-5.419	C
HETATM	627	C	0	-4.012	1.547	-5.901	C
HETATM	628	C	0	-3.069	0.512	-5.775	C
HETATM	629	O	0	-1.770	0.797	-6.002	O
HETATM	630	H	0	-9.733	-0.571	-4.734	H
HETATM	631	H	0	-8.045	1.632	-5.169	H
HETATM	632	H	0	-7.427	-0.594	-4.158	H
HETATM	633	H	0	-7.463	-1.293	-5.766	H
HETATM	634	H	0	-5.173	-2.041	-4.967	H
HETATM	635	H	0	-6.062	2.110	-5.806	H
HETATM	636	H	0	-2.749	-1.570	-5.284	H
HETATM	637	H	0	-3.675	2.530	-6.177	H
HETATM	638	H	0	-1.143	0.111	-5.675	H
HETATM	639	N	0	-8.983	0.096	-7.946	N
HETATM	640	C	0	-9.274	0.297	-9.364	C
HETATM	641	H	0	-9.579	-0.625	-9.813	H
HETATM	642	H	0	-8.397	0.661	-9.857	H
HETATM	643	H	0	-10.061	1.016	-9.458	H
HETATM	644	H	0	-9.493	-0.609	-7.436	H
HETATM	645	C	0	-9.701	5.735	-6.143	C
HETATM	646	H	0	-10.416	6.407	-5.718	H
HETATM	647	H	0	-10.213	4.940	-6.644	H

HETATM 648 H	0	-9.088	6.262	-6.845	H
HETATM 649 C	0	-8.880	5.171	-4.997	C
HETATM 650 O	0	-9.189	4.105	-4.478	O
HETATM 651 N	0	-7.890	5.926	-4.508	N
HETATM 652 C	0	-7.157	5.583	-3.275	C
HETATM 653 C	0	-8.117	5.332	-2.088	C
HETATM 654 O	0	-7.879	4.437	-1.289	O
HETATM 655 C	0	-6.109	6.647	-2.982	C
HETATM 656 H	0	-7.726	6.819	-4.945	H
HETATM 657 H	0	-6.639	4.640	-3.450	H
HETATM 658 H	0	-5.544	6.322	-2.111	H
HETATM 659 H	0	-6.586	7.604	-2.772	H
HETATM 660 H	0	-5.435	6.753	-3.833	H
HETATM 661 N	0	-9.200	6.111	-1.993	N
HETATM 662 C	0	-10.193	6.136	-0.913	C
HETATM 663 C	0	-11.199	4.984	-0.926	C
HETATM 664 O	0	-11.454	4.402	0.125	O
HETATM 665 C	0	-10.932	7.489	-0.942	C
HETATM 666 C	0	-10.060	8.699	-0.538	C
HETATM 667 C	0	-8.949	9.057	-1.528	C
HETATM 668 O	0	-9.033	8.827	-2.726	O
HETATM 669 N	0	-7.844	9.604	-1.076	N
HETATM 670 H	0	-9.250	6.856	-2.679	H
HETATM 671 H	0	-9.665	6.094	0.032	H
HETATM 672 H	0	-11.359	7.658	-1.932	H
HETATM 673 H	0	-11.758	7.437	-0.232	H
HETATM 674 H	0	-9.619	8.504	0.440	H
HETATM 675 H	0	-10.708	9.570	-0.445	H
HETATM 676 H	0	-7.184	9.862	-1.785	H
HETATM 677 H	0	-7.696	9.825	-0.094	H
HETATM 678 N	0	-11.792	4.666	-2.083	N
HETATM 679 C	0	-12.830	3.630	-2.212	C
HETATM 680 H	0	-13.064	3.478	-3.266	H
HETATM 681 C	0	-12.415	2.287	-1.617	C
HETATM 682 O	0	-13.216	1.597	-0.994	O
HETATM 683 H	0	-11.492	5.156	-2.913	H
HETATM 684 H	0	-13.735	3.961	-1.701	H
HETATM 685 N	0	-11.141	1.936	-1.802	N
HETATM 686 C	0	-10.526	0.714	-1.282	C
HETATM 687 C	0	-10.437	0.687	0.244	C
HETATM 688 O	0	-10.481	-0.411	0.784	O
HETATM 689 C	0	-9.141	0.515	-1.922	C
HETATM 690 C	0	-7.970	1.010	-1.080	C
HETATM 691 C	0	-6.705	1.102	-1.898	C
HETATM 692 N	0	-5.634	1.618	-1.068	N
HETATM 693 C	0	-4.771	2.499	-1.512	C
HETATM 694 N	0	-4.517	2.610	-2.842	N
HETATM 695 N	0	-4.114	3.294	-0.657	N
HETATM 696 H	0	-10.581	2.572	-2.354	H

HETATM 697 H	0	-11.196	-0.110	-1.556	H
HETATM 698 H	0	-8.983	-0.542	-2.154	H
HETATM 699 H	0	-9.098	1.046	-2.877	H
HETATM 700 H	0	-7.803	0.369	-0.207	H
HETATM 701 H	0	-8.170	2.014	-0.697	H
HETATM 702 H	0	-6.889	1.802	-2.724	H
HETATM 703 H	0	-6.430	0.141	-2.339	H
HETATM 704 H	0	-5.659	1.510	-0.025	H
HETATM 705 H	0	-4.355	3.536	-3.201	H
HETATM 706 H	0	-5.006	1.991	-3.477	H
HETATM 707 H	0	-4.345	3.082	0.331	H
HETATM 708 H	0	-3.143	3.501	-0.852	H
HETATM 709 N	0	-10.147	1.822	0.907	N
HETATM 710 C	0	-9.445	1.881	2.208	C
HETATM 711 C	0	-10.142	0.980	3.226	C
HETATM 712 O	0	-9.553	0.058	3.776	O
HETATM 713 C	0	-9.406	3.319	2.775	C
HETATM 714 C	0	-8.658	4.380	1.959	C
HETATM 715 C	0	-8.905	5.762	2.570	C
HETATM 716 C	0	-7.155	4.172	1.894	C
HETATM 717 H	0	-10.233	2.679	0.378	H
HETATM 718 H	0	-8.424	1.514	2.089	H
HETATM 719 H	0	-10.434	3.664	2.893	H
HETATM 720 H	0	-8.956	3.280	3.767	H
HETATM 721 H	0	-9.043	4.357	0.950	H
HETATM 722 H	0	-8.530	5.790	3.593	H
HETATM 723 H	0	-9.973	5.979	2.569	H
HETATM 724 H	0	-8.391	6.523	1.984	H
HETATM 725 H	0	-6.738	4.099	2.897	H
HETATM 726 H	0	-6.686	4.987	1.344	H
HETATM 727 H	0	-6.970	3.251	1.347	H
HETATM 728 N	0	-11.427	1.242	3.468	N
HETATM 729 C	0	-12.257	0.427	4.331	C
HETATM 730 H	0	-11.930	0.512	5.346	H
HETATM 731 H	0	-12.174	-0.592	4.014	H
HETATM 732 H	0	-13.277	0.741	4.257	H
HETATM 733 H	0	-11.840	1.985	2.924	H
HETATM 734 C	0	-12.030	-2.923	2.417	C
HETATM 735 H	0	-12.645	-3.772	2.205	H
HETATM 736 H	0	-12.114	-2.213	1.621	H
HETATM 737 H	0	-12.349	-2.471	3.333	H
HETATM 738 C	0	-10.584	-3.390	2.557	C
HETATM 739 O	0	-10.413	-4.534	2.963	O
HETATM 740 N	0	-9.546	-2.568	2.306	N
HETATM 741 C	0	-8.150	-2.934	2.653	C
HETATM 742 C	0	-8.041	-3.158	4.161	C
HETATM 743 O	0	-7.667	-4.252	4.570	O
HETATM 744 C	0	-7.034	-1.954	2.233	C
HETATM 745 C	0	-5.623	-2.551	2.506	C

HETATM 746 C	0	-5.264	-3.762	1.639	C
HETATM 747 C	0	-4.495	-1.561	2.262	C
HETATM 748 H	0	-9.752	-1.627	1.981	H
HETATM 749 H	0	-7.964	-3.883	2.160	H
HETATM 750 H	0	-7.111	-1.682	1.194	H
HETATM 751 H	0	-7.151	-1.039	2.805	H
HETATM 752 H	0	-5.552	-2.858	3.548	H
HETATM 753 H	0	-5.135	-3.454	0.606	H
HETATM 754 H	0	-6.026	-4.527	1.694	H
HETATM 755 H	0	-4.326	-4.193	1.989	H
HETATM 756 H	0	-4.576	-1.130	1.263	H
HETATM 757 H	0	-3.534	-2.060	2.375	H
HETATM 758 H	0	-4.544	-0.765	2.994	H
HETATM 759 N	0	-8.402	-2.161	4.975	N
HETATM 760 C	0	-8.456	-2.238	6.436	C
HETATM 761 C	0	-9.230	-3.469	6.917	C
HETATM 762 O	0	-8.829	-4.101	7.886	O
HETATM 763 C	0	-9.065	-0.964	7.056	C
HETATM 764 C	0	-8.135	0.234	7.132	C
HETATM 765 C	0	-8.432	1.415	6.426	C
HETATM 766 C	0	-6.963	0.165	7.911	C
HETATM 767 C	0	-7.540	2.503	6.451	C
HETATM 768 C	0	-6.062	1.248	7.933	C
HETATM 769 C	0	-6.346	2.416	7.193	C
HETATM 770 O	0	-5.454	3.441	7.162	O
HETATM 771 H	0	-8.646	-1.283	4.525	H
HETATM 772 H	0	-7.436	-2.348	6.807	H
HETATM 773 H	0	-9.971	-0.699	6.510	H
HETATM 774 H	0	-9.365	-1.192	8.080	H
HETATM 775 H	0	-9.339	1.483	5.844	H
HETATM 776 H	0	-6.735	-0.733	8.471	H
HETATM 777 H	0	-7.747	3.395	5.881	H
HETATM 778 H	0	-5.149	1.178	8.506	H
HETATM 779 H	0	-4.561	3.075	7.294	H
HETATM 780 N	0	-10.315	-3.834	6.230	N
HETATM 781 C	0	-11.050	-5.074	6.479	C
HETATM 782 H	0	-11.976	-5.067	5.905	H
HETATM 783 C	0	-10.265	-6.341	6.104	C
HETATM 784 O	0	-10.252	-7.297	6.868	O
HETATM 785 H	0	-10.548	-3.274	5.425	H
HETATM 786 H	0	-11.305	-5.135	7.538	H
HETATM 787 N	0	-9.617	-6.364	4.934	N
HETATM 788 C	0	-8.719	-7.445	4.491	C
HETATM 789 C	0	-7.458	-7.614	5.349	C
HETATM 790 O	0	-6.903	-8.707	5.404	O
HETATM 791 C	0	-8.366	-7.314	3.017	C
HETATM 792 O	0	-7.438	-6.285	2.777	O
HETATM 793 H	0	-9.720	-5.551	4.335	H
HETATM 794 H	0	-9.273	-8.378	4.599	H

HETATM 795 H	0	-9.274	-7.132	2.440	H
HETATM 796 H	0	-7.923	-8.255	2.695	H
HETATM 797 H	0	-7.563	-5.581	3.441	H
HETATM 798 N	0	-7.003	-6.537	5.991	N
HETATM 799 C	0	-5.978	-6.523	7.025	C
HETATM 800 C	0	-6.530	-6.998	8.386	C
HETATM 801 O	0	-5.852	-7.743	9.091	O
HETATM 802 C	0	-5.393	-5.107	7.111	C
HETATM 803 H	0	-7.471	-5.662	5.799	H
HETATM 804 H	0	-5.180	-7.212	6.741	H
HETATM 805 H	0	-4.588	-5.091	7.847	H
HETATM 806 H	0	-6.163	-4.398	7.414	H
HETATM 807 H	0	-4.994	-4.810	6.140	H
HETATM 808 N	0	-7.744	-6.561	8.757	N
HETATM 809 C	0	-8.478	-7.011	9.933	C
HETATM 810 H	0	-8.189	-6.430	10.783	H
HETATM 811 H	0	-8.209	-8.034	10.091	H
HETATM 812 H	0	-9.537	-6.938	9.795	H
HETATM 813 H	0	-8.198	-5.884	8.158	H
HETATM 814 N	0	3.033	-3.816	-1.687	N
HETATM 815 C	0	2.152	-2.808	-1.039	C
HETATM 816 C	0	2.456	-1.386	-1.606	C
HETATM 817 O	0	3.198	-1.332	-2.615	O
HETATM 818 O	0	2.005	-0.355	-1.068	O
HETATM 819 C	0	2.297	-2.994	0.487	C
HETATM 820 C	0	1.586	-2.005	1.424	C
HETATM 821 C	0	0.125	-1.759	1.116	C
HETATM 822 O	0	-0.626	-2.703	0.930	O
HETATM 823 N	0	-0.264	-0.459	1.094	N
HETATM 824 C	0	-1.611	-0.070	0.738	C
HETATM 825 C	0	-1.858	-0.263	-0.759	C
HETATM 826 O	0	-2.920	-0.652	-1.212	O
HETATM 827 C	0	-1.969	1.333	1.234	C
HETATM 828 S	0	-0.997	2.669	0.429	S
HETATM 829 N	0	-0.785	0.078	-1.518	N
HETATM 830 C	0	-0.850	0.155	-2.973	C
HETATM 831 C	0	-0.233	-1.012	-3.751	C
HETATM 832 O	0	0.110	-2.079	-3.195	O
HETATM 833 O	0	-0.121	-0.883	-4.986	O
HETATM 834 H	0	3.895	-3.938	-1.160	H
HETATM 835 H	0	3.256	-3.503	-2.622	H
HETATM 836 H	0	2.661	-4.769	-1.672	H
HETATM 837 H	0	1.113	-3.001	-1.304	H
HETATM 838 H	0	1.943	-3.997	0.729	H
HETATM 839 H	0	3.351	-2.945	0.742	H
HETATM 840 H	0	2.114	-1.054	1.407	H
HETATM 841 H	0	1.635	-2.399	2.436	H
HETATM 842 H	0	0.431	0.274	1.201	H
HETATM 843 H	0	-2.292	-0.752	1.239	H

HETATM	844	H	0	-3.042	1.489	1.101	H
HETATM	845	H	0	-1.778	1.350	2.303	H
HETATM	846	H	0	0.161	0.152	-1.140	H
HETATM	847	H	0	-1.890	0.241	-3.279	H
HETATM	848	H	0	-0.331	1.055	-3.291	H
HETATM	849	C	0	-5.220	1.746	2.725	C
HETATM	850	O	0	-6.219	1.185	3.158	O
HETATM	851	C	0	-4.179	2.240	3.747	C
HETATM	852	C	0	-3.440	3.511	3.335	C
HETATM	853	C	0	-1.952	3.553	3.680	C
HETATM	854	C	0	-1.145	4.503	2.792	C
HETATM	855	O	0	-4.899	1.865	1.478	O
HETATM	856	C	0	-1.338	4.312	1.258	C
HETATM	857	C	0	-0.431	5.269	0.527	C
HETATM	858	O	0	-1.574	5.825	3.018	O
HETATM	859	C	0	-0.624	6.588	0.416	C
HETATM	860	C	0	0.391	7.448	-0.180	C
HETATM	861	C	0	0.280	8.755	-0.457	C
HETATM	862	C	0	1.344	9.448	-0.990	C
HETATM	863	C	0	1.396	10.752	-1.367	C
HETATM	864	C	0	0.243	11.737	-1.334	C
HETATM	865	C	0	-0.079	12.181	-2.755	C
HETATM	866	C	0	-1.321	12.177	-3.308	C
HETATM	867	C	0	-2.565	11.735	-2.562	C
HETATM	868	C	0	-2.645	10.205	-2.514	C
HETATM	869	C	0	-3.547	9.734	-1.368	C
HETATM	870	C	0	-3.471	8.211	-1.259	C
HETATM	871	C	0	-4.311	7.709	-0.080	C
HETATM	872	H	0	-4.687	2.352	4.707	H
HETATM	873	H	0	-3.468	1.410	3.872	H
HETATM	874	H	0	-3.923	4.389	3.769	H
HETATM	875	H	0	-3.562	3.607	2.256	H
HETATM	876	H	0	-1.512	2.555	3.641	H
HETATM	877	H	0	-1.810	3.897	4.713	H
HETATM	878	H	0	-0.069	4.392	3.024	H
HETATM	879	H	0	-2.374	4.590	1.056	H
HETATM	880	H	0	0.506	4.869	0.155	H
HETATM	881	H	0	-1.515	7.048	0.834	H
HETATM	882	H	0	1.333	6.941	-0.396	H
HETATM	883	H	0	-0.658	9.259	-0.243	H
HETATM	884	H	0	2.261	8.884	-1.113	H
HETATM	885	H	0	2.341	11.121	-1.765	H
HETATM	886	H	0	0.557	12.613	-0.765	H
HETATM	887	H	0	-0.620	11.321	-0.825	H
HETATM	888	H	0	0.749	12.542	-3.366	H
HETATM	889	H	0	-1.432	12.532	-4.333	H
HETATM	890	H	0	-2.553	12.158	-1.556	H
HETATM	891	H	0	-3.449	12.126	-3.068	H
HETATM	892	H	0	-3.023	9.835	-3.468	H

HETATM 893 H	0	-1.644	9.798	-2.368	H
HETATM 894 H	0	-3.208	10.176	-0.428	H
HETATM 895 H	0	-4.576	10.046	-1.553	H
HETATM 896 H	0	-2.437	7.907	-1.114	H
HETATM 897 H	0	-3.815	7.767	-2.189	H
HETATM 898 H	0	-5.359	7.978	-0.220	H
HETATM 899 H	0	-4.226	6.624	-0.003	H
HETATM 900 H	0	-3.952	8.159	0.845	H
HETATM 901 O	0	6.683	3.419	10.654	O
HETATM 902 H	0	7.352	3.753	11.257	H
HETATM 903 H	0	6.470	2.549	11.004	H
HETATM 904 O	0	-4.655	11.219	2.335	O
HETATM 905 H	0	-4.245	10.464	2.798	H
HETATM 906 H	0	-4.126	11.970	2.666	H
HETATM 907 O	0	-4.756	6.825	3.149	O
HETATM 908 H	0	-4.685	6.080	2.543	H
HETATM 909 H	0	-4.972	6.384	4.000	H
HETATM 910 O	0	-7.126	10.488	1.609	O
HETATM 911 H	0	-7.615	11.260	1.909	H
HETATM 912 H	0	-6.193	10.756	1.770	H
HETATM 913 O	0	-3.323	9.130	3.469	O
HETATM 914 H	0	-3.745	8.258	3.327	H
HETATM 915 H	0	-2.538	9.103	2.904	H
HETATM 916 O	0	-0.220	12.116	4.307	O
HETATM 917 H	0	0.758	12.176	4.238	H
HETATM 918 H	0	-0.351	11.948	5.257	H
HETATM 919 O	0	-6.947	8.511	3.574	O
HETATM 920 H	0	-6.179	7.992	3.278	H
HETATM 921 H	0	-7.073	9.151	2.853	H
HETATM 922 O	0	-1.203	10.759	2.158	O
HETATM 923 H	0	-1.968	11.314	1.967	H
HETATM 924 H	0	-0.836	11.192	2.956	H
HETATM 925 O	0	-3.605	-1.469	5.920	O
HETATM 926 H	0	-4.467	-1.072	5.654	H
HETATM 927 H	0	-3.380	-2.007	5.156	H
HETATM 928 O	0	-4.633	7.960	6.889	O
HETATM 929 H	0	-5.601	8.034	6.847	H
HETATM 930 H	0	-4.479	7.102	6.469	H
HETATM 931 O	0	-5.872	-0.335	5.159	O
HETATM 932 H	0	-6.514	0.057	5.761	H
HETATM 933 H	0	-6.031	0.189	4.327	H
HETATM 934 O	0	-2.614	-0.010	7.931	O
HETATM 935 H	0	-2.982	-0.553	7.196	H
HETATM 936 H	0	-2.267	-0.677	8.527	H
HETATM 937 O	0	0.380	9.826	8.263	O
HETATM 938 H	0	1.023	10.324	8.777	H
HETATM 939 H	0	-0.139	10.528	7.819	H
HETATM 940 O	0	6.284	-1.985	10.108	O
HETATM 941 H	0	6.120	-2.579	9.359	H

HETATM 942 H	0	7.229	-2.041	10.242	H
HETATM 943 O	0	-3.741	12.774	6.134	O
HETATM 944 H	0	-3.731	11.796	6.120	H
HETATM 945 H	0	-4.524	12.985	6.649	H
HETATM 946 O	0	-1.162	11.564	6.865	O
HETATM 947 H	0	-1.661	12.384	6.973	H
HETATM 948 H	0	-1.859	10.938	6.577	H
HETATM 949 O	0	-5.485	5.673	5.481	O
HETATM 950 H	0	-5.556	4.848	5.995	H
HETATM 951 H	0	-6.275	6.175	5.760	H
HETATM 952 O	0	-2.897	2.520	7.125	O
HETATM 953 H	0	-2.762	2.305	6.194	H
HETATM 954 H	0	-2.746	1.647	7.556	H
HETATM 955 O	0	-2.809	12.831	3.548	O
HETATM 956 H	0	-3.200	13.012	4.423	H
HETATM 957 H	0	-1.857	12.836	3.747	H
HETATM 958 O	0	1.540	10.646	1.779	O
HETATM 959 H	0	1.729	10.287	0.903	H
HETATM 960 H	0	0.568	10.620	1.813	H
HETATM 961 O	0	-7.316	7.628	6.078	O
HETATM 962 H	0	-7.246	8.007	5.173	H
HETATM 963 H	0	-8.211	7.861	6.341	H
HETATM 964 O	0	2.472	11.844	4.019	O
HETATM 965 H	0	3.402	11.604	4.162	H
HETATM 966 H	0	2.279	11.447	3.147	H
HETATM 967 O	0	-2.563	5.088	8.012	O
HETATM 968 H	0	-3.335	5.163	8.583	H
HETATM 969 H	0	-2.559	4.137	7.779	H
HETATM 970 O	0	-3.285	10.103	6.009	O
HETATM 971 H	0	-3.267	9.787	5.082	H
HETATM 972 H	0	-3.739	9.359	6.461	H

RC (Head-to-tail orientation)

E = -2163.36945210 hartrees

HETATM 1 C	0	-15.068	-7.338	-7.468	C
HETATM 2 H	0	-15.596	-8.245	-7.259	H
HETATM 3 H	0	-14.281	-7.536	-8.166	H
HETATM 4 H	0	-15.743	-6.621	-7.886	H
HETATM 5 C	0	-14.435	-6.948	-6.133	C
HETATM 6 O	0	-13.222	-7.035	-5.976	O
HETATM 7 N	0	-15.248	-6.641	-5.119	N
HETATM 8 C	0	-14.839	-6.275	-3.742	C
HETATM 9 C	0	-14.001	-7.305	-3.004	C
HETATM 10 O	0	-12.933	-6.992	-2.481	O
HETATM 11 C	0	-16.117	-5.932	-2.965	C
HETATM 12 C	0	-15.879	-5.509	-1.507	C
HETATM 13 C	0	-15.042	-4.236	-1.401	C

HETATM	14	C	0	-17.235	-5.272	-0.864	C
HETATM	15	H	0	-16.230	-6.588	-5.345	H
HETATM	16	H	0	-14.230	-5.372	-3.812	H
HETATM	17	H	0	-16.628	-5.120	-3.482	H
HETATM	18	H	0	-16.778	-6.800	-2.969	H
HETATM	19	H	0	-15.382	-6.309	-0.958	H
HETATM	20	H	0	-15.036	-3.892	-0.367	H
HETATM	21	H	0	-15.466	-3.458	-2.033	H
HETATM	22	H	0	-14.015	-4.435	-1.705	H
HETATM	23	H	0	-17.084	-4.952	0.159	H
HETATM	24	H	0	-17.821	-6.191	-0.859	H
HETATM	25	H	0	-17.787	-4.503	-1.404	H
HETATM	26	N	0	-14.494	-8.540	-2.959	N
HETATM	27	C	0	-13.727	-9.653	-2.420	C
HETATM	28	H	0	-14.255	-10.589	-2.604	H
HETATM	29	C	0	-12.318	-9.751	-3.047	C
HETATM	30	O	0	-11.359	-10.098	-2.362	O
HETATM	31	H	0	-15.397	-8.704	-3.378	H
HETATM	32	H	0	-13.610	-9.525	-1.343	H
HETATM	33	N	0	-12.179	-9.397	-4.331	N
HETATM	34	C	0	-10.911	-9.302	-5.062	C
HETATM	35	C	0	-10.050	-8.118	-4.689	C
HETATM	36	O	0	-8.852	-8.289	-4.532	O
HETATM	37	H	0	-12.999	-9.058	-4.810	H
HETATM	38	H	0	-10.334	-10.212	-4.895	H
HETATM	39	H	0	-11.123	-9.233	-6.129	H
HETATM	40	N	0	-10.620	-6.933	-4.493	N
HETATM	41	C	0	-9.886	-5.812	-3.887	C
HETATM	42	C	0	-9.219	-6.205	-2.595	C
HETATM	43	O	0	-8.055	-5.895	-2.396	O
HETATM	44	C	0	-10.800	-4.590	-3.654	C
HETATM	45	C	0	-10.115	-3.497	-2.821	C
HETATM	46	C	0	-11.234	-3.996	-4.996	C
HETATM	47	H	0	-11.609	-6.843	-4.701	H
HETATM	48	H	0	-9.091	-5.512	-4.569	H
HETATM	49	H	0	-11.693	-4.899	-3.116	H
HETATM	50	H	0	-9.159	-3.226	-3.262	H
HETATM	51	H	0	-9.950	-3.841	-1.801	H
HETATM	52	H	0	-10.753	-2.621	-2.762	H
HETATM	53	H	0	-11.749	-4.747	-5.595	H
HETATM	54	H	0	-10.363	-3.637	-5.541	H
HETATM	55	H	0	-11.922	-3.169	-4.825	H
HETATM	56	N	0	-9.942	-6.887	-1.720	N
HETATM	57	C	0	-9.366	-7.408	-0.496	C
HETATM	58	C	0	-8.285	-8.486	-0.715	C
HETATM	59	O	0	-7.341	-8.535	0.073	O
HETATM	60	C	0	-10.512	-7.930	0.391	C
HETATM	61	C	0	-11.203	-6.797	1.174	C
HETATM	62	C	0	-12.611	-7.214	1.596	C

HETATM	63	C	0	-10.388	-6.440	2.421	C
HETATM	64	H	0	-10.915	-7.066	-1.946	H
HETATM	65	H	0	-8.868	-6.590	0.026	H
HETATM	66	H	0	-11.243	-8.441	-0.237	H
HETATM	67	H	0	-10.126	-8.663	1.100	H
HETATM	68	H	0	-11.294	-5.912	0.543	H
HETATM	69	H	0	-12.570	-8.116	2.201	H
HETATM	70	H	0	-13.218	-7.398	0.709	H
HETATM	71	H	0	-13.074	-6.418	2.178	H
HETATM	72	H	0	-10.927	-5.718	3.031	H
HETATM	73	H	0	-9.430	-6.008	2.135	H
HETATM	74	H	0	-10.212	-7.329	3.025	H
HETATM	75	N	0	-8.388	-9.337	-1.746	N
HETATM	76	C	0	-7.291	-10.213	-2.199	C
HETATM	77	C	0	-6.071	-9.358	-2.662	C
HETATM	78	O	0	-4.947	-9.580	-2.217	O
HETATM	79	C	0	-7.789	-11.191	-3.278	C
HETATM	80	C	0	-6.723	-12.208	-3.728	C
HETATM	81	C	0	-6.317	-13.164	-2.602	C
HETATM	82	C	0	-7.271	-13.043	-4.885	C
HETATM	83	H	0	-9.214	-9.267	-2.325	H
HETATM	84	H	0	-6.960	-10.792	-1.337	H
HETATM	85	H	0	-8.657	-11.730	-2.897	H
HETATM	86	H	0	-8.098	-10.626	-4.154	H
HETATM	87	H	0	-5.843	-11.676	-4.080	H
HETATM	88	H	0	-7.196	-13.667	-2.202	H
HETATM	89	H	0	-5.806	-12.613	-1.813	H
HETATM	90	H	0	-5.624	-13.909	-2.991	H
HETATM	91	H	0	-8.159	-13.591	-4.572	H
HETATM	92	H	0	-6.510	-13.746	-5.223	H
HETATM	93	H	0	-7.522	-12.387	-5.719	H
HETATM	94	N	0	-6.276	-8.346	-3.515	N
HETATM	95	C	0	-5.242	-7.438	-4.042	C
HETATM	96	C	0	-4.572	-6.556	-2.957	C
HETATM	97	O	0	-3.344	-6.471	-2.905	O
HETATM	98	C	0	-5.763	-6.624	-5.228	C
HETATM	99	C	0	-6.173	-7.469	-6.451	C
HETATM	100	C	0	-5.108	-8.445	-6.939	C
HETATM	101	N	0	-3.931	-7.998	-7.318	N
HETATM	102	O	0	-5.320	-9.643	-6.989	O
HETATM	103	H	0	-7.224	-8.234	-3.853	H
HETATM	104	H	0	-4.437	-8.070	-4.417	H
HETATM	105	H	0	-6.619	-6.038	-4.898	H
HETATM	106	H	0	-4.971	-5.943	-5.539	H
HETATM	107	H	0	-6.428	-6.806	-7.276	H
HETATM	108	H	0	-7.064	-8.042	-6.214	H
HETATM	109	H	0	-3.322	-8.710	-7.684	H
HETATM	110	H	0	-3.652	-7.025	-7.276	H
HETATM	111	N	0	-5.350	-5.936	-2.063	N

HETATM 112 C	0	-4.911	-5.252	-0.838	C
HETATM 113 C	0	-4.114	-6.195	0.053	C
HETATM 114 O	0	-3.037	-5.822	0.519	O
HETATM 115 C	0	-6.124	-4.655	-0.125	C
HETATM 116 H	0	-6.346	-6.025	-2.209	H
HETATM 117 H	0	-4.248	-4.435	-1.127	H
HETATM 118 H	0	-5.773	-4.077	0.727	H
HETATM 119 H	0	-6.792	-5.445	0.219	H
HETATM 120 H	0	-6.664	-3.994	-0.806	H
HETATM 121 N	0	-4.610	-7.423	0.247	N
HETATM 122 C	0	-3.834	-8.468	0.892	C
HETATM 123 C	0	-2.432	-8.644	0.271	C
HETATM 124 O	0	-1.449	-8.667	1.010	O
HETATM 125 C	0	-4.595	-9.783	1.066	C
HETATM 126 C	0	-3.742	-10.891	1.649	C
HETATM 127 C	0	-3.465	-10.914	3.031	C
HETATM 128 C	0	-3.195	-11.875	0.804	C
HETATM 129 C	0	-2.658	-11.933	3.574	C
HETATM 130 C	0	-2.378	-12.888	1.341	C
HETATM 131 C	0	-2.111	-12.920	2.726	C
HETATM 132 O	0	-1.311	-13.892	3.235	O
HETATM 133 H	0	-5.512	-7.666	-0.146	H
HETATM 134 H	0	-3.639	-8.115	1.904	H
HETATM 135 H	0	-5.425	-9.596	1.743	H
HETATM 136 H	0	-5.009	-10.118	0.121	H
HETATM 137 H	0	-3.895	-10.160	3.679	H
HETATM 138 H	0	-3.398	-11.848	-0.261	H
HETATM 139 H	0	-2.463	-11.962	4.636	H
HETATM 140 H	0	-1.952	-13.650	0.706	H
HETATM 141 H	0	-1.362	-13.927	4.192	H
HETATM 142 N	0	-2.298	-8.710	-1.057	N
HETATM 143 C	0	-0.988	-8.773	-1.719	C
HETATM 144 C	0	-0.067	-7.585	-1.436	C
HETATM 145 O	0	1.071	-7.795	-1.032	O
HETATM 146 C	0	-1.143	-9.069	-3.217	C
HETATM 147 C	0	-1.862	-10.360	-3.584	C
HETATM 148 C	0	-2.648	-10.399	-4.751	C
HETATM 149 C	0	-1.706	-11.537	-2.821	C
HETATM 150 C	0	-3.280	-11.590	-5.146	C
HETATM 151 C	0	-2.345	-12.728	-3.212	C
HETATM 152 C	0	-3.130	-12.755	-4.377	C
HETATM 153 H	0	-3.142	-8.742	-1.621	H
HETATM 154 H	0	-0.462	-9.623	-1.287	H
HETATM 155 H	0	-1.648	-8.230	-3.694	H
HETATM 156 H	0	-0.146	-9.137	-3.645	H
HETATM 157 H	0	-2.762	-9.516	-5.360	H
HETATM 158 H	0	-1.091	-11.551	-1.936	H
HETATM 159 H	0	-3.882	-11.607	-6.045	H
HETATM 160 H	0	-2.223	-13.628	-2.627	H

HETATM 161 H	0	-3.615	-13.670	-4.688	H
HETATM 162 N	0	-0.507	-6.343	-1.616	N
HETATM 163 C	0	0.291	-5.142	-1.288	C
HETATM 164 C	0	0.678	-5.114	0.197	C
HETATM 165 O	0	1.833	-4.847	0.505	O
HETATM 166 C	0	-0.539	-3.911	-1.662	C
HETATM 167 O	0	-0.875	-3.995	-3.033	O
HETATM 168 H	0	-1.442	-6.219	-1.996	H
HETATM 169 H	0	1.206	-5.132	-1.875	H
HETATM 170 H	0	0.033	-3.003	-1.479	H
HETATM 171 H	0	-1.453	-3.887	-1.065	H
HETATM 172 H	0	-1.646	-3.402	-3.200	H
HETATM 173 N	0	-0.230	-5.442	1.125	N
HETATM 174 C	0	0.077	-5.653	2.551	C
HETATM 175 C	0	1.172	-6.690	2.776	C
HETATM 176 O	0	2.095	-6.472	3.561	O
HETATM 177 C	0	-1.195	-6.073	3.304	C
HETATM 178 C	0	-2.197	-4.938	3.559	C
HETATM 179 C	0	-3.514	-5.554	4.034	C
HETATM 180 C	0	-1.675	-3.979	4.629	C
HETATM 181 H	0	-1.172	-5.652	0.806	H
HETATM 182 H	0	0.448	-4.722	2.972	H
HETATM 183 H	0	-1.690	-6.862	2.743	H
HETATM 184 H	0	-0.906	-6.495	4.265	H
HETATM 185 H	0	-2.379	-4.379	2.642	H
HETATM 186 H	0	-3.354	-6.145	4.935	H
HETATM 187 H	0	-3.927	-6.188	3.252	H
HETATM 188 H	0	-4.233	-4.772	4.255	H
HETATM 189 H	0	-2.431	-3.225	4.829	H
HETATM 190 H	0	-0.777	-3.472	4.279	H
HETATM 191 H	0	-1.467	-4.524	5.549	H
HETATM 192 N	0	1.078	-7.822	2.090	N
HETATM 193 C	0	2.138	-8.812	2.093	C
HETATM 194 C	0	3.450	-8.292	1.523	C
HETATM 195 O	0	4.475	-8.561	2.130	O
HETATM 196 C	0	1.705	-10.100	1.365	C
HETATM 197 C	0	0.671	-10.939	2.133	C
HETATM 198 C	0	1.236	-11.567	3.401	C
HETATM 199 N	0	1.979	-12.646	3.301	N
HETATM 200 O	0	1.023	-11.095	4.510	O
HETATM 201 H	0	0.266	-7.962	1.496	H
HETATM 202 H	0	2.346	-9.072	3.132	H
HETATM 203 H	0	1.293	-9.849	0.391	H
HETATM 204 H	0	2.586	-10.721	1.195	H
HETATM 205 H	0	0.317	-11.734	1.478	H
HETATM 206 H	0	-0.184	-10.323	2.403	H
HETATM 207 H	0	2.314	-13.050	4.157	H
HETATM 208 H	0	2.135	-13.080	2.407	H
HETATM 209 N	0	3.460	-7.549	0.414	N

HETATM 210 C	0	4.665	-6.871	-0.088	C
HETATM 211 C	0	5.220	-5.881	0.937	C
HETATM 212 O	0	6.426	-5.831	1.124	O
HETATM 213 C	0	4.443	-6.158	-1.433	C
HETATM 214 C	0	5.719	-5.467	-1.930	C
HETATM 215 C	0	4.066	-7.106	-2.568	C
HETATM 216 H	0	2.575	-7.423	-0.069	H
HETATM 217 H	0	5.425	-7.629	-0.254	H
HETATM 218 H	0	3.652	-5.422	-1.316	H
HETATM 219 H	0	6.532	-6.191	-1.960	H
HETATM 220 H	0	5.994	-4.643	-1.273	H
HETATM 221 H	0	5.574	-5.075	-2.935	H
HETATM 222 H	0	3.769	-6.512	-3.425	H
HETATM 223 H	0	3.251	-7.766	-2.280	H
HETATM 224 H	0	4.920	-7.700	-2.876	H
HETATM 225 N	0	4.375	-5.104	1.617	N
HETATM 226 C	0	4.750	-4.173	2.692	C
HETATM 227 C	0	5.485	-4.865	3.821	C
HETATM 228 O	0	6.635	-4.547	4.133	O
HETATM 229 C	0	3.501	-3.412	3.223	C
HETATM 230 C	0	3.083	-2.339	2.206	C
HETATM 231 C	0	3.739	-2.746	4.596	C
HETATM 232 C	0	1.624	-1.878	2.308	C
HETATM 233 H	0	3.394	-5.176	1.366	H
HETATM 234 H	0	5.432	-3.427	2.287	H
HETATM 235 H	0	2.677	-4.110	3.334	H
HETATM 236 H	0	3.743	-1.484	2.319	H
HETATM 237 H	0	3.222	-2.734	1.207	H
HETATM 238 H	0	3.822	-3.499	5.381	H
HETATM 239 H	0	2.903	-2.103	4.864	H
HETATM 240 H	0	4.656	-2.158	4.567	H
HETATM 241 H	0	1.456	-1.066	1.600	H
HETATM 242 H	0	1.397	-1.525	3.311	H
HETATM 243 H	0	0.955	-2.700	2.062	H
HETATM 244 N	0	4.798	-5.835	4.411	N
HETATM 245 C	0	5.376	-6.784	5.337	C
HETATM 246 C	0	6.679	-7.373	4.738	C
HETATM 247 O	0	7.696	-7.398	5.420	O
HETATM 248 C	0	4.335	-7.868	5.614	C
HETATM 249 O	0	4.799	-8.836	6.528	O
HETATM 250 H	0	3.851	-5.996	4.079	H
HETATM 251 H	0	5.622	-6.281	6.271	H
HETATM 252 H	0	4.070	-8.365	4.680	H
HETATM 253 H	0	3.437	-7.401	6.022	H
HETATM 254 H	0	4.070	-9.489	6.599	H
HETATM 255 N	0	6.711	-7.770	3.453	N
HETATM 256 C	0	7.870	-8.316	2.727	C
HETATM 257 C	0	9.080	-7.399	2.620	C
HETATM 258 O	0	10.206	-7.857	2.823	O

HETATM 259 C	0	7.501	-8.914	1.363	C
HETATM 260 H	0	5.835	-7.752	2.948	H
HETATM 261 H	0	8.207	-9.161	3.327	H
HETATM 262 H	0	8.352	-9.477	0.978	H
HETATM 263 H	0	7.270	-8.130	0.650	H
HETATM 264 H	0	6.660	-9.599	1.462	H
HETATM 265 N	0	8.866	-6.110	2.346	N
HETATM 266 C	0	9.901	-5.079	2.417	C
HETATM 267 C	0	10.637	-5.167	3.766	C
HETATM 268 O	0	11.854	-5.029	3.805	O
HETATM 269 C	0	9.317	-3.658	2.262	C
HETATM 270 C	0	8.396	-3.444	1.051	C
HETATM 271 C	0	8.562	-2.067	0.404	C
HETATM 272 N	0	9.762	-2.042	-0.448	N
HETATM 273 C	0	9.826	-2.166	-1.757	C
HETATM 274 N	0	8.768	-2.214	-2.488	N
HETATM 275 N	0	10.969	-2.244	-2.363	N
HETATM 276 H	0	7.903	-5.847	2.149	H
HETATM 277 H	0	10.632	-5.255	1.631	H
HETATM 278 H	0	8.756	-3.394	3.159	H
HETATM 279 H	0	10.154	-2.965	2.210	H
HETATM 280 H	0	7.368	-3.527	1.387	H
HETATM 281 H	0	8.577	-4.212	0.303	H
HETATM 282 H	0	8.641	-1.307	1.182	H
HETATM 283 H	0	7.669	-1.840	-0.179	H
HETATM 284 H	0	10.655	-2.082	0.023	H
HETATM 285 H	0	8.775	-2.253	-3.491	H
HETATM 286 H	0	7.835	-2.165	-2.079	H
HETATM 287 H	0	11.803	-1.944	-1.885	H
HETATM 288 H	0	10.983	-2.343	-3.371	H
HETATM 289 N	0	9.907	-5.410	4.864	N
HETATM 290 C	0	10.383	-5.433	6.269	C
HETATM 291 C	0	10.848	-6.817	6.773	C
HETATM 292 O	0	11.846	-6.862	7.492	O
HETATM 293 C	0	9.333	-4.799	7.188	C
HETATM 294 C	0	9.070	-3.306	6.884	C
HETATM 295 C	0	9.135	-2.423	8.126	C
HETATM 296 N	0	8.225	-2.870	9.196	N
HETATM 297 C	0	6.987	-2.468	9.395	C
HETATM 298 N	0	6.365	-1.611	8.578	N
HETATM 299 N	0	6.299	-2.889	10.493	N
HETATM 300 H	0	8.913	-5.530	4.697	H
HETATM 301 H	0	11.268	-4.789	6.305	H
HETATM 302 H	0	8.394	-5.366	7.177	H
HETATM 303 H	0	9.721	-4.883	8.207	H
HETATM 304 H	0	8.106	-3.178	6.374	H
HETATM 305 H	0	9.857	-2.924	6.222	H
HETATM 306 H	0	8.914	-1.378	7.903	H
HETATM 307 H	0	10.154	-2.405	8.518	H

HETATM 308 H	0	8.533	-3.661	9.759	H
HETATM 309 H	0	5.548	-1.152	8.976	H
HETATM 310 H	0	6.868	-1.045	7.890	H
HETATM 311 H	0	6.735	-3.607	11.066	H
HETATM 312 H	0	5.298	-3.019	10.386	H
HETATM 313 N	0	10.214	-7.927	6.380	N
HETATM 314 C	0	10.712	-9.311	6.513	C
HETATM 315 C	0	12.091	-9.417	5.802	C
HETATM 316 O	0	13.096	-9.740	6.430	O
HETATM 317 C	0	9.672	-10.277	5.930	C
HETATM 318 H	0	9.347	-7.782	5.881	H
HETATM 319 H	0	10.858	-9.539	7.569	H
HETATM 320 H	0	10.001	-11.304	6.092	H
HETATM 321 H	0	9.552	-10.107	4.861	H
HETATM 322 H	0	8.711	-10.130	6.424	H
HETATM 323 N	0	12.154	-9.090	4.501	N
HETATM 324 C	0	13.317	-9.274	3.617	C
HETATM 325 H	0	12.964	-9.359	2.589	H
HETATM 326 C	0	14.396	-8.140	3.654	C
HETATM 327 O	0	15.554	-8.428	3.367	O
HETATM 328 H	0	11.296	-8.775	4.061	H
HETATM 329 H	0	13.814	-10.210	3.876	H
HETATM 330 N	0	14.070	-6.861	3.943	N
HETATM 331 C	0	14.990	-5.680	3.982	C
HETATM 332 H	0	15.974	-5.991	4.333	H
HETATM 333 C	0	15.129	-5.029	2.615	C
HETATM 334 O	0	16.199	-5.067	2.007	O
HETATM 335 H	0	13.095	-6.670	4.133	H
HETATM 336 H	0	14.580	-4.944	4.671	H
HETATM 337 N	0	14.038	-4.433	2.135	N
HETATM 338 C	0	13.883	-3.966	0.754	C
HETATM 339 C	0	13.360	-2.520	0.764	C
HETATM 340 O	0	12.159	-2.298	0.864	O
HETATM 341 C	0	13.045	-4.933	-0.100	C
HETATM 342 C	0	13.494	-4.752	-1.545	C
HETATM 343 C	0	13.251	-6.399	0.305	C
HETATM 344 H	0	13.218	-4.459	2.733	H
HETATM 345 H	0	14.879	-3.930	0.312	H
HETATM 346 H	0	11.984	-4.699	-0.026	H
HETATM 347 H	0	12.916	-5.395	-2.195	H
HETATM 348 H	0	14.551	-4.993	-1.659	H
HETATM 349 H	0	13.316	-3.728	-1.848	H
HETATM 350 H	0	14.311	-6.605	0.445	H
HETATM 351 H	0	12.869	-7.051	-0.469	H
HETATM 352 H	0	12.715	-6.609	1.231	H
HETATM 353 N	0	14.237	-1.507	0.680	N
HETATM 354 C	0	13.855	-0.072	0.631	C
HETATM 355 C	0	12.870	0.212	-0.495	C
HETATM 356 O	0	12.935	-0.449	-1.533	O

HETATM 357 C	0	15.089	0.815	0.465	C
HETATM 358 O	0	15.863	0.808	1.651	O
HETATM 359 H	0	15.219	-1.749	0.746	H
HETATM 360 H	0	13.386	0.155	1.583	H
HETATM 361 H	0	14.771	1.840	0.266	H
HETATM 362 H	0	15.687	0.463	-0.378	H
HETATM 363 H	0	16.147	-0.120	1.838	H
HETATM 364 N	0	11.935	1.153	-0.306	N
HETATM 365 C	0	10.776	1.290	-1.174	C
HETATM 366 C	0	10.980	1.320	-2.676	C
HETATM 367 O	0	10.337	0.530	-3.366	O
HETATM 368 C	0	10.012	2.522	-0.680	C
HETATM 369 C	0	10.390	2.584	0.793	C
HETATM 370 C	0	11.834	2.100	0.801	C
HETATM 371 H	0	10.132	0.439	-0.971	H
HETATM 372 H	0	10.355	3.427	-1.174	H
HETATM 373 H	0	8.939	2.404	-0.823	H
HETATM 374 H	0	9.774	1.880	1.354	H
HETATM 375 H	0	10.297	3.594	1.190	H
HETATM 376 H	0	12.051	1.650	1.768	H
HETATM 377 H	0	12.504	2.942	0.620	H
HETATM 378 N	0	11.858	2.181	-3.212	N
HETATM 379 C	0	11.933	2.327	-4.647	C
HETATM 380 C	0	12.619	1.160	-5.351	C
HETATM 381 O	0	12.735	1.152	-6.579	O
HETATM 382 C	0	12.689	3.642	-4.863	C
HETATM 383 C	0	13.647	3.684	-3.678	C
HETATM 384 C	0	12.805	3.080	-2.559	C
HETATM 385 H	0	10.938	2.421	-5.078	H
HETATM 386 H	0	13.216	3.678	-5.817	H
HETATM 387 H	0	11.989	4.472	-4.783	H
HETATM 388 H	0	13.965	4.701	-3.444	H
HETATM 389 H	0	14.507	3.043	-3.877	H
HETATM 390 H	0	12.270	3.875	-2.045	H
HETATM 391 H	0	13.458	2.553	-1.865	H
HETATM 392 N	0	13.058	0.155	-4.592	N
HETATM 393 C	0	13.489	-1.109	-5.140	C
HETATM 394 C	0	12.302	-1.829	-5.776	C
HETATM 395 O	0	11.570	-2.581	-5.134	O
HETATM 396 C	0	14.291	-1.905	-4.102	C
HETATM 397 C	0	15.472	-1.155	-3.448	C
HETATM 398 C	0	16.146	-2.062	-2.417	C
HETATM 399 C	0	16.532	-0.732	-4.466	C
HETATM 400 H	0	12.889	0.209	-3.596	H
HETATM 401 H	0	14.186	-0.890	-5.950	H
HETATM 402 H	0	13.608	-2.235	-3.328	H
HETATM 403 H	0	14.703	-2.775	-4.602	H
HETATM 404 H	0	15.114	-0.264	-2.934	H
HETATM 405 H	0	16.548	-2.949	-2.906	H

HETATM 406 H	0	15.415	-2.368	-1.673	H
HETATM 407 H	0	16.952	-1.523	-1.920	H
HETATM 408 H	0	16.887	-1.599	-5.023	H
HETATM 409 H	0	17.372	-0.268	-3.949	H
HETATM 410 H	0	16.114	-0.000	-5.156	H
HETATM 411 N	0	12.174	-1.631	-7.090	N
HETATM 412 C	0	11.453	-2.494	-8.038	C
HETATM 413 C	0	12.111	-3.884	-8.169	C
HETATM 414 O	0	12.089	-4.515	-9.227	O
HETATM 415 C	0	11.300	-1.776	-9.395	C
HETATM 416 O	0	10.542	-2.561	-10.287	O
HETATM 417 C	0	12.621	-1.431	-10.086	C
HETATM 418 H	0	12.720	-0.857	-7.450	H
HETATM 419 H	0	10.450	-2.662	-7.647	H
HETATM 420 H	0	10.758	-0.846	-9.227	H
HETATM 421 H	0	13.203	-2.331	-10.282	H
HETATM 422 H	0	13.203	-0.750	-9.467	H
HETATM 423 H	0	12.409	-0.937	-11.035	H
HETATM 424 H	0	11.069	-3.365	-10.431	H
HETATM 425 N	0	12.717	-4.369	-7.088	N
HETATM 426 C	0	13.725	-5.410	-7.075	C
HETATM 427 H	0	14.569	-5.098	-7.690	H
HETATM 428 C	0	14.252	-5.728	-5.649	C
HETATM 429 O	0	13.900	-5.016	-4.716	O
HETATM 430 H	0	12.549	-3.909	-6.200	H
HETATM 431 N	0	15.098	-6.756	-5.440	N
HETATM 432 C	0	15.742	-7.065	-4.133	C
HETATM 433 C	0	15.985	-8.557	-3.881	C
HETATM 434 O	0	16.156	-9.301	-4.848	O
HETATM 435 H	0	15.327	-7.367	-6.211	H
HETATM 436 H	0	16.702	-6.553	-4.083	H
HETATM 437 H	0	15.107	-6.676	-3.339	H
HETATM 438 N	0	15.993	-9.004	-2.605	N
HETATM 439 C	0	15.873	-10.416	-2.232	C
HETATM 440 C	0	14.765	-11.093	-3.089	C
HETATM 441 O	0	13.664	-10.544	-3.171	O
HETATM 442 C	0	15.544	-10.428	-0.734	C
HETATM 443 C	0	16.161	-9.124	-0.235	C
HETATM 444 C	0	15.942	-8.175	-1.412	C
HETATM 445 H	0	16.838	-10.895	-2.396	H
HETATM 446 H	0	14.463	-10.395	-0.581	H
HETATM 447 H	0	15.973	-11.296	-0.234	H
HETATM 448 H	0	17.230	-9.262	-0.067	H
HETATM 449 H	0	15.671	-8.764	0.670	H
HETATM 450 H	0	16.711	-7.401	-1.425	H
HETATM 451 H	0	14.953	-7.728	-1.345	H
HETATM 452 N	0	15.007	-12.228	-3.770	N
HETATM 453 C	0	14.089	-12.761	-4.794	C
HETATM 454 C	0	12.762	-13.284	-4.253	C

HETATM 455	O	0	11.795 -13.326 -5.004	O
HETATM 456	C	0	14.883 -13.860 -5.511	C
HETATM 457	C	0	15.891 -14.320 -4.459	C
HETATM 458	C	0	16.219 -13.029 -3.710	C
HETATM 459	H	0	13.860 -11.975 -5.514	H
HETATM 460	H	0	14.248 -14.680 -5.848	H
HETATM 461	H	0	15.417 -13.424 -6.357	H
HETATM 462	H	0	16.779 -14.761 -4.913	H
HETATM 463	H	0	15.415 -15.028 -3.779	H
HETATM 464	H	0	17.027 -12.502 -4.219	H
HETATM 465	H	0	16.499 -13.252 -2.679	H
HETATM 466	N	0	12.673 -13.621 -2.961	N
HETATM 467	C	0	11.377 -13.839 -2.324	C
HETATM 468	H	0	13.316 -6.326 -7.498	H
HETATM 469	H	0	11.528 -14.191 -1.305	H
HETATM 470	H	0	10.823 -14.599 -2.876	H
HETATM 471	C	0	10.547 -12.565 -2.282	C
HETATM 472	O	0	9.372 -12.591 -2.636	O
HETATM 473	N	0	11.161 -11.437 -1.902	N
HETATM 474	C	0	10.531 -10.133 -2.089	C
HETATM 475	C	0	10.155 -9.889 -3.551	C
HETATM 476	O	0	9.013 -9.544 -3.823	O
HETATM 477	C	0	11.336 -8.957 -1.511	C
HETATM 478	C	0	10.886 -7.619 -2.086	C
HETATM 479	C	0	9.839 -6.893 -1.485	C
HETATM 480	C	0	11.442 -7.159 -3.298	C
HETATM 481	C	0	9.340 -5.736 -2.111	C
HETATM 482	C	0	10.918 -6.023 -3.935	C
HETATM 483	C	0	9.864 -5.314 -3.344	C
HETATM 484	H	0	12.158 -11.486 -1.754	H
HETATM 485	H	0	9.582 -10.150 -1.550	H
HETATM 486	H	0	11.219 -8.948 -0.427	H
HETATM 487	H	0	12.394 -9.080 -1.723	H
HETATM 488	H	0	9.395 -7.237 -0.563	H
HETATM 489	H	0	12.254 -7.696 -3.766	H
HETATM 490	H	0	8.529 -5.180 -1.671	H
HETATM 491	H	0	11.321 -5.693 -4.882	H
HETATM 492	H	0	9.455 -4.451 -3.847	H
HETATM 493	N	0	11.094 -10.029 -4.486	N
HETATM 494	C	0	10.854 -9.693 -5.889	C
HETATM 495	H	0	11.782 -9.799 -6.450	H
HETATM 496	H	0	10.535 -8.654 -5.962	H
HETATM 497	C	0	9.791 -10.583 -6.554	C
HETATM 498	N	0	9.781 -11.882 -6.241	N
HETATM 499	H	0	10.537 -12.227 -5.661	H
HETATM 500	O	0	8.960 -10.091 -7.312	O
HETATM 501	H	0	12.023 -10.292 -4.173	H
HETATM 502	C	0	8.686 -12.820 -6.511	C
HETATM 503	H	0	8.595 -12.971 -7.587	H

HETATM 504 H	0	8.900 -13.777 -6.036	H
HETATM 505 C	0	7.359 -12.291 -5.979	C
HETATM 506 O	0	6.387 -12.195 -6.721	O
HETATM 507 N	0	7.324 -11.919 -4.698	N
HETATM 508 C	0	6.151 -11.340 -4.031	C
HETATM 509 C	0	5.647 -10.038 -4.650	C
HETATM 510 O	0	4.450 -9.887 -4.881	O
HETATM 511 C	0	6.359 -11.298 -2.498	C
HETATM 512 C	0	5.342 -10.455 -1.725	C
HETATM 513 C	0	6.254 -12.723 -1.931	C
HETATM 514 H	0	8.167 -12.045 -4.146	H
HETATM 515 H	0	5.330 -12.037 -4.199	H
HETATM 516 H	0	7.348 -10.903 -2.274	H
HETATM 517 H	0	4.329 -10.660 -2.075	H
HETATM 518 H	0	5.585 -9.410 -1.866	H
HETATM 519 H	0	5.407 -10.663 -0.657	H
HETATM 520 H	0	5.237 -13.099 -2.043	H
HETATM 521 H	0	6.527 -12.722 -0.875	H
HETATM 522 H	0	6.933 -13.393 -2.456	H
HETATM 523 N	0	6.552 -9.125 -4.974	N
HETATM 524 C	0	6.325 -7.938 -5.788	C
HETATM 525 C	0	5.697 -8.256 -7.107	C
HETATM 526 O	0	4.627 -7.758 -7.431	O
HETATM 527 C	0	7.671 -7.203 -5.931	C
HETATM 528 C	0	7.706 -6.015 -6.876	C
HETATM 529 C	0	7.544 -4.719 -6.361	C
HETATM 530 C	0	7.963 -6.193 -8.251	C
HETATM 531 C	0	7.620 -3.599 -7.209	C
HETATM 532 C	0	8.048 -5.077 -9.106	C
HETATM 533 C	0	7.866 -3.777 -8.587	C
HETATM 534 O	0	7.953 -2.696 -9.407	O
HETATM 535 H	0	7.507 -9.339 -4.711	H
HETATM 536 H	0	5.634 -7.279 -5.261	H
HETATM 537 H	0	7.981 -6.871 -4.939	H
HETATM 538 H	0	8.428 -7.905 -6.266	H
HETATM 539 H	0	7.377 -4.594 -5.301	H
HETATM 540 H	0	8.095 -7.189 -8.655	H
HETATM 541 H	0	7.510 -2.608 -6.795	H
HETATM 542 H	0	8.231 -5.212 -10.162	H
HETATM 543 H	0	8.745 -2.765 -9.968	H
HETATM 544 N	0	6.368 -9.097 -7.867	N
HETATM 545 C	0	5.901 -9.436 -9.175	C
HETATM 546 H	0	6.616 -10.112 -9.642	H
HETATM 547 C	0	4.539 -10.108 -9.191	C
HETATM 548 O	0	3.698 -9.764 -10.015	O
HETATM 549 H	0	7.240 -9.493 -7.527	H
HETATM 550 H	0	5.841 -8.531 -9.781	H
HETATM 551 N	0	4.315 -11.033 -8.261	N
HETATM 552 C	0	3.011 -11.603 -7.993	C

HETATM 553	C	0	1.940 -10.506 -7.695	C
HETATM 554	O	0	0.879 -10.498 -8.315	O
HETATM 555	C	0	3.129 -12.622 -6.853	C
HETATM 556	H	0	5.082 -11.293 -7.650	H
HETATM 557	H	0	2.681 -12.133 -8.888	H
HETATM 558	H	0	3.466 -12.132 -5.940	H
HETATM 559	H	0	3.843 -13.401 -7.126	H
HETATM 560	H	0	2.156 -13.081 -6.674	H
HETATM 561	N	0	2.201 -9.582 -6.757	N
HETATM 562	C	0	1.322 -8.470 -6.328	C
HETATM 563	C	0	1.032 -7.425 -7.428	C
HETATM 564	O	0	-0.120 -7.011 -7.573	O
HETATM 565	C	0	1.956 -7.839 -5.087	C
HETATM 566	C	0	1.229 -6.593 -4.558	C
HETATM 567	C	0	1.730 -5.285 -5.160	C
HETATM 568	O	0	2.903 -5.116 -5.457	O
HETATM 569	N	0	0.899 -4.279 -5.273	N
HETATM 570	H	0	3.095 -9.667 -6.284	H
HETATM 571	H	0	0.360 -8.896 -6.041	H
HETATM 572	H	0	1.962 -8.592 -4.299	H
HETATM 573	H	0	2.997 -7.599 -5.301	H
HETATM 574	H	0	1.423 -6.537 -3.495	H
HETATM 575	H	0	0.153 -6.691 -4.704	H
HETATM 576	H	0	1.266 -3.417 -5.674	H
HETATM 577	H	0	-0.006 -4.296 -4.822	H
HETATM 578	N	0	2.057 -6.942 -8.139	N
HETATM 579	C	0	1.962 -6.008 -9.280	C
HETATM 580	C	0	1.298 -6.717 -10.487	C
HETATM 581	O	0	0.457 -6.108 -11.144	O
HETATM 582	C	0	3.345 -5.437 -9.671	C
HETATM 583	C	0	3.244 -4.432 -10.828	C
HETATM 584	C	0	4.008 -4.681 -8.510	C
HETATM 585	H	0	2.976 -7.294 -7.889	H
HETATM 586	H	0	1.316 -5.176 -8.997	H
HETATM 587	H	0	4.000 -6.254 -9.975	H
HETATM 588	H	0	2.856 -4.920 -11.722	H
HETATM 589	H	0	4.230 -4.032 -11.063	H
HETATM 590	H	0	2.579 -3.612 -10.553	H
HETATM 591	H	0	3.335 -3.912 -8.141	H
HETATM 592	H	0	4.942 -4.229 -8.840	H
HETATM 593	H	0	4.233 -5.359 -7.693	H
HETATM 594	N	0	1.653 -7.981 -10.793	N
HETATM 595	C	0	1.029 -8.828 -11.824	C
HETATM 596	H	0	0.782 -9.789 -11.422	H
HETATM 597	H	0	1.669 -8.950 -12.672	H
HETATM 598	H	0	0.133 -8.326 -12.122	H
HETATM 599	H	0	2.356 -8.429 -10.215	H
HETATM 600	C	0	13.207 5.330 -9.264	C
HETATM 601	H	0	12.990 5.814 -10.193	H

HETATM 602 H	0	13.375	4.288	-9.435	H
HETATM 603 H	0	14.084	5.766	-8.831	H
HETATM 604 C	0	12.032	5.537	-8.374	C
HETATM 605 O	0	10.948	5.125	-8.759	O
HETATM 606 N	0	12.226	6.273	-7.274	N
HETATM 607 C	0	11.163	6.845	-6.440	C
HETATM 608 H	0	11.537	7.719	-5.908	H
HETATM 609 C	0	9.923	7.250	-7.232	C
HETATM 610 O	0	8.850	6.719	-6.994	O
HETATM 611 H	0	13.179	6.520	-7.037	H
HETATM 612 H	0	10.828	6.113	-5.703	H
HETATM 613 N	0	10.081	8.137	-8.218	N
HETATM 614 C	0	9.015	8.554	-9.143	C
HETATM 615 H	0	9.398	9.330	-9.806	H
HETATM 616 C	0	8.428	7.437	-10.008	C
HETATM 617 O	0	7.215	7.249	-9.992	O
HETATM 618 H	0	11.005	8.524	-8.314	H
HETATM 619 H	0	8.200	8.988	-8.562	H
HETATM 620 N	0	9.278	6.715	-10.757	N
HETATM 621 C	0	8.918	5.514	-11.535	C
HETATM 622 H	0	9.814	4.944	-11.777	H
HETATM 623 C	0	7.961	4.622	-10.742	C
HETATM 624 O	0	6.821	4.400	-11.137	O
HETATM 625 H	0	10.257	6.933	-10.665	H
HETATM 626 H	0	8.425	5.814	-12.460	H
HETATM 627 N	0	8.420	4.158	-9.581	N
HETATM 628 C	0	7.691	3.306	-8.644	C
HETATM 629 C	0	6.483	3.923	-7.981	C
HETATM 630 O	0	5.449	3.273	-7.979	O
HETATM 631 C	0	8.672	2.787	-7.572	C
HETATM 632 C	0	9.215	1.356	-7.756	C
HETATM 633 C	0	8.217	0.248	-8.147	C
HETATM 634 N	0	6.990	0.222	-7.332	N
HETATM 635 C	0	5.841	-0.358	-7.640	C
HETATM 636 N	0	5.648	-1.150	-8.647	N
HETATM 637 N	0	4.795	-0.203	-6.914	N
HETATM 638 H	0	9.354	4.459	-9.317	H
HETATM 639 H	0	7.291	2.463	-9.202	H
HETATM 640 H	0	9.520	3.464	-7.476	H
HETATM 641 H	0	8.185	2.843	-6.612	H
HETATM 642 H	0	9.695	1.063	-6.821	H
HETATM 643 H	0	9.992	1.387	-8.521	H
HETATM 644 H	0	8.728	-0.708	-8.037	H
HETATM 645 H	0	7.950	0.371	-9.198	H
HETATM 646 H	0	6.978	0.770	-6.466	H
HETATM 647 H	0	4.693	-1.485	-8.781	H
HETATM 648 H	0	6.431	-1.520	-9.163	H
HETATM 649 H	0	4.924	0.239	-6.005	H
HETATM 650 H	0	3.908	-0.587	-7.238	H

HETATM	651	N	0	6.575	5.134	-7.442	N
HETATM	652	C	0	5.412	5.853	-6.943	C
HETATM	653	C	0	4.277	5.863	-8.021	C
HETATM	654	O	0	3.123	5.589	-7.689	O
HETATM	655	C	0	5.801	7.294	-6.587	C
HETATM	656	H	0	7.479	5.591	-7.419	H
HETATM	657	H	0	5.036	5.350	-6.051	H
HETATM	658	H	0	4.946	7.796	-6.137	H
HETATM	659	H	0	6.103	7.835	-7.484	H
HETATM	660	H	0	6.630	7.306	-5.884	H
HETATM	661	N	0	4.590	6.140	-9.305	N
HETATM	662	C	0	3.715	5.998	-10.497	C
HETATM	663	H	0	4.275	6.277	-11.390	H
HETATM	664	C	0	3.208	4.567	-10.672	C
HETATM	665	O	0	1.996	4.383	-10.662	O
HETATM	666	H	0	5.559	6.389	-9.485	H
HETATM	667	H	0	2.858	6.665	-10.399	H
HETATM	668	N	0	4.086	3.558	-10.800	N
HETATM	669	C	0	3.686	2.133	-10.911	C
HETATM	670	C	0	2.757	1.718	-9.760	C
HETATM	671	O	0	1.728	1.115	-10.028	O
HETATM	672	C	0	4.856	1.154	-11.133	C
HETATM	673	C	0	4.353	-0.280	-11.362	C
HETATM	674	C	0	5.651	1.487	-12.404	C
HETATM	675	H	0	5.072	3.801	-10.830	H
HETATM	676	H	0	3.073	2.065	-11.810	H
HETATM	677	H	0	5.523	1.181	-10.271	H
HETATM	678	H	0	3.729	-0.321	-12.256	H
HETATM	679	H	0	3.759	-0.624	-10.518	H
HETATM	680	H	0	5.196	-0.957	-11.493	H
HETATM	681	H	0	5.005	1.411	-13.280	H
HETATM	682	H	0	6.485	0.795	-12.514	H
HETATM	683	H	0	6.046	2.495	-12.365	H
HETATM	684	N	0	3.033	2.099	-8.511	N
HETATM	685	C	0	2.172	1.911	-7.338	C
HETATM	686	C	0	0.819	2.586	-7.476	C
HETATM	687	O	0	-0.220	1.998	-7.205	O
HETATM	688	C	0	2.918	2.400	-6.072	C
HETATM	689	C	0	2.258	1.901	-4.796	C
HETATM	690	O	0	1.112	2.209	-4.527	O
HETATM	691	N	0	2.927	1.136	-3.975	N
HETATM	692	H	0	3.905	2.592	-8.375	H
HETATM	693	H	0	1.994	0.850	-7.219	H
HETATM	694	H	0	2.933	3.487	-6.044	H
HETATM	695	H	0	3.954	2.072	-6.083	H
HETATM	696	H	0	2.469	0.772	-3.139	H
HETATM	697	H	0	3.913	0.946	-4.122	H
HETATM	698	N	0	0.803	3.850	-7.862	N
HETATM	699	C	0	-0.461	4.517	-8.072	C

HETATM 700 C	0	-1.296	3.910	-9.216	C
HETATM 701 O	0	-2.497	3.695	-9.042	O
HETATM 702 C	0	-0.235	6.016	-8.315	C
HETATM 703 S	0	0.388	6.815	-6.809	S
HETATM 704 H	0	1.679	4.319	-8.071	H
HETATM 705 H	0	-1.077	4.408	-7.179	H
HETATM 706 H	0	-1.185	6.478	-8.590	H
HETATM 707 H	0	0.473	6.160	-9.135	H
HETATM 708 H	0	1.656	6.391	-6.961	H
HETATM 709 N	0	-0.666	3.645	-10.365	N
HETATM 710 C	0	-1.196	2.859	-11.479	C
HETATM 711 H	0	-0.414	2.691	-12.219	H
HETATM 712 C	0	-1.710	1.474	-10.971	C
HETATM 713 O	0	-2.826	1.114	-11.307	O
HETATM 714 H	0	0.320	3.879	-10.410	H
HETATM 715 H	0	-2.024	3.392	-11.947	H
HETATM 716 N	0	-0.969	0.703	-10.143	N
HETATM 717 C	0	-1.310	-0.664	-9.642	C
HETATM 718 C	0	-2.414	-0.679	-8.572	C
HETATM 719 O	0	-3.258	-1.576	-8.564	O
HETATM 720 C	0	-0.061	-1.505	-9.295	C
HETATM 721 C	0	0.356	-1.319	-7.841	C
HETATM 722 C	0	1.805	-1.642	-7.493	C
HETATM 723 O	0	2.022	-1.942	-6.304	O
HETATM 724 O	0	2.763	-1.446	-8.275	O
HETATM 725 H	0	-0.047	1.053	-9.914	H
HETATM 726 H	0	-1.760	-1.177	-10.493	H
HETATM 727 H	0	-0.291	-2.560	-9.448	H
HETATM 728 H	0	0.750	-1.244	-9.973	H
HETATM 729 H	0	-0.308	-1.917	-7.213	H
HETATM 730 H	0	0.199	-0.287	-7.577	H
HETATM 731 N	0	-2.450	0.318	-7.684	N
HETATM 732 C	0	-3.565	0.540	-6.759	C
HETATM 733 C	0	-4.829	1.052	-7.448	C
HETATM 734 O	0	-5.946	0.836	-6.975	O
HETATM 735 C	0	-3.171	1.454	-5.594	C
HETATM 736 C	0	-2.484	0.767	-4.428	C
HETATM 737 C	0	-1.195	0.227	-4.582	C
HETATM 738 C	0	-3.094	0.751	-3.157	C
HETATM 739 C	0	-0.478	-0.236	-3.467	C
HETATM 740 C	0	-2.381	0.280	-2.037	C
HETATM 741 C	0	-1.049	-0.168	-2.181	C
HETATM 742 O	0	-0.301	-0.459	-1.085	O
HETATM 743 H	0	-1.686	0.987	-7.700	H
HETATM 744 H	0	-3.840	-0.422	-6.325	H
HETATM 745 H	0	-2.532	2.258	-5.960	H
HETATM 746 H	0	-4.078	1.918	-5.207	H
HETATM 747 H	0	-0.715	0.218	-5.548	H
HETATM 748 H	0	-4.090	1.148	-3.026	H

HETATM 749 H	0	0.532	-0.598	-3.600	H
HETATM 750 H	0	-2.831	0.302	-1.056	H
HETATM 751 H	0	0.652	-0.460	-1.351	H
HETATM 752 N	0	-4.668	1.739	-8.570	N
HETATM 753 C	0	-5.743	2.337	-9.336	C
HETATM 754 H	0	-5.311	2.753	-10.247	H
HETATM 755 C	0	-6.887	1.425	-9.757	C
HETATM 756 O	0	-8.027	1.801	-9.516	O
HETATM 757 H	0	-3.718	1.895	-8.890	H
HETATM 758 H	0	-6.154	3.170	-8.771	H
HETATM 759 N	0	-6.655	0.254	-10.370	N
HETATM 760 C	0	-7.676	-0.761	-10.568	C
HETATM 761 C	0	-8.521	-1.059	-9.335	C
HETATM 762 O	0	-9.721	-1.259	-9.467	O
HETATM 763 C	0	-6.925	-2.010	-11.039	C
HETATM 764 C	0	-5.747	-1.423	-11.809	C
HETATM 765 C	0	-5.427	-0.152	-11.025	C
HETATM 766 H	0	-8.340	-0.428	-11.367	H
HETATM 767 H	0	-6.549	-2.574	-10.183	H
HETATM 768 H	0	-7.548	-2.643	-11.672	H
HETATM 769 H	0	-6.063	-1.160	-12.820	H
HETATM 770 H	0	-4.897	-2.105	-11.835	H
HETATM 771 H	0	-5.103	0.623	-11.718	H
HETATM 772 H	0	-4.661	-0.363	-10.282	H
HETATM 773 N	0	-7.925	-1.081	-8.139	N
HETATM 774 C	0	-8.660	-1.285	-6.891	C
HETATM 775 C	0	-9.470	-0.028	-6.507	C
HETATM 776 O	0	-10.606	-0.163	-6.069	O
HETATM 777 C	0	-7.718	-1.637	-5.728	C
HETATM 778 C	0	-6.607	-2.657	-6.015	C
HETATM 779 C	0	-5.998	-3.080	-4.677	C
HETATM 780 C	0	-7.098	-3.903	-6.751	C
HETATM 781 H	0	-6.937	-0.869	-8.091	H
HETATM 782 H	0	-9.356	-2.110	-7.030	H
HETATM 783 H	0	-7.241	-0.728	-5.362	H
HETATM 784 H	0	-8.342	-2.013	-4.920	H
HETATM 785 H	0	-5.837	-2.178	-6.620	H
HETATM 786 H	0	-6.733	-3.603	-4.066	H
HETATM 787 H	0	-5.641	-2.201	-4.140	H
HETATM 788 H	0	-5.148	-3.735	-4.851	H
HETATM 789 H	0	-7.827	-4.440	-6.148	H
HETATM 790 H	0	-6.239	-4.534	-6.966	H
HETATM 791 H	0	-7.549	-3.642	-7.706	H
HETATM 792 N	0	-8.913	1.185	-6.652	N
HETATM 793 C	0	-9.649	2.470	-6.603	C
HETATM 794 C	0	-10.868	2.411	-7.512	C
HETATM 795 O	0	-11.978	2.501	-7.014	O
HETATM 796 C	0	-8.675	3.631	-6.875	C
HETATM 797 C	0	-9.265	4.885	-7.491	C

HETATM 798 C	0	-9.850	5.873	-6.678	C
HETATM 799 C	0	-9.186	5.083	-8.884	C
HETATM 800 C	0	-10.330	7.061	-7.259	C
HETATM 801 C	0	-9.689	6.260	-9.463	C
HETATM 802 C	0	-10.257	7.253	-8.648	C
HETATM 803 H	0	-7.951	1.190	-6.973	H
HETATM 804 H	0	-10.039	2.605	-5.594	H
HETATM 805 H	0	-8.191	3.897	-5.936	H
HETATM 806 H	0	-7.880	3.286	-7.525	H
HETATM 807 H	0	-9.909	5.727	-5.608	H
HETATM 808 H	0	-8.740	4.331	-9.518	H
HETATM 809 H	0	-10.752	7.838	-6.645	H
HETATM 810 H	0	-9.634	6.405	-10.533	H
HETATM 811 H	0	-10.636	8.164	-9.091	H
HETATM 812 N	0	-10.670	2.151	-8.801	N
HETATM 813 C	0	-11.706	1.852	-9.780	C
HETATM 814 H	0	-11.243	1.460	-10.685	H
HETATM 815 C	0	-12.740	0.839	-9.290	C
HETATM 816 O	0	-13.927	1.148	-9.251	O
HETATM 817 H	0	-9.706	2.061	-9.093	H
HETATM 818 H	0	-12.233	2.772	-10.032	H
HETATM 819 N	0	-12.289	-0.356	-8.904	N
HETATM 820 C	0	-13.115	-1.448	-8.399	C
HETATM 821 C	0	-14.001	-1.030	-7.252	C
HETATM 822 O	0	-15.224	-1.042	-7.349	O
HETATM 823 C	0	-12.243	-2.668	-8.082	C
HETATM 824 H	0	-11.299	-0.539	-9.017	H
HETATM 825 H	0	-13.789	-1.739	-9.207	H
HETATM 826 H	0	-12.871	-3.485	-7.724	H
HETATM 827 H	0	-11.512	-2.415	-7.319	H
HETATM 828 H	0	-11.722	-2.995	-8.983	H
HETATM 829 N	0	-13.365	-0.653	-6.161	N
HETATM 830 C	0	-14.068	-0.266	-4.958	C
HETATM 831 C	0	-14.925	0.982	-5.159	C
HETATM 832 O	0	-15.983	1.064	-4.555	O
HETATM 833 C	0	-13.128	-0.033	-3.768	C
HETATM 834 O	0	-11.912	-0.727	-3.856	O
HETATM 835 C	0	-13.774	-0.572	-2.503	C
HETATM 836 H	0	-12.355	-0.634	-6.196	H
HETATM 837 H	0	-14.746	-1.081	-4.704	H
HETATM 838 H	0	-12.912	1.030	-3.663	H
HETATM 839 H	0	-14.742	-0.101	-2.338	H
HETATM 840 H	0	-13.111	-0.354	-1.674	H
HETATM 841 H	0	-13.904	-1.651	-2.579	H
HETATM 842 H	0	-11.428	-0.410	-4.639	H
HETATM 843 N	0	-14.501	1.953	-5.975	N
HETATM 844 C	0	-15.267	3.161	-6.294	C
HETATM 845 C	0	-16.518	2.871	-7.125	C
HETATM 846 O	0	-17.583	3.362	-6.776	O

HETATM 847 C	0	-14.370	4.226	-6.949	C
HETATM 848 C	0	-15.042	5.594	-7.177	C
HETATM 849 C	0	-15.433	6.275	-5.862	C
HETATM 850 C	0	-14.062	6.519	-7.900	C
HETATM 851 H	0	-13.603	1.844	-6.436	H
HETATM 852 H	0	-15.623	3.564	-5.347	H
HETATM 853 H	0	-13.499	4.385	-6.312	H
HETATM 854 H	0	-14.029	3.845	-7.913	H
HETATM 855 H	0	-15.927	5.475	-7.800	H
HETATM 856 H	0	-14.568	6.345	-5.205	H
HETATM 857 H	0	-16.222	5.701	-5.374	H
HETATM 858 H	0	-15.825	7.271	-6.069	H
HETATM 859 H	0	-13.167	6.664	-7.297	H
HETATM 860 H	0	-14.536	7.481	-8.095	H
HETATM 861 H	0	-13.778	6.074	-8.854	H
HETATM 862 N	0	-16.410	2.092	-8.201	N
HETATM 863 C	0	-17.559	1.643	-8.994	C
HETATM 864 H	0	-17.206	1.078	-9.856	H
HETATM 865 C	0	-18.511	0.761	-8.198	C
HETATM 866 O	0	-19.721	0.932	-8.294	O
HETATM 867 H	0	-15.489	1.737	-8.444	H
HETATM 868 H	0	-18.114	2.511	-9.350	H
HETATM 869 N	0	-17.968	-0.169	-7.406	N
HETATM 870 C	0	-18.755	-0.973	-6.466	C
HETATM 871 C	0	-19.467	-0.103	-5.414	C
HETATM 872 O	0	-20.646	-0.316	-5.154	O
HETATM 873 C	0	-17.938	-2.106	-5.814	C
HETATM 874 C	0	-18.729	-2.854	-4.730	C
HETATM 875 C	0	-17.547	-3.171	-6.853	C
HETATM 876 H	0	-16.960	-0.283	-7.424	H
HETATM 877 H	0	-19.558	-1.445	-7.034	H
HETATM 878 H	0	-17.036	-1.692	-5.362	H
HETATM 879 H	0	-19.659	-3.243	-5.147	H
HETATM 880 H	0	-18.979	-2.185	-3.908	H
HETATM 881 H	0	-18.142	-3.677	-4.333	H
HETATM 882 H	0	-18.440	-3.675	-7.223	H
HETATM 883 H	0	-16.878	-3.900	-6.399	H
HETATM 884 H	0	-17.041	-2.712	-7.700	H
HETATM 885 N	0	-18.766	0.840	-4.776	N
HETATM 886 C	0	-19.327	1.736	-3.761	C
HETATM 887 C	0	-20.307	2.788	-4.310	C
HETATM 888 O	0	-21.213	3.214	-3.595	O
HETATM 889 C	0	-18.195	2.432	-2.994	C
HETATM 890 H	0	-17.784	0.942	-4.995	H
HETATM 891 H	0	-19.892	1.130	-3.050	H
HETATM 892 H	0	-18.621	3.061	-2.211	H
HETATM 893 H	0	-17.616	3.055	-3.676	H
HETATM 894 H	0	-17.544	1.693	-2.530	H
HETATM 895 N	0	-20.082	3.263	-5.538	N

HETATM 896 C	0	-20.905	4.247	-6.215	C
HETATM 897 H	0	-21.910	3.879	-6.218	H
HETATM 898 H	0	-20.572	4.384	-7.222	H
HETATM 899 H	0	-20.869	5.183	-5.697	H
HETATM 900 H	0	-19.277	2.900	-6.035	H
HETATM 901 C	0	-15.470	11.722	-2.061	C
HETATM 902 H	0	-16.392	11.223	-1.848	H
HETATM 903 H	0	-15.394	11.898	-3.114	H
HETATM 904 H	0	-15.440	12.655	-1.539	H
HETATM 905 C	0	-14.289	10.863	-1.625	C
HETATM 906 O	0	-13.160	11.299	-1.791	O
HETATM 907 N	0	-14.503	9.629	-1.145	N
HETATM 908 C	0	-13.456	8.632	-0.786	C
HETATM 909 C	0	-12.441	8.454	-1.920	C
HETATM 910 O	0	-11.235	8.454	-1.697	O
HETATM 911 C	0	-14.138	7.328	-0.358	C
HETATM 912 S	0	-15.477	7.670	0.824	S
HETATM 913 H	0	-15.460	9.364	-0.958	H
HETATM 914 H	0	-12.904	9.020	0.072	H
HETATM 915 H	0	-13.399	6.676	0.111	H
HETATM 916 H	0	-14.559	6.836	-1.233	H
HETATM 917 H	0	-15.920	6.415	0.979	H
HETATM 918 N	0	-12.939	8.399	-3.154	N
HETATM 919 C	0	-12.119	8.475	-4.354	C
HETATM 920 C	0	-11.238	9.716	-4.473	C
HETATM 921 O	0	-10.049	9.605	-4.755	O
HETATM 922 H	0	-13.943	8.402	-3.247	H
HETATM 923 H	0	-11.468	7.600	-4.380	H
HETATM 924 H	0	-12.765	8.434	-5.231	H
HETATM 925 N	0	-11.815	10.895	-4.250	N
HETATM 926 C	0	-11.083	12.155	-4.146	C
HETATM 927 H	0	-11.775	12.957	-3.889	H
HETATM 928 C	0	-9.973	12.121	-3.085	C
HETATM 929 O	0	-8.869	12.595	-3.337	O
HETATM 930 H	0	-12.774	10.897	-3.938	H
HETATM 931 H	0	-10.627	12.387	-5.109	H
HETATM 932 N	0	-10.248	11.543	-1.908	N
HETATM 933 C	0	-9.251	11.320	-0.842	C
HETATM 934 C	0	-8.121	10.432	-1.296	C
HETATM 935 O	0	-6.970	10.807	-1.107	O
HETATM 936 C	0	-9.879	10.800	0.471	C
HETATM 937 C	0	-8.835	10.685	1.594	C
HETATM 938 C	0	-10.973	11.742	0.991	C
HETATM 939 H	0	-11.206	11.239	-1.771	H
HETATM 940 H	0	-8.803	12.289	-0.618	H
HETATM 941 H	0	-10.318	9.819	0.305	H
HETATM 942 H	0	-8.051	9.978	1.321	H
HETATM 943 H	0	-9.311	10.327	2.506	H
HETATM 944 H	0	-8.380	11.658	1.782	H

HETATM 945 H	0	-10.562	12.739	1.159	H
HETATM 946 H	0	-11.381	11.360	1.927	H
HETATM 947 H	0	-11.786	11.815	0.274	H
HETATM 948 N	0	-8.421	9.283	-1.903	N
HETATM 949 C	0	-7.401	8.483	-2.572	C
HETATM 950 C	0	-6.556	9.302	-3.527	C
HETATM 951 O	0	-5.332	9.237	-3.464	O
HETATM 952 C	0	-8.023	7.248	-3.244	C
HETATM 953 C	0	-7.033	6.437	-4.066	C
HETATM 954 C	0	-6.222	5.461	-3.452	C
HETATM 955 C	0	-6.900	6.688	-5.447	C
HETATM 956 C	0	-5.275	4.751	-4.217	C
HETATM 957 C	0	-5.958	5.979	-6.215	C
HETATM 958 C	0	-5.136	5.012	-5.599	C
HETATM 959 O	0	-4.187	4.358	-6.317	O
HETATM 960 H	0	-9.400	9.035	-2.006	H
HETATM 961 H	0	-6.718	8.116	-1.808	H
HETATM 962 H	0	-8.453	6.609	-2.473	H
HETATM 963 H	0	-8.838	7.559	-3.895	H
HETATM 964 H	0	-6.318	5.267	-2.391	H
HETATM 965 H	0	-7.521	7.439	-5.922	H
HETATM 966 H	0	-4.632	4.013	-3.760	H
HETATM 967 H	0	-5.860	6.185	-7.270	H
HETATM 968 H	0	-4.191	4.554	-7.259	H
HETATM 969 N	0	-7.205	10.095	-4.370	N
HETATM 970 C	0	-6.511	10.987	-5.288	C
HETATM 971 H	0	-5.557	11.286	-4.909	H
HETATM 972 H	0	-7.087	11.856	-5.531	H
HETATM 973 H	0	-8.227	10.037	-4.304	H
HETATM 974 H	0	-6.334	10.448	-6.220	H
HETATM 975 N	0	-4.549	12.263	-1.592	N
HETATM 976 O	0	-3.108	13.824	-2.256	O
HETATM 977 C	0	-4.262	13.412	-2.214	C
HETATM 978 C	0	-5.325	14.188	-2.993	C
HETATM 979 H	0	-6.303	13.756	-3.035	H
HETATM 980 H	0	-4.883	14.167	-3.967	H
HETATM 981 H	0	-5.397	15.200	-2.655	H
HETATM 982 C	0	-3.540	11.463	-0.859	C
HETATM 983 C	0	-2.468	10.827	-1.752	C
HETATM 984 O	0	-1.286	10.901	-1.425	O
HETATM 985 C	0	-4.258	10.475	0.050	C
HETATM 986 H	0	-5.509	11.931	-1.591	H
HETATM 987 H	0	-3.005	12.154	-0.205	H
HETATM 988 H	0	-3.525	9.961	0.657	H
HETATM 989 H	0	-4.819	9.761	-0.545	H
HETATM 990 H	0	-4.944	11.009	0.709	H
HETATM 991 N	0	-2.825	10.210	-2.883	N
HETATM 992 C	0	-1.836	9.676	-3.830	C
HETATM 993 C	0	-0.953	10.763	-4.485	C

HETATM 994 O	0	0.197	10.451	-4.788	O
HETATM 995 C	0	-2.446	8.693	-4.846	C
HETATM 996 C	0	-2.760	7.300	-4.257	C
HETATM 997 C	0	-1.614	6.751	-3.394	C
HETATM 998 N	0	-1.754	5.330	-3.055	N
HETATM 999 C	0	-1.072	4.344	-3.595	C
HETATM 1000 N	0	-0.375	4.479	-4.678	N
HETATM 1001 N	0	-1.052	3.181	-3.036	N
HETATM 1002 H	0	-3.819	10.111	-3.080	H
HETATM 1003 H	0	-1.120	9.131	-3.242	H
HETATM 1004 H	0	-3.348	9.119	-5.288	H
HETATM 1005 H	0	-1.726	8.549	-5.652	H
HETATM 1006 H	0	-2.935	6.618	-5.089	H
HETATM 1007 H	0	-3.664	7.344	-3.653	H
HETATM 1008 H	0	-1.574	7.307	-2.458	H
HETATM 1009 H	0	-0.671	6.917	-3.915	H
HETATM 1010 H	0	-2.220	5.080	-2.191	H
HETATM 1011 H	0	0.165	3.662	-4.943	H
HETATM 1012 H	0	-0.312	5.352	-5.165	H
HETATM 1013 H	0	-1.587	3.026	-2.191	H
HETATM 1014 H	0	-0.473	2.451	-3.442	H
HETATM 1015 N	0	-1.405	12.024	-4.620	N
HETATM 1016 C	0	-0.551	13.188	-4.934	C
HETATM 1017 H	0	-0.977	13.853	-5.655	H
HETATM 1018 H	0	0.380	12.812	-5.302	H
HETATM 1019 H	0	-0.387	13.714	-4.017	H
HETATM 1020 H	0	-2.341	12.198	-4.286	H
HETATM 1021 C	0	0.985	13.859	-1.542	C
HETATM 1022 H	0	-0.034	13.537	-1.475	H
HETATM 1023 H	0	1.189	14.192	-2.538	H
HETATM 1024 H	0	1.151	14.662	-0.855	H
HETATM 1025 C	0	1.943	12.716	-1.336	C
HETATM 1026 O	0	3.124	12.958	-1.131	O
HETATM 1027 N	0	1.470	11.484	-1.514	N
HETATM 1028 C	0	2.297	10.275	-1.582	C
HETATM 1029 C	0	3.343	10.389	-2.701	C
HETATM 1030 O	0	4.522	10.350	-2.389	O
HETATM 1031 C	0	1.426	9.031	-1.767	C
HETATM 1032 C	0	2.154	7.770	-2.194	C
HETATM 1033 C	0	2.944	7.063	-1.271	C
HETATM 1034 C	0	2.032	7.299	-3.517	C
HETATM 1035 C	0	3.569	5.857	-1.648	C
HETATM 1036 C	0	2.647	6.090	-3.896	C
HETATM 1037 C	0	3.393	5.352	-2.954	C
HETATM 1038 O	0	3.962	4.179	-3.328	O
HETATM 1039 H	0	0.468	11.382	-1.633	H
HETATM 1040 H	0	2.841	10.169	-0.642	H
HETATM 1041 H	0	0.876	8.832	-0.847	H
HETATM 1042 H	0	0.710	9.263	-2.537	H

HETATM 1043	H	0	3.054	7.449	-0.269	H
HETATM 1044	H	0	1.464	7.861	-4.245	H
HETATM 1045	H	0	4.162	5.296	-0.944	H
HETATM 1046	H	0	2.558	5.705	-4.900	H
HETATM 1047	H	0	4.317	3.678	-2.574	H
HETATM 1048	N	0	2.953	10.566	-3.973	N
HETATM 1049	C	0	3.870	10.773	-5.112	C
HETATM 1050	H	0	3.299	11.053	-5.997	H
HETATM 1051	C	0	4.920	11.871	-4.827	C
HETATM 1052	O	0	6.102	11.625	-5.026	O
HETATM 1053	H	0	1.956	10.543	-4.166	H
HETATM 1054	H	0	4.398	9.843	-5.317	H
HETATM 1055	N	0	4.514	13.054	-4.329	N
HETATM 1056	C	0	5.398	14.169	-3.904	C
HETATM 1057	H	0	4.795	14.983	-3.503	H
HETATM 1058	C	0	6.408	13.761	-2.862	C
HETATM 1059	O	0	7.620	13.844	-3.058	O
HETATM 1060	H	0	3.525	13.146	-4.163	H
HETATM 1061	H	0	5.943	14.541	-4.773	H
HETATM 1062	N	0	5.868	13.301	-1.746	N
HETATM 1063	C	0	6.635	12.795	-0.641	C
HETATM 1064	C	0	7.625	11.748	-1.013	C
HETATM 1065	O	0	8.797	11.896	-0.725	O
HETATM 1066	H	0	4.856	13.254	-1.675	H
HETATM 1067	H	0	7.172	13.624	-0.178	H
HETATM 1068	H	0	5.952	12.378	0.099	H
HETATM 1069	N	0	7.139	10.705	-1.652	N
HETATM 1070	C	0	7.920	9.581	-2.087	C
HETATM 1071	C	0	8.998	9.936	-3.092	C
HETATM 1072	O	0	10.134	9.475	-2.973	O
HETATM 1073	C	0	6.971	8.502	-2.645	C
HETATM 1074	C	0	7.510	7.103	-2.906	C
HETATM 1075	C	0	6.657	6.183	-3.542	C
HETATM 1076	C	0	8.814	6.697	-2.553	C
HETATM 1077	C	0	7.113	4.903	-3.905	C
HETATM 1078	C	0	9.283	5.428	-2.939	C
HETATM 1079	C	0	8.441	4.535	-3.625	C
HETATM 1080	O	0	8.917	3.323	-3.995	O
HETATM 1081	H	0	6.151	10.710	-1.873	H
HETATM 1082	H	0	8.430	9.174	-1.215	H
HETATM 1083	H	0	6.133	8.383	-1.962	H
HETATM 1084	H	0	6.553	8.874	-3.582	H
HETATM 1085	H	0	5.650	6.480	-3.793	H
HETATM 1086	H	0	9.490	7.337	-2.008	H
HETATM 1087	H	0	6.463	4.208	-4.416	H
HETATM 1088	H	0	10.295	5.127	-2.723	H
HETATM 1089	H	0	8.219	2.750	-4.386	H
HETATM 1090	N	0	8.660	10.776	-4.065	N
HETATM 1091	C	0	9.646	11.327	-4.962	C

HETATM 1092	C	0	10.845	11.956	-4.220	C
HETATM 1093	O	0	11.991	11.733	-4.617	O
HETATM 1094	C	0	8.993	12.309	-5.941	C
HETATM 1095	H	0	7.703	11.106	-4.142	H
HETATM 1096	H	0	10.050	10.503	-5.552	H
HETATM 1097	H	0	9.751	12.711	-6.615	H
HETATM 1098	H	0	8.530	13.134	-5.400	H
HETATM 1099	H	0	8.237	11.795	-6.534	H
HETATM 1100	N	0	10.592	12.675	-3.117	N
HETATM 1101	C	0	11.612	13.147	-2.169	C
HETATM 1102	H	0	11.189	13.942	-1.555	H
HETATM 1103	C	0	12.162	12.037	-1.230	C
HETATM 1104	O	0	13.311	11.635	-1.404	O
HETATM 1105	H	0	9.613	12.831	-2.896	H
HETATM 1106	H	0	12.462	13.552	-2.720	H
HETATM 1107	N	0	11.402	11.558	-0.226	N
HETATM 1108	C	0	11.796	10.610	0.852	C
HETATM 1109	C	0	10.826	9.440	1.171	C
HETATM 1110	O	0	9.600	9.541	1.064	O
HETATM 1111	C	0	12.165	11.377	2.137	C
HETATM 1112	O	0	11.247	11.182	3.207	O
HETATM 1113	H	0	10.442	11.873	-0.227	H
HETATM 1114	H	0	12.718	10.136	0.512	H
HETATM 1115	H	0	12.252	12.443	1.923	H
HETATM 1116	H	0	13.145	11.031	2.464	H
HETATM 1117	H	0	11.714	11.450	4.023	H
HETATM 1118	N	0	11.388	8.335	1.689	N
HETATM 1119	C	0	10.715	7.106	2.149	C
HETATM 1120	C	0	9.828	7.271	3.402	C
HETATM 1121	O	0	9.211	6.300	3.851	O
HETATM 1122	C	0	11.792	6.046	2.423	C
HETATM 1123	H	0	12.394	8.356	1.806	H
HETATM 1124	H	0	10.084	6.742	1.338	H
HETATM 1125	H	0	11.330	5.107	2.723	H
HETATM 1126	H	0	12.456	6.381	3.215	H
HETATM 1127	H	0	12.386	5.873	1.531	H
HETATM 1128	N	0	9.735	8.478	3.968	N
HETATM 1129	C	0	8.908	8.791	5.139	C
HETATM 1130	C	0	7.880	9.893	4.836	C
HETATM 1131	O	0	6.730	9.748	5.229	O
HETATM 1132	C	0	9.771	9.232	6.331	C
HETATM 1133	C	0	10.623	8.126	6.961	C
HETATM 1134	C	0	11.860	7.755	6.158	C
HETATM 1135	O	0	12.699	8.593	5.824	O
HETATM 1136	N	0	12.037	6.493	5.851	N
HETATM 1137	H	0	10.259	9.220	3.519	H
HETATM 1138	H	0	8.354	7.911	5.447	H
HETATM 1139	H	0	10.396	10.075	6.045	H
HETATM 1140	H	0	9.095	9.578	7.111	H

HETATM 1141 H	0	9.997	7.247	7.111	H
HETATM 1142 H	0	10.961	8.469	7.939	H
HETATM 1143 H	0	12.891	6.222	5.376	H
HETATM 1144 H	0	11.352	5.800	6.142	H
HETATM 1145 N	0	8.226	10.961	4.104	N
HETATM 1146 C	0	7.266	12.008	3.685	C
HETATM 1147 C	0	6.088	11.423	2.888	C
HETATM 1148 O	0	4.956	11.883	3.003	O
HETATM 1149 C	0	8.006	13.062	2.840	C
HETATM 1150 C	0	9.057	13.888	3.604	C
HETATM 1151 C	0	9.857	14.730	2.610	C
HETATM 1152 C	0	8.421	14.829	4.627	C
HETATM 1153 H	0	9.190	11.050	3.804	H
HETATM 1154 H	0	6.844	12.482	4.573	H
HETATM 1155 H	0	8.497	12.550	2.011	H
HETATM 1156 H	0	7.271	13.749	2.417	H
HETATM 1157 H	0	9.747	13.224	4.122	H
HETATM 1158 H	0	10.625	15.295	3.138	H
HETATM 1159 H	0	9.197	15.424	2.088	H
HETATM 1160 H	0	10.340	14.080	1.881	H
HETATM 1161 H	0	7.919	14.252	5.403	H
HETATM 1162 H	0	7.700	15.486	4.140	H
HETATM 1163 H	0	9.194	15.435	5.101	H
HETATM 1164 N	0	6.349	10.360	2.116	N
HETATM 1165 C	0	5.337	9.485	1.488	C
HETATM 1166 C	0	4.240	9.013	2.455	C
HETATM 1167 O	0	3.134	8.723	2.004	O
HETATM 1168 C	0	6.013	8.284	0.808	C
HETATM 1169 C	0	6.475	7.180	1.758	C
HETATM 1170 C	0	7.139	6.004	1.048	C
HETATM 1171 N	0	7.535	5.028	2.054	N
HETATM 1172 C	0	7.449	3.691	2.008	C
HETATM 1173 N	0	6.991	3.040	0.955	N
HETATM 1174 N	0	7.874	2.978	3.065	N
HETATM 1175 H	0	7.330	10.122	2.023	H
HETATM 1176 H	0	4.828	10.090	0.731	H
HETATM 1177 H	0	5.315	7.843	0.089	H
HETATM 1178 H	0	6.879	8.626	0.238	H
HETATM 1179 H	0	5.625	6.771	2.313	H
HETATM 1180 H	0	7.169	7.603	2.497	H
HETATM 1181 H	0	8.008	6.322	0.459	H
HETATM 1182 H	0	6.423	5.550	0.360	H
HETATM 1183 H	0	7.972	5.418	2.888	H
HETATM 1184 H	0	6.887	1.995	1.068	H
HETATM 1185 H	0	6.483	3.510	0.219	H
HETATM 1186 H	0	8.273	3.444	3.871	H
HETATM 1187 H	0	7.596	2.004	3.156	H
HETATM 1188 N	0	4.565	8.804	3.734	N
HETATM 1189 C	0	3.838	7.902	4.624	C

HETATM 1190	C	0	2.457	8.367	5.018	C
HETATM 1191	O	0	1.507	7.634	4.772	O
HETATM 1192	C	0	4.658	7.462	5.851	C
HETATM 1193	C	0	5.845	6.539	5.523	C
HETATM 1194	C	0	6.688	6.305	6.775	C
HETATM 1195	C	0	5.401	5.163	5.018	C
HETATM 1196	H	0	5.450	9.172	4.056	H
HETATM 1197	H	0	3.645	7.001	4.045	H
HETATM 1198	H	0	5.014	8.341	6.379	H
HETATM 1199	H	0	3.998	6.929	6.536	H
HETATM 1200	H	0	6.468	7.004	4.762	H
HETATM 1201	H	0	6.111	5.756	7.516	H
HETATM 1202	H	0	6.982	7.264	7.204	H
HETATM 1203	H	0	7.586	5.743	6.522	H
HETATM 1204	H	0	6.270	4.521	4.900	H
HETATM 1205	H	0	4.900	5.247	4.056	H
HETATM 1206	H	0	4.719	4.713	5.740	H
HETATM 1207	N	0	2.311	9.529	5.637	N
HETATM 1208	C	0	0.990	9.968	6.046	C
HETATM 1209	C	0	-0.060	10.009	4.901	C
HETATM 1210	O	0	-1.158	9.484	5.095	O
HETATM 1211	C	0	1.103	11.271	6.851	C
HETATM 1212	H	0	3.130	10.082	5.881	H
HETATM 1213	H	0	0.618	9.219	6.746	H
HETATM 1214	H	0	1.598	12.053	6.279	H
HETATM 1215	H	0	1.690	11.085	7.752	H
HETATM 1216	H	0	0.109	11.609	7.144	H
HETATM 1217	N	0	0.228	10.560	3.703	N
HETATM 1218	C	0	-0.611	10.381	2.508	C
HETATM 1219	C	0	-0.771	8.913	2.063	C
HETATM 1220	O	0	-1.849	8.538	1.606	O
HETATM 1221	C	0	0.075	11.202	1.416	C
HETATM 1222	C	0	0.980	12.185	2.147	C
HETATM 1223	C	0	1.371	11.412	3.396	C
HETATM 1224	H	0	-1.593	10.808	2.703	H
HETATM 1225	H	0	0.692	10.546	0.806	H
HETATM 1226	H	0	-0.653	11.738	0.810	H
HETATM 1227	H	0	0.410	13.072	2.428	H
HETATM 1228	H	0	1.855	12.459	1.556	H
HETATM 1229	H	0	1.591	12.117	4.194	H
HETATM 1230	H	0	2.247	10.802	3.189	H
HETATM 1231	N	0	0.249	8.050	2.169	N
HETATM 1232	C	0	0.081	6.604	1.943	C
HETATM 1233	C	0	-0.981	6.018	2.867	C
HETATM 1234	O	0	-1.953	5.445	2.388	O
HETATM 1235	C	0	1.415	5.848	2.021	C
HETATM 1236	C	0	1.283	4.372	1.608	C
HETATM 1237	C	0	0.847	4.178	0.155	C
HETATM 1238	C	0	2.631	3.693	1.789	C

HETATM 1239	H	0	1.151	8.385	2.491	H
HETATM 1240	H	0	-0.290	6.495	0.926	H
HETATM 1241	H	0	2.141	6.329	1.373	H
HETATM 1242	H	0	1.792	5.884	3.040	H
HETATM 1243	H	0	0.562	3.879	2.256	H
HETATM 1244	H	0	1.496	4.731	-0.518	H
HETATM 1245	H	0	-0.176	4.516	0.022	H
HETATM 1246	H	0	0.896	3.120	-0.106	H
HETATM 1247	H	0	3.026	3.894	2.782	H
HETATM 1248	H	0	3.337	4.037	1.034	H
HETATM 1249	H	0	2.480	2.620	1.688	H
HETATM 1250	N	0	-0.836	6.218	4.173	N
HETATM 1251	C	0	-1.850	5.874	5.157	C
HETATM 1252	C	0	-3.216	6.489	4.848	C
HETATM 1253	O	0	-4.203	5.776	4.917	O
HETATM 1254	C	0	-1.364	6.176	6.582	C
HETATM 1255	C	0	-0.300	5.206	7.069	C
HETATM 1256	C	0	1.035	5.624	7.227	C
HETATM 1257	C	0	-0.647	3.871	7.360	C
HETATM 1258	C	0	2.025	4.710	7.636	C
HETATM 1259	C	0	0.338	2.955	7.778	C
HETATM 1260	C	0	1.682	3.368	7.902	C
HETATM 1261	O	0	2.639	2.501	8.322	O
HETATM 1262	H	0	-0.002	6.709	4.478	H
HETATM 1263	H	0	-2.001	4.796	5.099	H
HETATM 1264	H	0	-0.990	7.200	6.631	H
HETATM 1265	H	0	-2.215	6.103	7.261	H
HETATM 1266	H	0	1.304	6.653	7.038	H
HETATM 1267	H	0	-1.672	3.539	7.253	H
HETATM 1268	H	0	3.049	5.029	7.761	H
HETATM 1269	H	0	0.070	1.929	7.986	H
HETATM 1270	H	0	2.228	1.721	8.740	H
HETATM 1271	N	0	-3.312	7.766	4.477	N
HETATM 1272	C	0	-4.570	8.404	4.085	C
HETATM 1273	C	0	-5.221	7.792	2.803	C
HETATM 1274	O	0	-6.410	7.488	2.824	O
HETATM 1275	C	0	-4.337	9.910	3.929	C
HETATM 1276	H	0	-2.460	8.317	4.489	H
HETATM 1277	H	0	-5.283	8.260	4.895	H
HETATM 1278	H	0	-3.653	10.097	3.104	H
HETATM 1279	H	0	-3.911	10.320	4.846	H
HETATM 1280	H	0	-5.285	10.407	3.719	H
HETATM 1281	N	0	-4.490	7.616	1.689	N
HETATM 1282	C	0	-4.948	6.958	0.433	C
HETATM 1283	C	0	-5.319	5.459	0.717	C
HETATM 1284	O	0	-6.383	5.020	0.286	O
HETATM 1285	C	0	-3.892	7.011	-0.679	C
HETATM 1286	O	0	-2.629	6.569	-0.226	O
HETATM 1287	H	0	-3.522	7.903	1.757	H

HETATM 1288	H	0	-5.850	7.458	0.083	H
HETATM 1289	H	0	-3.788	8.022	-1.062	H
HETATM 1290	H	0	-4.218	6.375	-1.503	H
HETATM 1291	H	0	-2.288	7.223	0.412	H
HETATM 1292	N	0	-4.503	4.674	1.459	N
HETATM 1293	C	0	-4.764	3.290	1.971	C
HETATM 1294	C	0	-6.038	3.274	2.774	C
HETATM 1295	O	0	-6.911	2.451	2.545	O
HETATM 1296	C	0	-3.570	2.842	2.808	C
HETATM 1297	H	0	-3.634	5.099	1.765	H
HETATM 1298	H	0	-4.880	2.613	1.124	H
HETATM 1299	H	0	-3.693	1.798	3.071	H
HETATM 1300	H	0	-3.500	3.437	3.719	H
HETATM 1301	H	0	-2.651	2.955	2.240	H
HETATM 1302	N	0	-6.155	4.236	3.682	N
HETATM 1303	C	0	-7.343	4.476	4.462	C
HETATM 1304	C	0	-8.590	4.790	3.643	C
HETATM 1305	O	0	-9.644	4.272	3.975	O
HETATM 1306	C	0	-7.066	5.486	5.583	C
HETATM 1307	C	0	-8.279	5.867	6.450	C
HETATM 1308	C	0	-7.906	6.233	7.901	C
HETATM 1309	N	0	-6.594	6.902	8.040	N
HETATM 1310	C	0	-6.231	8.120	7.698	C
HETATM 1311	N	0	-7.069	8.958	7.155	N
HETATM 1312	N	0	-5.010	8.525	7.894	N
HETATM 1313	H	0	-5.343	4.820	3.851	H
HETATM 1314	H	0	-7.581	3.538	4.966	H
HETATM 1315	H	0	-6.308	5.034	6.223	H
HETATM 1316	H	0	-6.662	6.402	5.158	H
HETATM 1317	H	0	-8.985	5.037	6.490	H
HETATM 1318	H	0	-8.787	6.712	5.983	H
HETATM 1319	H	0	-7.861	5.304	8.474	H
HETATM 1320	H	0	-8.697	6.844	8.338	H
HETATM 1321	H	0	-5.846	6.295	8.371	H
HETATM 1322	H	0	-6.799	9.894	6.927	H
HETATM 1323	H	0	-8.010	8.636	7.021	H
HETATM 1324	H	0	-4.366	7.926	8.409	H
HETATM 1325	H	0	-4.709	9.440	7.626	H
HETATM 1326	N	0	-8.514	5.591	2.587	N
HETATM 1327	C	0	-9.621	5.796	1.647	C
HETATM 1328	C	0	-10.009	4.533	0.890	C
HETATM 1329	O	0	-11.195	4.305	0.679	O
HETATM 1330	C	0	-9.227	6.918	0.686	C
HETATM 1331	H	0	-7.627	6.049	2.417	H
HETATM 1332	H	0	-10.490	6.138	2.206	H
HETATM 1333	H	0	-8.980	7.815	1.250	H
HETATM 1334	H	0	-10.066	7.128	0.028	H
HETATM 1335	H	0	-8.371	6.625	0.080	H
HETATM 1336	N	0	-9.034	3.702	0.518	N

HETATM 1337 C	0	-9.313	2.355	0.043	C
HETATM 1338 C	0	-10.006	1.508	1.096	C
HETATM 1339 O	0	-11.027	0.902	0.814	O
HETATM 1340 C	0	-8.034	1.706	-0.529	C
HETATM 1341 C	0	-8.281	0.390	-1.298	C
HETATM 1342 C	0	-9.003	0.601	-2.632	C
HETATM 1343 C	0	-6.944	-0.282	-1.614	C
HETATM 1344 H	0	-8.072	3.996	0.653	H
HETATM 1345 H	0	-10.023	2.459	-0.778	H
HETATM 1346 H	0	-7.540	2.413	-1.196	H
HETATM 1347 H	0	-7.351	1.495	0.292	H
HETATM 1348 H	0	-8.871	-0.287	-0.682	H
HETATM 1349 H	0	-8.395	1.199	-3.309	H
HETATM 1350 H	0	-9.971	1.074	-2.473	H
HETATM 1351 H	0	-9.187	-0.370	-3.094	H
HETATM 1352 H	0	-6.345	0.352	-2.266	H
HETATM 1353 H	0	-7.121	-1.239	-2.106	H
HETATM 1354 H	0	-6.394	-0.466	-0.691	H
HETATM 1355 N	0	-9.488	1.506	2.316	N
HETATM 1356 C	0	-10.081	0.832	3.457	C
HETATM 1357 C	0	-11.516	1.286	3.751	C
HETATM 1358 O	0	-12.377	0.488	4.118	O
HETATM 1359 C	0	-9.183	0.971	4.693	C
HETATM 1360 C	0	-8.805	-0.282	5.427	C
HETATM 1361 C	0	-7.680	-0.371	6.169	C
HETATM 1362 C	0	-9.444	-1.606	5.506	C
HETATM 1363 N	0	-7.578	-1.635	6.708	N
HETATM 1364 C	0	-8.627	-2.438	6.330	C
HETATM 1365 C	0	-10.601	-2.219	4.966	C
HETATM 1366 C	0	-8.934	-3.777	6.607	C
HETATM 1367 C	0	-10.912	-3.567	5.226	C
HETATM 1368 C	0	-10.080	-4.348	6.040	C
HETATM 1369 H	0	-8.608	1.991	2.443	H
HETATM 1370 H	0	-10.131	-0.222	3.195	H
HETATM 1371 H	0	-8.248	1.439	4.398	H
HETATM 1372 H	0	-9.649	1.656	5.400	H
HETATM 1373 H	0	-6.963	0.433	6.294	H
HETATM 1374 H	0	-6.786	-1.939	7.271	H
HETATM 1375 H	0	-11.270	-1.664	4.335	H
HETATM 1376 H	0	-8.299	-4.363	7.250	H
HETATM 1377 H	0	-11.800	-4.009	4.795	H
HETATM 1378 H	0	-10.319	-5.384	6.233	H
HETATM 1379 N	0	-11.764	2.580	3.605	N
HETATM 1380 C	0	-13.041	3.257	3.724	C
HETATM 1381 C	0	-14.003	2.881	2.613	C
HETATM 1382 O	0	-15.093	2.420	2.923	O
HETATM 1383 C	0	-12.760	4.773	3.783	C
HETATM 1384 C	0	-13.958	5.734	3.684	C
HETATM 1385 C	0	-14.931	5.604	4.850	C

HETATM 1386	C	0	-13.436	7.172	3.666	C
HETATM 1387	H	0	-10.951	3.155	3.420	H
HETATM 1388	H	0	-13.502	2.960	4.666	H
HETATM 1389	H	0	-12.218	4.983	4.706	H
HETATM 1390	H	0	-12.105	5.013	2.955	H
HETATM 1391	H	0	-14.493	5.550	2.753	H
HETATM 1392	H	0	-14.420	5.810	5.790	H
HETATM 1393	H	0	-15.343	4.600	4.869	H
HETATM 1394	H	0	-15.751	6.311	4.729	H
HETATM 1395	H	0	-12.878	7.379	4.579	H
HETATM 1396	H	0	-14.274	7.866	3.596	H
HETATM 1397	H	0	-12.789	7.319	2.802	H
HETATM 1398	N	0	-13.605	3.054	1.350	N
HETATM 1399	C	0	-14.320	2.531	0.191	C
HETATM 1400	C	0	-14.646	1.040	0.395	C
HETATM 1401	O	0	-15.797	0.686	0.228	O
HETATM 1402	C	0	-13.504	2.708	-1.106	C
HETATM 1403	C	0	-13.559	4.097	-1.753	C
HETATM 1404	C	0	-12.555	4.190	-2.901	C
HETATM 1405	C	0	-14.947	4.391	-2.332	C
HETATM 1406	H	0	-12.678	3.437	1.201	H
HETATM 1407	H	0	-15.274	3.048	0.096	H
HETATM 1408	H	0	-12.467	2.435	-0.915	H
HETATM 1409	H	0	-13.894	2.014	-1.844	H
HETATM 1410	H	0	-13.302	4.844	-1.011	H
HETATM 1411	H	0	-12.793	3.462	-3.676	H
HETATM 1412	H	0	-11.552	3.996	-2.521	H
HETATM 1413	H	0	-12.570	5.190	-3.333	H
HETATM 1414	H	0	-15.246	3.585	-3.004	H
HETATM 1415	H	0	-14.935	5.323	-2.894	H
HETATM 1416	H	0	-15.684	4.471	-1.534	H
HETATM 1417	N	0	-13.692	0.174	0.770	N
HETATM 1418	C	0	-13.896	-1.268	1.051	C
HETATM 1419	C	0	-14.961	-1.456	2.120	C
HETATM 1420	O	0	-15.908	-2.197	1.902	O
HETATM 1421	C	0	-12.574	-1.989	1.384	C
HETATM 1422	C	0	-12.776	-3.368	2.022	C
HETATM 1423	C	0	-11.758	-2.221	0.105	C
HETATM 1424	H	0	-12.751	0.543	0.844	H
HETATM 1425	H	0	-14.300	-1.727	0.150	H
HETATM 1426	H	0	-11.992	-1.380	2.074	H
HETATM 1427	H	0	-11.805	-3.829	2.186	H
HETATM 1428	H	0	-13.373	-4.004	1.368	H
HETATM 1429	H	0	-13.272	-3.277	2.988	H
HETATM 1430	H	0	-12.334	-2.813	-0.607	H
HETATM 1431	H	0	-10.837	-2.751	0.338	H
HETATM 1432	H	0	-11.494	-1.273	-0.358	H
HETATM 1433	N	0	-14.836	-0.791	3.264	N
HETATM 1434	C	0	-15.797	-0.902	4.354	C

HETATM 1435	C	0	-17.174	-0.232	4.090	C
HETATM 1436	O	0	-18.156	-0.605	4.730	O
HETATM 1437	C	0	-15.117	-0.410	5.630	C
HETATM 1438	H	0	-14.019	-0.207	3.396	H
HETATM 1439	H	0	-16.010	-1.962	4.502	H
HETATM 1440	H	0	-14.277	-1.063	5.871	H
HETATM 1441	H	0	-15.827	-0.437	6.458	H
HETATM 1442	H	0	-14.743	0.601	5.486	H
HETATM 1443	N	0	-17.273	0.748	3.182	N
HETATM 1444	C	0	-18.528	1.283	2.622	C
HETATM 1445	C	0	-19.119	0.256	1.611	C
HETATM 1446	O	0	-20.229	-0.212	1.825	O
HETATM 1447	C	0	-18.278	2.634	1.926	C
HETATM 1448	C	0	-18.026	3.811	2.885	C
HETATM 1449	C	0	-17.478	4.998	2.092	C
HETATM 1450	C	0	-19.300	4.257	3.604	C
HETATM 1451	H	0	-16.407	1.055	2.752	H
HETATM 1452	H	0	-19.265	1.409	3.415	H
HETATM 1453	H	0	-17.423	2.527	1.259	H
HETATM 1454	H	0	-19.144	2.876	1.307	H
HETATM 1455	H	0	-17.289	3.530	3.633	H
HETATM 1456	H	0	-18.199	5.299	1.331	H
HETATM 1457	H	0	-16.544	4.706	1.615	H
HETATM 1458	H	0	-17.294	5.834	2.766	H
HETATM 1459	H	0	-20.064	4.538	2.878	H
HETATM 1460	H	0	-19.082	5.111	4.245	H
HETATM 1461	H	0	-19.680	3.449	4.227	H
HETATM 1462	N	0	-18.372	-0.135	0.561	N
HETATM 1463	C	0	-18.651	-1.175	-0.459	C
HETATM 1464	C	0	-19.144	-2.488	0.159	C
HETATM 1465	O	0	-20.022	-3.152	-0.384	O
HETATM 1466	C	0	-17.410	-1.388	-1.333	C
HETATM 1467	H	0	-17.467	0.306	0.483	H
HETATM 1468	H	0	-19.457	-0.812	-1.100	H
HETATM 1469	H	0	-17.613	-2.160	-2.072	H
HETATM 1470	H	0	-16.570	-1.701	-0.715	H
HETATM 1471	H	0	-17.157	-0.464	-1.852	H
HETATM 1472	N	0	-18.541	-2.874	1.280	N
HETATM 1473	C	0	-18.898	-4.052	2.044	C
HETATM 1474	C	0	-20.135	-3.908	2.936	C
HETATM 1475	O	0	-20.767	-4.911	3.264	O
HETATM 1476	C	0	-17.707	-4.455	2.930	C
HETATM 1477	H	0	-17.746	-2.327	1.585	H
HETATM 1478	H	0	-19.108	-4.869	1.352	H
HETATM 1479	H	0	-17.950	-5.374	3.466	H
HETATM 1480	H	0	-17.503	-3.665	3.653	H
HETATM 1481	H	0	-16.816	-4.627	2.330	H
HETATM 1482	N	0	-20.431	-2.690	3.392	N
HETATM 1483	C	0	-21.666	-2.380	4.078	C

HETATM 1484 H	0	-21.835	-3.008	4.928	H
HETATM 1485 H	0	-22.440	-2.541	3.357	H
HETATM 1486 H	0	-21.672	-1.355	4.385	H
HETATM 1487 H	0	-19.903	-1.913	3.016	H
HETATM 1488 N	0	4.272	-2.762	-5.189	N
HETATM 1489 C	0	4.320	-2.244	-3.797	C
HETATM 1490 C	0	5.773	-2.348	-3.238	C
HETATM 1491 O	0	6.644	-2.693	-4.074	O
HETATM 1492 O	0	6.042	-2.127	-2.033	O
HETATM 1493 C	0	3.207	-2.928	-2.985	C
HETATM 1494 C	0	3.131	-2.560	-1.492	C
HETATM 1495 C	0	3.058	-1.072	-1.216	C
HETATM 1496 O	0	2.201	-0.402	-1.776	O
HETATM 1497 N	0	3.950	-0.575	-0.336	N
HETATM 1498 C	0	4.070	0.830	-0.039	C
HETATM 1499 C	0	4.977	1.559	-1.032	C
HETATM 1500 O	0	4.929	2.782	-1.163	O
HETATM 1501 C	0	4.626	1.003	1.386	C
HETATM 1502 S	0	6.217	0.133	1.634	S
HETATM 1503 N	0	5.814	0.765	-1.720	N
HETATM 1504 C	0	6.825	1.265	-2.642	C
HETATM 1505 C	0	6.436	1.097	-4.093	C
HETATM 1506 O	0	5.493	0.348	-4.402	O
HETATM 1507 O	0	7.066	1.744	-4.941	O
HETATM 1508 H	0	5.186	-2.613	-5.595	H
HETATM 1509 H	0	3.526	-2.302	-5.713	H
HETATM 1510 H	0	4.037	-3.752	-5.225	H
HETATM 1511 H	0	4.092	-1.179	-3.807	H
HETATM 1512 H	0	2.253	-2.653	-3.439	H
HETATM 1513 H	0	3.316	-4.006	-3.068	H
HETATM 1514 H	0	3.978	-2.993	-0.961	H
HETATM 1515 H	0	2.229	-2.990	-1.078	H
HETATM 1516 H	0	4.645	-1.172	0.113	H
HETATM 1517 H	0	3.084	1.293	-0.126	H
HETATM 1518 H	0	3.870	0.657	2.097	H
HETATM 1519 H	0	4.748	2.075	1.572	H
HETATM 1520 H	0	5.899	-0.222	-1.501	H
HETATM 1521 H	0	7.013	2.320	-2.463	H
HETATM 1522 H	0	7.753	0.715	-2.495	H
HETATM 1523 O	0	10.948	-6.924	-8.073	O
HETATM 1524 H	0	10.036	-6.636	-7.980	H
HETATM 1525 H	0	11.337	-6.272	-8.670	H
HETATM 1526 O	0	22.004	-2.043	3.032	O
HETATM 1527 H	0	22.754	-2.583	2.765	H
HETATM 1528 H	0	22.373	-1.455	3.696	H
HETATM 1529 O	0	16.304	5.929	-5.207	O
HETATM 1530 H	0	15.486	6.455	-5.098	H
HETATM 1531 H	0	16.915	6.565	-5.586	H
HETATM 1532 O	0	13.860	8.626	3.244	O

HETATM 1533 H	0	13.450	8.548	4.119	H
HETATM 1534 H	0	14.661	9.158	3.432	H
HETATM 1535 O	0	4.734	10.914	6.664	O
HETATM 1536 H	0	5.118	10.803	7.543	H
HETATM 1537 H	0	5.459	10.620	6.090	H
HETATM 1538 O	0	8.035	11.997	7.351	O
HETATM 1539 H	0	7.577	11.239	7.763	H
HETATM 1540 H	0	7.636	12.751	7.786	H
HETATM 1541 O	0	4.753	8.180	9.120	O
HETATM 1542 H	0	3.783	8.286	9.069	H
HETATM 1543 H	0	4.850	7.267	9.439	H
HETATM 1544 O	0	14.253	-1.380	4.299	O
HETATM 1545 H	0	13.525	-1.839	4.778	H
HETATM 1546 H	0	15.024	-1.944	4.492	H
HETATM 1547 O	0	-3.007	-3.070	-6.319	O
HETATM 1548 H	0	-2.768	-3.984	-6.565	H
HETATM 1549 H	0	-3.126	-2.633	-7.182	H
HETATM 1550 O	0	-8.986	3.963	-3.344	O
HETATM 1551 H	0	-8.179	4.354	-3.689	H
HETATM 1552 H	0	-8.754	3.050	-3.174	H
HETATM 1553 O	0	-14.777	1.559	8.031	O
HETATM 1554 H	0	-14.146	0.934	8.444	H
HETATM 1555 H	0	-15.433	1.667	8.742	H
HETATM 1556 O	0	-16.444	-4.486	6.498	O
HETATM 1557 H	0	-16.656	-3.943	7.287	H
HETATM 1558 H	0	-17.209	-4.333	5.933	H
HETATM 1559 O	0	-16.388	2.543	6.025	O
HETATM 1560 H	0	-16.005	2.487	5.139	H
HETATM 1561 H	0	-15.740	2.074	6.588	H
HETATM 1562 O	0	-10.205	-1.387	8.898	O
HETATM 1563 H	0	-10.464	-1.065	8.017	H
HETATM 1564 H	0	-11.012	-1.846	9.192	H
HETATM 1565 O	0	-13.393	3.738	7.210	O
HETATM 1566 H	0	-14.039	4.408	7.466	H
HETATM 1567 H	0	-13.823	2.917	7.521	H
HETATM 1568 O	0	3.222	-7.663	9.354	O
HETATM 1569 H	0	3.313	-6.792	8.924	H
HETATM 1570 H	0	2.538	-8.095	8.804	H
HETATM 1571 O	0	-5.829	-4.410	6.315	O
HETATM 1572 H	0	-6.568	-4.314	5.707	H
HETATM 1573 H	0	-6.081	-5.197	6.841	H
HETATM 1574 O	0	17.163	3.863	-3.678	O
HETATM 1575 H	0	16.788	4.613	-4.186	H
HETATM 1576 H	0	17.829	3.515	-4.274	H
HETATM 1577 O	0	16.308	3.646	-1.128	O
HETATM 1578 H	0	16.626	3.727	-2.052	H
HETATM 1579 H	0	17.039	3.181	-0.688	H
HETATM 1580 O	0	16.448	-2.999	4.750	O
HETATM 1581 H	0	16.223	-3.492	5.562	H

HETATM 1582 H	0	17.252	-3.455	4.444	H
HETATM 1583 O	0	17.990	2.173	0.551	O
HETATM 1584 H	0	18.624	1.439	0.403	H
HETATM 1585 H	0	17.245	1.708	0.972	H
HETATM 1586 O	0	19.433	-2.182	2.211	O
HETATM 1587 H	0	19.173	-3.035	2.611	H
HETATM 1588 H	0	20.363	-2.094	2.509	H
HETATM 1589 O	0	18.409	-4.457	3.349	O
HETATM 1590 H	0	17.682	-4.725	2.747	H
HETATM 1591 H	0	18.838	-5.295	3.551	H
HETATM 1592 O	0	19.398	-0.136	0.366	O
HETATM 1593 H	0	19.372	-0.843	1.040	H
HETATM 1594 H	0	20.084	-0.438	-0.233	H
HETATM 1595 O	0	16.750	-1.637	2.206	O
HETATM 1596 H	0	16.535	-2.065	3.051	H
HETATM 1597 H	0	17.710	-1.797	2.127	H
HETATM 1598 O	0	-2.283	-5.698	-6.618	O
HETATM 1599 H	0	-2.089	-5.949	-5.710	H
HETATM 1600 H	0	-1.530	-6.078	-7.116	H
HETATM 1601 O	0	1.071	0.390	-12.586	O
HETATM 1602 H	0	1.290	0.547	-11.654	H
HETATM 1603 H	0	0.830	-0.537	-12.610	H
HETATM 1604 O	0	-8.256	-12.470	0.683	O
HETATM 1605 H	0	-7.912	-13.176	0.129	H
HETATM 1606 H	0	-9.060	-12.172	0.194	H
HETATM 1607 O	0	-10.506	-11.560	-0.303	O
HETATM 1608 H	0	-11.155	-11.302	0.380	H
HETATM 1609 H	0	-10.804	-11.065	-1.089	H
HETATM 1610 O	0	-6.207	-12.028	3.643	O
HETATM 1611 H	0	-6.762	-11.409	3.136	H
HETATM 1612 H	0	-5.466	-12.198	3.053	H
HETATM 1613 O	0	2.735	-10.576	6.553	O
HETATM 1614 H	0	3.247	-11.357	6.859	H
HETATM 1615 H	0	2.179	-10.932	5.836	H
HETATM 1616 O	0	4.519	-12.359	7.508	O
HETATM 1617 H	0	4.743	-13.178	7.957	H
HETATM 1618 H	0	5.186	-11.732	7.848	H
HETATM 1619 O	0	14.518	-7.056	7.122	O
HETATM 1620 H	0	13.569	-6.989	7.335	H
HETATM 1621 H	0	14.624	-8.004	6.968	H
HETATM 1622 O	0	14.984	7.212	1.134	O
HETATM 1623 H	0	14.542	7.717	1.837	H
HETATM 1624 H	0	15.916	7.227	1.414	H
HETATM 1625 O	0	15.127	8.280	7.154	O
HETATM 1626 H	0	14.292	8.508	6.709	H
HETATM 1627 H	0	15.361	9.087	7.626	H
HETATM 1628 O	0	17.872	9.652	1.911	O
HETATM 1629 H	0	17.847	8.676	1.931	H
HETATM 1630 H	0	18.464	9.845	1.180	H

HETATM 1631	O	0	13.845	10.060	-3.617	O
HETATM 1632	H	0	13.999	10.565	-2.799	H
HETATM 1633	H	0	13.273	10.674	-4.119	H
HETATM 1634	O	0	14.939	4.187	2.468	O
HETATM 1635	H	0	15.899	4.159	2.308	H
HETATM 1636	H	0	14.578	4.393	1.587	H
HETATM 1637	O	0	17.727	4.250	2.253	O
HETATM 1638	H	0	18.352	3.951	2.920	H
HETATM 1639	H	0	17.887	3.621	1.518	H
HETATM 1640	O	0	17.450	6.973	2.319	O
HETATM 1641	H	0	17.636	6.022	2.192	H
HETATM 1642	H	0	17.251	7.025	3.272	H
HETATM 1643	O	0	14.883	12.341	4.361	O
HETATM 1644	H	0	14.055	12.127	4.826	H
HETATM 1645	H	0	14.953	13.295	4.446	H
HETATM 1646	O	0	10.176	4.493	7.176	O
HETATM 1647	H	0	9.326	4.135	7.507	H
HETATM 1648	H	0	10.820	3.821	7.466	H
HETATM 1649	O	0	16.082	9.971	3.885	O
HETATM 1650	H	0	16.765	10.048	3.181	H
HETATM 1651	H	0	15.809	10.903	4.024	H
HETATM 1652	O	0	14.674	5.626	7.601	O
HETATM 1653	H	0	14.743	5.374	6.667	H
HETATM 1654	H	0	14.942	6.564	7.583	H
HETATM 1655	O	0	14.038	1.255	3.820	O
HETATM 1656	H	0	14.205	0.298	3.970	H
HETATM 1657	H	0	14.703	1.473	3.146	H
HETATM 1658	O	0	6.719	9.935	8.593	O
HETATM 1659	H	0	7.462	9.407	8.945	H
HETATM 1660	H	0	5.956	9.354	8.799	H
HETATM 1661	O	0	12.167	2.771	7.902	O
HETATM 1662	H	0	12.548	3.413	8.536	H
HETATM 1663	H	0	12.663	2.960	7.078	H
HETATM 1664	O	0	16.440	7.478	4.847	O
HETATM 1665	H	0	16.406	8.388	4.482	H
HETATM 1666	H	0	16.280	7.642	5.792	H
HETATM 1667	O	0	2.037	8.042	9.200	O
HETATM 1668	H	0	1.085	8.254	9.163	H
HETATM 1669	H	0	2.095	7.418	9.943	H
HETATM 1670	O	0	11.802	6.131	-0.920	O
HETATM 1671	H	0	12.644	5.712	-0.676	H
HETATM 1672	H	0	12.053	6.742	-1.636	H
HETATM 1673	O	0	11.583	1.019	10.066	O
HETATM 1674	H	0	12.094	0.185	10.030	H
HETATM 1675	H	0	11.923	1.514	9.303	H
HETATM 1676	O	0	14.163	7.576	-4.983	O
HETATM 1677	H	0	14.325	8.504	-4.742	H
HETATM 1678	H	0	13.457	7.337	-4.359	H
HETATM 1679	O	0	14.202	4.964	-0.126	O

HETATM 1680	H	0	14.549	5.831	0.178	H
HETATM 1681	H	0	14.976	4.555	-0.570	H
HETATM 1682	O	0	14.581	5.474	4.776	O
HETATM 1683	H	0	14.685	5.017	3.909	H
HETATM 1684	H	0	15.263	6.175	4.714	H
HETATM 1685	O	0	5.304	3.149	8.696	O
HETATM 1686	H	0	4.399	2.907	8.428	H
HETATM 1687	H	0	5.513	2.439	9.350	H
HETATM 1688	O	0	10.532	5.950	9.527	O
HETATM 1689	H	0	11.422	5.621	9.745	H
HETATM 1690	H	0	10.392	5.588	8.637	H
HETATM 1691	O	0	12.310	7.919	-2.931	O
HETATM 1692	H	0	12.925	8.672	-3.018	H
HETATM 1693	H	0	11.443	8.371	-2.948	H
HETATM 1694	O	0	12.596	11.407	5.583	O
HETATM 1695	H	0	12.667	10.448	5.736	H
HETATM 1696	H	0	12.162	11.729	6.383	H
HETATM 1697	O	0	7.986	3.290	8.222	O
HETATM 1698	H	0	7.009	3.232	8.283	H
HETATM 1699	H	0	8.269	2.442	8.634	H
HETATM 1700	O	0	11.132	-2.870	11.304	O
HETATM 1701	H	0	11.743	-2.242	10.875	H
HETATM 1702	H	0	11.381	-3.713	10.888	H
HETATM 1703	O	0	8.520	8.056	9.493	O
HETATM 1704	H	0	7.941	7.308	9.704	H
HETATM 1705	H	0	9.399	7.677	9.630	H
HETATM 1706	O	0	15.741	-4.641	6.944	O
HETATM 1707	H	0	16.337	-4.716	7.696	H
HETATM 1708	H	0	15.327	-5.534	6.919	H
HETATM 1709	O	0	2.621	6.133	11.124	O
HETATM 1710	H	0	2.826	6.221	12.061	H
HETATM 1711	H	0	3.488	5.877	10.741	H
HETATM 1712	O	0	7.811	5.399	10.052	O
HETATM 1713	H	0	8.752	5.525	10.258	H
HETATM 1714	H	0	7.833	4.638	9.448	H
HETATM 1715	O	0	13.101	3.235	5.397	O
HETATM 1716	H	0	13.599	4.044	5.181	H
HETATM 1717	H	0	13.498	2.581	4.782	H
HETATM 1718	O	0	13.072	4.761	9.528	O
HETATM 1719	H	0	13.686	5.119	8.844	H
HETATM 1720	H	0	13.633	4.710	10.309	H
HETATM 1721	O	0	-2.535	3.618	-0.676	O
HETATM 1722	H	0	-2.133	2.892	-0.150	H
HETATM 1723	H	0	-2.542	4.355	-0.053	H
HETATM 1724	O	0	-9.353	-12.656	5.402	O
HETATM 1725	H	0	-9.602	-12.759	4.455	H
HETATM 1726	H	0	-9.903	-13.315	5.835	H
HETATM 1727	O	0	-18.516	3.082	8.874	O
HETATM 1728	H	0	-19.408	3.379	9.082	H

HETATM 1729 H	0	-18.667	2.422	8.169	H
HETATM 1730 O	0	-5.446	2.557	7.205	O
HETATM 1731 H	0	-5.158	3.395	7.602	H
HETATM 1732 H	0	-6.420	2.611	7.284	H
HETATM 1733 O	0	-8.125	2.714	7.627	O
HETATM 1734 H	0	-8.251	2.695	8.593	H
HETATM 1735 H	0	-9.048	2.718	7.312	H
HETATM 1736 O	0	-4.799	4.799	8.806	O
HETATM 1737 H	0	-5.369	4.363	9.481	H
HETATM 1738 H	0	-3.918	4.766	9.225	H
HETATM 1739 O	0	-7.958	-0.034	9.512	O
HETATM 1740 H	0	-8.795	-0.521	9.360	H
HETATM 1741 H	0	-7.576	-0.006	8.627	H
HETATM 1742 O	0	-5.495	-3.261	10.441	O
HETATM 1743 H	0	-4.726	-3.855	10.330	H
HETATM 1744 H	0	-6.245	-3.877	10.328	H
HETATM 1745 O	0	-11.225	-4.057	11.708	O
HETATM 1746 H	0	-10.378	-3.561	11.634	H
HETATM 1747 H	0	-11.317	-4.189	12.657	H
HETATM 1748 O	0	-2.866	-2.410	-3.727	O
HETATM 1749 H	0	-2.993	-2.657	-4.670	H
HETATM 1750 H	0	-2.685	-1.463	-3.777	H
HETATM 1751 O	0	-12.695	-4.872	8.113	O
HETATM 1752 H	0	-13.033	-5.743	8.402	H
HETATM 1753 H	0	-13.014	-4.828	7.193	H
HETATM 1754 O	0	-12.943	0.009	9.259	O
HETATM 1755 H	0	-12.470	-0.046	8.401	H
HETATM 1756 H	0	-12.927	-0.914	9.568	H
HETATM 1757 O	0	-7.829	-10.296	2.222	O
HETATM 1758 H	0	-7.612	-9.596	1.582	H
HETATM 1759 H	0	-8.014	-11.062	1.640	H
HETATM 1760 O	0	-13.480	-7.433	8.740	O
HETATM 1761 H	0	-14.282	-7.393	8.170	H
HETATM 1762 H	0	-13.805	-7.900	9.516	H
HETATM 1763 O	0	-11.960	-7.332	5.425	O
HETATM 1764 H	0	-12.532	-6.553	5.515	H
HETATM 1765 H	0	-11.521	-7.393	6.293	H
HETATM 1766 O	0	-18.648	1.234	6.779	O
HETATM 1767 H	0	-18.835	0.595	6.069	H
HETATM 1768 H	0	-17.920	1.763	6.399	H
HETATM 1769 O	0	-8.292	-8.490	6.995	O
HETATM 1770 H	0	-9.188	-8.279	7.319	H
HETATM 1771 H	0	-8.480	-8.968	6.162	H
HETATM 1772 O	0	-17.215	-3.084	8.683	O
HETATM 1773 H	0	-16.460	-2.870	9.281	H
HETATM 1774 H	0	-17.859	-3.463	9.290	H
HETATM 1775 O	0	-5.739	-0.533	11.129	O
HETATM 1776 H	0	-5.698	-1.507	11.170	H
HETATM 1777 H	0	-6.572	-0.381	10.640	H

HETATM 1778	O	0	-15.301	-7.466	4.492	O
HETATM 1779	H	0	-15.995	-7.455	3.825	H
HETATM 1780	H	0	-14.850	-8.319	4.316	H
HETATM 1781	O	0	-14.166	-9.905	4.057	O
HETATM 1782	H	0	-13.197	-9.806	4.144	H
HETATM 1783	H	0	-14.362	-10.656	4.624	H
HETATM 1784	O	0	-15.249	-2.447	10.339	O
HETATM 1785	H	0	-15.327	-1.677	10.942	H
HETATM 1786	H	0	-14.292	-2.519	10.209	H
HETATM 1787	O	0	-12.080	-10.937	1.837	O
HETATM 1788	H	0	-13.036	-10.929	1.959	H
HETATM 1789	H	0	-11.770	-10.403	2.598	H
HETATM 1790	O	0	-11.686	0.164	6.920	O
HETATM 1791	H	0	-11.996	0.098	6.003	H
HETATM 1792	H	0	-11.321	1.068	6.963	H
HETATM 1793	O	0	-15.675	-7.129	7.235	O
HETATM 1794	H	0	-15.620	-7.414	6.307	H
HETATM 1795	H	0	-16.085	-6.253	7.157	H
HETATM 1796	O	0	-10.320	-5.400	9.455	O
HETATM 1797	H	0	-11.007	-5.061	8.852	H
HETATM 1798	H	0	-10.648	-5.105	10.325	H
HETATM 1799	O	0	-16.073	4.346	8.170	O
HETATM 1800	H	0	-16.223	3.918	7.311	H
HETATM 1801	H	0	-16.935	4.226	8.599	H
HETATM 1802	O	0	-17.561	-0.300	8.810	O
HETATM 1803	H	0	-17.520	-1.252	8.614	H
HETATM 1804	H	0	-18.076	0.061	8.066	H
HETATM 1805	O	0	-11.689	2.342	10.058	O
HETATM 1806	H	0	-12.106	1.464	9.967	H
HETATM 1807	H	0	-12.460	2.902	10.279	H
HETATM 1808	O	0	-10.891	2.758	7.478	O
HETATM 1809	H	0	-11.065	2.667	8.436	H
HETATM 1810	H	0	-11.684	3.253	7.185	H
HETATM 1811	O	0	-11.482	-9.589	4.117	O
HETATM 1812	H	0	-10.555	-9.764	4.378	H
HETATM 1813	H	0	-11.641	-8.710	4.532	H
HETATM 1814	O	0	-8.883	-9.995	4.768	O
HETATM 1815	H	0	-8.920	-10.927	5.058	H
HETATM 1816	H	0	-8.451	-10.059	3.893	H
HETATM 1817	O	0	-12.521	-2.699	9.733	O
HETATM 1818	H	0	-12.662	-3.427	9.089	H
HETATM 1819	H	0	-12.170	-3.177	10.513	H
HETATM 1820	O	0	-16.515	1.687	10.200	O
HETATM 1821	H	0	-16.887	0.863	9.802	H
HETATM 1822	H	0	-17.220	2.327	9.990	H
HETATM 1823	O	0	-8.848	2.477	10.267	O
HETATM 1824	H	0	-8.637	1.525	10.225	H
HETATM 1825	H	0	-9.815	2.482	10.395	H
HETATM 1826	O	0	-14.250	3.476	10.314	O

HETATM 1827	H	0	-14.725	4.029	9.677	H
HETATM 1828	H	0	-14.930	2.843	10.585	H
HETATM 1829	O	0	-15.388	-0.222	11.875	O
HETATM 1830	H	0	-15.745	0.513	11.347	H
HETATM 1831	H	0	-15.506	0.077	12.780	H
HETATM 1832	O	0	-13.949	-5.324	5.621	O
HETATM 1833	H	0	-14.749	-4.848	5.913	H
HETATM 1834	H	0	-14.339	-6.051	5.097	H
HETATM 1835	O	0	-10.814	-7.611	7.908	O
HETATM 1836	H	0	-10.466	-6.936	8.521	H
HETATM 1837	H	0	-11.710	-7.765	8.260	H
HETATM 1838	O	0	-6.535	-6.532	7.827	O
HETATM 1839	H	0	-5.660	-6.951	7.958	H
HETATM 1840	H	0	-7.093	-7.278	7.526	H
HETATM 1841	O	0	-5.230	-1.645	8.300	O
HETATM 1842	H	0	-5.400	-2.094	9.152	H
HETATM 1843	H	0	-4.622	-2.279	7.866	H
HETATM 1844	O	0	-0.434	-7.923	10.372	O
HETATM 1845	H	0	-0.748	-8.544	9.696	H
HETATM 1846	H	0	-0.741	-7.060	10.051	H
HETATM 1847	O	0	9.225	-5.361	10.607	O
HETATM 1848	H	0	10.169	-5.349	10.369	H
HETATM 1849	H	0	8.904	-6.189	10.191	H
HETATM 1850	O	0	0.877	-5.963	7.296	O
HETATM 1851	H	0	1.093	-6.917	7.367	H
HETATM 1852	H	0	1.749	-5.547	7.428	H
HETATM 1853	O	0	-1.788	-1.439	7.309	O
HETATM 1854	H	0	-2.408	-0.687	7.247	H
HETATM 1855	H	0	-2.390	-2.213	7.242	H
HETATM 1856	O	0	-1.635	-7.106	6.732	O
HETATM 1857	H	0	-0.806	-6.610	6.825	H
HETATM 1858	H	0	-1.362	-7.897	6.236	H
HETATM 1859	O	0	3.456	-5.182	8.201	O
HETATM 1860	H	0	3.355	-4.453	8.832	H
HETATM 1861	H	0	4.428	-5.301	8.186	H
HETATM 1862	O	0	7.971	-0.027	11.603	O
HETATM 1863	H	0	8.127	-0.893	12.022	H
HETATM 1864	H	0	8.679	0.518	12.009	H
HETATM 1865	O	0	-6.349	3.606	10.614	O
HETATM 1866	H	0	-5.971	3.033	11.307	H
HETATM 1867	H	0	-7.277	3.307	10.577	H
HETATM 1868	O	0	-6.109	-10.042	7.760	O
HETATM 1869	H	0	-6.903	-9.508	7.580	H
HETATM 1870	H	0	-6.305	-10.870	7.268	H
HETATM 1871	O	0	5.653	-8.410	10.228	O
HETATM 1872	H	0	5.688	-7.752	10.946	H
HETATM 1873	H	0	4.746	-8.267	9.883	H
HETATM 1874	O	0	1.834	-7.095	11.642	O
HETATM 1875	H	0	0.950	-7.441	11.408	H

HETATM 1876 H	0	2.380	-7.429	10.908	H
HETATM 1877 O	0	-7.614	-4.874	9.714	O
HETATM 1878 H	0	-8.544	-5.162	9.629	H
HETATM 1879 H	0	-7.158	-5.487	9.102	H
HETATM 1880 O	0	3.251	-5.086	12.604	O
HETATM 1881 H	0	2.976	-4.979	13.521	H
HETATM 1882 H	0	2.675	-5.827	12.295	H
HETATM 1883 O	0	-1.262	1.611	0.603	O
HETATM 1884 H	0	-0.847	0.900	0.084	H
HETATM 1885 H	0	-1.190	1.295	1.510	H
HETATM 1886 O	0	-3.786	0.460	7.499	O
HETATM 1887 H	0	-4.326	1.256	7.299	H
HETATM 1888 H	0	-4.469	-0.217	7.688	H
HETATM 1889 O	0	6.212	-10.345	8.381	O
HETATM 1890 H	0	5.943	-9.767	7.643	H
HETATM 1891 H	0	5.991	-9.793	9.158	H
HETATM 1892 O	0	5.603	-5.997	11.544	O
HETATM 1893 H	0	6.293	-5.561	12.085	H
HETATM 1894 H	0	4.779	-5.721	11.992	H
HETATM 1895 O	0	7.594	-4.464	12.507	O
HETATM 1896 H	0	8.306	-4.883	11.978	H
HETATM 1897 H	0	8.045	-3.678	12.873	H
HETATM 1898 O	0	-3.736	-9.940	8.939	O
HETATM 1899 H	0	-4.596	-10.022	8.460	H
HETATM 1900 H	0	-3.916	-10.408	9.761	H
HETATM 1901 O	0	6.068	-5.600	8.856	O
HETATM 1902 H	0	5.880	-5.773	9.798	H
HETATM 1903 H	0	6.825	-6.181	8.687	H
HETATM 1904 O	0	-3.905	-7.294	8.205	O
HETATM 1905 H	0	-3.125	-7.196	7.616	H
HETATM 1906 H	0	-3.823	-8.219	8.505	H
HETATM 1907 O	0	1.331	-8.594	7.679	O
HETATM 1908 H	0	1.815	-9.339	7.264	H
HETATM 1909 H	0	0.507	-9.024	7.985	H
HETATM 1910 O	0	-1.000	-9.475	5.388	O
HETATM 1911 H	0	-0.207	-10.004	5.173	H
HETATM 1912 H	0	-1.501	-9.507	4.566	H
HETATM 1913 O	0	-3.479	-4.975	9.555	O
HETATM 1914 H	0	-3.741	-5.851	9.204	H
HETATM 1915 H	0	-2.514	-5.084	9.674	H
HETATM 1916 O	0	-3.213	0.233	10.178	O
HETATM 1917 H	0	-4.058	-0.118	10.517	H
HETATM 1918 H	0	-3.399	0.365	9.230	H
HETATM 1919 O	0	-10.073	-12.727	2.835	O
HETATM 1920 H	0	-10.804	-12.269	2.391	H
HETATM 1921 H	0	-9.397	-12.785	2.140	H
HETATM 1922 O	0	-1.126	-9.677	8.208	O
HETATM 1923 H	0	-1.223	-9.729	7.242	H
HETATM 1924 H	0	-2.034	-9.866	8.520	H

HETATM 1925 O	0	-6.795	-12.149	6.261	O
HETATM 1926 H	0	-7.709	-12.453	6.130	H
HETATM 1927 H	0	-6.448	-12.165	5.346	H
HETATM 1928 O	0	3.425	-3.398	10.476	O
HETATM 1929 H	0	3.396	-3.964	11.278	H
HETATM 1930 H	0	2.468	-3.299	10.267	H
HETATM 1931 O	0	-2.432	4.912	10.183	O
HETATM 1932 H	0	-2.577	4.082	10.688	H
HETATM 1933 H	0	-1.456	4.995	10.214	H
HETATM 1934 O	0	-0.640	8.622	9.260	O
HETATM 1935 H	0	-0.784	9.469	9.689	H
HETATM 1936 H	0	-1.491	8.166	9.370	H
HETATM 1937 O	0	11.855	-5.015	9.635	O
HETATM 1938 H	0	11.982	-5.873	9.203	H
HETATM 1939 H	0	12.353	-4.422	9.035	H
HETATM 1940 O	0	9.102	-2.222	12.897	O
HETATM 1941 H	0	9.844	-2.464	12.294	H
HETATM 1942 H	0	9.563	-1.930	13.689	H
HETATM 1943 O	0	0.050	2.473	11.170	O
HETATM 1944 H	0	-0.874	2.448	11.468	H
HETATM 1945 H	0	0.174	3.407	10.930	H
HETATM 1946 O	0	-3.542	-3.451	7.312	O
HETATM 1947 H	0	-3.447	-4.058	8.073	H
HETATM 1948 H	0	-4.254	-3.882	6.790	H
HETATM 1949 O	0	1.521	0.572	9.930	O
HETATM 1950 H	0	1.124	1.264	10.502	H
HETATM 1951 H	0	0.768	-0.045	9.832	H
HETATM 1952 O	0	5.849	1.163	10.358	O
HETATM 1953 H	0	6.534	0.761	10.927	H
HETATM 1954 H	0	5.137	0.495	10.372	H
HETATM 1955 O	0	0.561	-2.854	7.068	O
HETATM 1956 H	0	0.383	-3.615	6.506	H
HETATM 1957 H	0	-0.243	-2.310	6.978	H
HETATM 1958 O	0	10.194	1.275	12.391	O
HETATM 1959 H	0	10.767	1.211	11.601	H
HETATM 1960 H	0	10.746	1.732	13.028	H
HETATM 1961 O	0	-3.155	7.472	9.818	O
HETATM 1962 H	0	-3.421	7.647	10.727	H
HETATM 1963 H	0	-2.888	6.526	9.864	H
HETATM 1964 O	0	8.123	-7.524	9.382	O
HETATM 1965 H	0	8.623	-8.349	9.226	H
HETATM 1966 H	0	7.276	-7.876	9.715	H
HETATM 1967 O	0	12.842	-1.421	9.760	O
HETATM 1968 H	0	12.303	-1.308	8.929	H
HETATM 1969 H	0	13.473	-2.097	9.484	H
HETATM 1970 O	0	0.905	-3.079	9.712	O
HETATM 1971 H	0	0.897	-3.018	8.731	H
HETATM 1972 H	0	0.324	-2.334	9.960	H
HETATM 1973 O	0	-0.736	-0.915	9.741	O

HETATM 1974	H	0	-1.052	-1.117	8.837	H
HETATM 1975	H	0	-1.533	-0.530	10.151	H
HETATM 1976	O	0	5.051	5.546	10.038	O
HETATM 1977	H	0	5.996	5.624	10.271	H
HETATM 1978	H	0	5.041	4.693	9.563	H
HETATM 1979	O	0	-8.978	-2.824	10.977	O
HETATM 1980	H	0	-8.344	-3.455	10.592	H
HETATM 1981	H	0	-9.232	-2.277	10.217	H
HETATM 1982	O	0	0.265	5.077	10.271	O
HETATM 1983	H	0	1.071	5.463	10.669	H
HETATM 1984	H	0	0.491	5.048	9.329	H
HETATM 1985	O	0	13.255	-3.595	7.778	O
HETATM 1986	H	0	12.834	-3.075	7.058	H
HETATM 1987	H	0	14.088	-3.889	7.374	H
HETATM 1988	O	0	3.934	-0.720	9.930	O
HETATM 1989	H	0	3.086	-0.229	9.920	H
HETATM 1990	H	0	3.654	-1.613	10.197	H
HETATM 1991	O	0	8.947	0.999	9.248	O
HETATM 1992	H	0	9.873	0.936	9.550	H
HETATM 1993	H	0	8.463	0.596	9.993	H
HETATM 1994	O	0	8.829	-10.150	9.208	O
HETATM 1995	H	0	7.955	-10.392	8.850	H
HETATM 1996	H	0	9.113	-10.945	9.665	H
HETATM 1997	O	0	-2.763	2.558	11.464	O
HETATM 1998	H	0	-3.572	2.497	12.004	H
HETATM 1999	H	0	-2.799	1.711	10.973	H
HETATM 2000	O	0	-0.760	-5.311	9.423	O
HETATM 2001	H	0	-0.259	-5.530	8.616	H
HETATM 2002	H	0	-0.220	-4.598	9.806	H
HETATM 2003	O	0	-5.290	1.814	12.435	O
HETATM 2004	H	0	-5.556	1.642	13.344	H
HETATM 2005	H	0	-5.436	0.947	12.000	H
HETATM 2006	C	0	11.787	-1.105	6.392	C
HETATM 2007	O	0	11.564	-1.046	7.630	O
HETATM 2008	C	0	11.602	0.236	5.619	C
HETATM 2009	C	0	10.326	0.984	5.985	C
HETATM 2010	C	0	9.087	0.373	5.332	C
HETATM 2011	C	0	7.810	1.034	5.775	C
HETATM 2012	O	0	12.224	-2.104	5.769	O
HETATM 2013	C	0	6.471	0.516	5.461	C
HETATM 2014	C	0	5.301	1.411	5.383	C
HETATM 2015	O	0	7.031	0.394	6.790	O
HETATM 2016	C	0	4.129	1.048	4.855	C
HETATM 2017	C	0	2.950	1.904	4.808	C
HETATM 2018	C	0	1.709	1.435	4.638	C
HETATM 2019	C	0	0.604	2.251	4.576	C
HETATM 2020	C	0	-0.688	1.840	4.512	C
HETATM 2021	C	0	-1.159	0.404	4.661	C
HETATM 2022	C	0	-1.583	-0.222	3.341	C

HETATM 2023	C	0	-2.809	-0.774	3.120	C
HETATM 2024	C	0	-3.900	-0.840	4.184	C
HETATM 2025	C	0	-5.010	-1.835	3.837	C
HETATM 2026	C	0	-6.003	-1.353	2.772	C
HETATM 2027	C	0	-7.155	-2.365	2.706	C
HETATM 2028	C	0	-8.125	-2.060	1.566	C
HETATM 2029	H	0	12.462	0.848	5.908	H
HETATM 2030	H	0	11.663	0.066	4.538	H
HETATM 2031	H	0	10.237	0.952	7.074	H
HETATM 2032	H	0	10.390	2.044	5.687	H
HETATM 2033	H	0	9.020	-0.698	5.553	H
HETATM 2034	H	0	9.172	0.456	4.240	H
HETATM 2035	H	0	7.885	2.112	5.949	H
HETATM 2036	H	0	6.413	-0.422	4.913	H
HETATM 2037	H	0	5.428	2.388	5.850	H
HETATM 2038	H	0	4.035	0.049	4.440	H
HETATM 2039	H	0	3.133	2.966	4.977	H
HETATM 2040	H	0	1.594	0.359	4.562	H
HETATM 2041	H	0	0.774	3.327	4.605	H
HETATM 2042	H	0	-1.451	2.610	4.490	H
HETATM 2043	H	0	-1.993	0.439	5.356	H
HETATM 2044	H	0	-0.399	-0.220	5.128	H
HETATM 2045	H	0	-0.841	-0.277	2.548	H
HETATM 2046	H	0	-3.003	-1.225	2.147	H
HETATM 2047	H	0	-4.335	0.143	4.361	H
HETATM 2048	H	0	-3.458	-1.182	5.118	H
HETATM 2049	H	0	-5.559	-2.047	4.754	H
HETATM 2050	H	0	-4.551	-2.759	3.493	H
HETATM 2051	H	0	-6.398	-0.371	3.042	H
HETATM 2052	H	0	-5.503	-1.287	1.804	H
HETATM 2053	H	0	-7.703	-2.344	3.645	H
HETATM 2054	H	0	-6.762	-3.374	2.582	H
HETATM 2055	H	0	-8.518	-1.051	1.671	H
HETATM 2056	H	0	-7.617	-2.153	0.607	H
HETATM 2057	H	0	-8.948	-2.772	1.603	H

TS (head-to-tail orientation, from scan between GSH and C6 of LTA₄, not optimized)

HETATM 1	C	0	-15.068	-7.338	-7.468	C
HETATM 2	H	0	-15.596	-8.245	-7.259	H
HETATM 3	H	0	-14.281	-7.536	-8.166	H
HETATM 4	H	0	-15.743	-6.621	-7.886	H
HETATM 5	C	0	-14.435	-6.948	-6.133	C
HETATM 6	O	0	-13.222	-7.035	-5.976	O
HETATM 7	N	0	-15.249	-6.641	-5.119	N
HETATM 8	C	0	-14.839	-6.275	-3.742	C
HETATM 9	C	0	-14.001	-7.305	-3.005	C
HETATM 10	O	0	-12.933	-6.992	-2.481	O
HETATM 11	C	0	-16.117	-5.931	-2.964	C

HETATM	12	C	0	-15.878	-5.509	-1.507	C
HETATM	13	C	0	-15.041	-4.235	-1.401	C
HETATM	14	C	0	-17.233	-5.272	-0.863	C
HETATM	15	H	0	-16.230	-6.588	-5.345	H
HETATM	16	H	0	-14.230	-5.372	-3.813	H
HETATM	17	H	0	-16.628	-5.120	-3.482	H
HETATM	18	H	0	-16.778	-6.800	-2.968	H
HETATM	19	H	0	-15.380	-6.308	-0.958	H
HETATM	20	H	0	-15.035	-3.891	-0.368	H
HETATM	21	H	0	-15.466	-3.457	-2.034	H
HETATM	22	H	0	-14.014	-4.433	-1.707	H
HETATM	23	H	0	-17.081	-4.951	0.161	H
HETATM	24	H	0	-17.819	-6.191	-0.857	H
HETATM	25	H	0	-17.786	-4.503	-1.402	H
HETATM	26	N	0	-14.494	-8.540	-2.959	N
HETATM	27	C	0	-13.727	-9.653	-2.420	C
HETATM	28	H	0	-14.255	-10.589	-2.604	H
HETATM	29	C	0	-12.318	-9.751	-3.047	C
HETATM	30	O	0	-11.359	-10.098	-2.363	O
HETATM	31	H	0	-15.397	-8.704	-3.377	H
HETATM	32	H	0	-13.610	-9.525	-1.343	H
HETATM	33	N	0	-12.179	-9.397	-4.331	N
HETATM	34	C	0	-10.911	-9.302	-5.062	C
HETATM	35	C	0	-10.049	-8.118	-4.690	C
HETATM	36	O	0	-8.852	-8.289	-4.534	O
HETATM	37	H	0	-12.999	-9.057	-4.811	H
HETATM	38	H	0	-10.335	-10.212	-4.895	H
HETATM	39	H	0	-11.123	-9.234	-6.129	H
HETATM	40	N	0	-10.620	-6.933	-4.493	N
HETATM	41	C	0	-9.886	-5.812	-3.887	C
HETATM	42	C	0	-9.219	-6.205	-2.596	C
HETATM	43	O	0	-8.055	-5.896	-2.397	O
HETATM	44	C	0	-10.800	-4.590	-3.654	C
HETATM	45	C	0	-10.115	-3.497	-2.821	C
HETATM	46	C	0	-11.235	-3.997	-4.995	C
HETATM	47	H	0	-11.610	-6.844	-4.699	H
HETATM	48	H	0	-9.091	-5.512	-4.569	H
HETATM	49	H	0	-11.693	-4.899	-3.115	H
HETATM	50	H	0	-9.160	-3.226	-3.262	H
HETATM	51	H	0	-9.949	-3.842	-1.801	H
HETATM	52	H	0	-10.754	-2.621	-2.761	H
HETATM	53	H	0	-11.749	-4.747	-5.595	H
HETATM	54	H	0	-10.364	-3.636	-5.540	H
HETATM	55	H	0	-11.923	-3.170	-4.824	H
HETATM	56	N	0	-9.941	-6.887	-1.720	N
HETATM	57	C	0	-9.366	-7.407	-0.496	C

HETATM	58	C	0	-8.285	-8.486	-0.715	C
HETATM	59	O	0	-7.340	-8.534	0.073	O
HETATM	60	C	0	-10.513	-7.931	0.389	C
HETATM	61	C	0	-11.205	-6.798	1.172	C
HETATM	62	C	0	-12.614	-7.214	1.590	C
HETATM	63	C	0	-10.391	-6.442	2.420	C
HETATM	64	H	0	-10.914	-7.065	-1.946	H
HETATM	65	H	0	-8.869	-6.590	0.027	H
HETATM	66	H	0	-11.243	-8.442	-0.239	H
HETATM	67	H	0	-10.127	-8.664	1.099	H
HETATM	68	H	0	-11.294	-5.912	0.541	H
HETATM	69	H	0	-12.574	-8.117	2.194	H
HETATM	70	H	0	-13.219	-7.396	0.702	H
HETATM	71	H	0	-13.077	-6.418	2.172	H
HETATM	72	H	0	-10.931	-5.721	3.030	H
HETATM	73	H	0	-9.432	-6.011	2.137	H
HETATM	74	H	0	-10.218	-7.332	3.024	H
HETATM	75	N	0	-8.388	-9.337	-1.746	N
HETATM	76	C	0	-7.291	-10.213	-2.199	C
HETATM	77	C	0	-6.071	-9.358	-2.662	C
HETATM	78	O	0	-4.947	-9.582	-2.218	O
HETATM	79	C	0	-7.789	-11.191	-3.278	C
HETATM	80	C	0	-6.723	-12.207	-3.729	C
HETATM	81	C	0	-6.316	-13.163	-2.603	C
HETATM	82	C	0	-7.271	-13.042	-4.886	C
HETATM	83	H	0	-9.214	-9.268	-2.324	H
HETATM	84	H	0	-6.960	-10.792	-1.337	H
HETATM	85	H	0	-8.657	-11.730	-2.897	H
HETATM	86	H	0	-8.099	-10.626	-4.154	H
HETATM	87	H	0	-5.843	-11.675	-4.082	H
HETATM	88	H	0	-7.194	-13.667	-2.203	H
HETATM	89	H	0	-5.805	-12.612	-1.815	H
HETATM	90	H	0	-5.623	-13.908	-2.993	H
HETATM	91	H	0	-8.159	-13.592	-4.572	H
HETATM	92	H	0	-6.510	-13.745	-5.225	H
HETATM	93	H	0	-7.524	-12.386	-5.720	H
HETATM	94	N	0	-6.276	-8.346	-3.515	N
HETATM	95	C	0	-5.242	-7.438	-4.042	C
HETATM	96	C	0	-4.571	-6.555	-2.958	C
HETATM	97	O	0	-3.344	-6.470	-2.907	O
HETATM	98	C	0	-5.764	-6.624	-5.227	C
HETATM	99	C	0	-6.171	-7.469	-6.451	C
HETATM	100	C	0	-5.101	-8.437	-6.944	C
HETATM	101	N	0	-3.925	-7.982	-7.319	N
HETATM	102	O	0	-5.307	-9.635	-7.002	O
HETATM	103	H	0	-7.224	-8.233	-3.851	H

HETATM 104 H	0	-4.438	-8.070	-4.417	H
HETATM 105 H	0	-6.621	-6.040	-4.898	H
HETATM 106 H	0	-4.973	-5.941	-5.538	H
HETATM 107 H	0	-6.433	-6.806	-7.274	H
HETATM 108 H	0	-7.058	-8.049	-6.213	H
HETATM 109 H	0	-3.313	-8.690	-7.688	H
HETATM 110 H	0	-3.650	-7.009	-7.270	H
HETATM 111 N	0	-5.349	-5.935	-2.064	N
HETATM 112 C	0	-4.911	-5.252	-0.838	C
HETATM 113 C	0	-4.110	-6.195	0.048	C
HETATM 114 O	0	-3.029	-5.825	0.507	O
HETATM 115 C	0	-6.126	-4.663	-0.121	C
HETATM 116 H	0	-6.346	-6.024	-2.210	H
HETATM 117 H	0	-4.251	-4.432	-1.125	H
HETATM 118 H	0	-5.779	-4.092	0.737	H
HETATM 119 H	0	-6.792	-5.458	0.215	H
HETATM 120 H	0	-6.667	-3.999	-0.797	H
HETATM 121 N	0	-4.608	-7.422	0.247	N
HETATM 122 C	0	-3.834	-8.468	0.892	C
HETATM 123 C	0	-2.433	-8.646	0.271	C
HETATM 124 O	0	-1.449	-8.671	1.009	O
HETATM 125 C	0	-4.598	-9.782	1.066	C
HETATM 126 C	0	-3.745	-10.891	1.649	C
HETATM 127 C	0	-3.472	-10.917	3.031	C
HETATM 128 C	0	-3.196	-11.873	0.802	C
HETATM 129 C	0	-2.666	-11.937	3.574	C
HETATM 130 C	0	-2.380	-12.886	1.339	C
HETATM 131 C	0	-2.116	-12.922	2.725	C
HETATM 132 O	0	-1.317	-13.894	3.234	O
HETATM 133 H	0	-5.514	-7.663	-0.140	H
HETATM 134 H	0	-3.638	-8.116	1.904	H
HETATM 135 H	0	-5.427	-9.594	1.743	H
HETATM 136 H	0	-5.012	-10.116	0.121	H
HETATM 137 H	0	-3.903	-10.165	3.681	H
HETATM 138 H	0	-3.397	-11.843	-0.262	H
HETATM 139 H	0	-2.474	-11.969	4.636	H
HETATM 140 H	0	-1.952	-13.647	0.704	H
HETATM 141 H	0	-1.370	-13.933	4.190	H
HETATM 142 N	0	-2.299	-8.712	-1.057	N
HETATM 143 C	0	-0.988	-8.773	-1.719	C
HETATM 144 C	0	-0.068	-7.584	-1.432	C
HETATM 145 O	0	1.069	-7.794	-1.026	O
HETATM 146 C	0	-1.142	-9.067	-3.218	C
HETATM 147 C	0	-1.862	-10.357	-3.587	C
HETATM 148 C	0	-2.646	-10.395	-4.755	C
HETATM 149 C	0	-1.709	-11.535	-2.823	C

HETATM 150 C	0	-3.278	-11.585	-5.152	C
HETATM 151 C	0	-2.349	-12.725	-3.216	C
HETATM 152 C	0	-3.131	-12.751	-4.382	C
HETATM 153 H	0	-3.142	-8.743	-1.622	H
HETATM 154 H	0	-0.462	-9.623	-1.289	H
HETATM 155 H	0	-1.646	-8.227	-3.694	H
HETATM 156 H	0	-0.145	-9.135	-3.645	H
HETATM 157 H	0	-2.758	-9.512	-5.364	H
HETATM 158 H	0	-1.095	-11.550	-1.937	H
HETATM 159 H	0	-3.879	-11.601	-6.052	H
HETATM 160 H	0	-2.229	-13.625	-2.631	H
HETATM 161 H	0	-3.617	-13.665	-4.695	H
HETATM 162 N	0	-0.509	-6.343	-1.612	N
HETATM 163 C	0	0.291	-5.142	-1.288	C
HETATM 164 C	0	0.680	-5.104	0.197	C
HETATM 165 O	0	1.830	-4.815	0.507	O
HETATM 166 C	0	-0.539	-3.911	-1.663	C
HETATM 167 O	0	-0.888	-4.003	-3.030	O
HETATM 168 H	0	-1.443	-6.219	-1.992	H
HETATM 169 H	0	1.206	-5.134	-1.876	H
HETATM 170 H	0	0.039	-3.004	-1.492	H
HETATM 171 H	0	-1.447	-3.880	-1.058	H
HETATM 172 H	0	-1.654	-3.403	-3.196	H
HETATM 173 N	0	-0.226	-5.444	1.124	N
HETATM 174 C	0	0.077	-5.653	2.551	C
HETATM 175 C	0	1.169	-6.693	2.780	C
HETATM 176 O	0	2.088	-6.480	3.571	O
HETATM 177 C	0	-1.198	-6.071	3.302	C
HETATM 178 C	0	-2.207	-4.941	3.551	C
HETATM 179 C	0	-3.526	-5.565	4.010	C
HETATM 180 C	0	-1.702	-3.981	4.630	C
HETATM 181 H	0	-1.165	-5.666	0.802	H
HETATM 182 H	0	0.445	-4.719	2.971	H
HETATM 183 H	0	-1.687	-6.864	2.742	H
HETATM 184 H	0	-0.910	-6.489	4.266	H
HETATM 185 H	0	-2.383	-4.380	2.634	H
HETATM 186 H	0	-3.374	-6.155	4.912	H
HETATM 187 H	0	-3.926	-6.200	3.223	H
HETATM 188 H	0	-4.253	-4.789	4.223	H
HETATM 189 H	0	-2.460	-3.226	4.821	H
HETATM 190 H	0	-0.799	-3.476	4.292	H
HETATM 191 H	0	-1.508	-4.528	5.552	H
HETATM 192 N	0	1.077	-7.823	2.090	N
HETATM 193 C	0	2.138	-8.812	2.093	C
HETATM 194 C	0	3.450	-8.287	1.528	C
HETATM 195 O	0	4.474	-8.555	2.134	O

HETATM 196 C	0	1.709 -10.099	1.362	C
HETATM 197 C	0	0.674 -10.941	2.127	C
HETATM 198 C	0	1.242 -11.580	3.388	C
HETATM 199 N	0	1.976 -12.664	3.279	N
HETATM 200 O	0	1.038 -11.111	4.501	O
HETATM 201 H	0	0.266 -7.962	1.493	H
HETATM 202 H	0	2.344 -9.074	3.132	H
HETATM 203 H	0	1.297 -9.847	0.388	H
HETATM 204 H	0	2.590 -10.719	1.192	H
HETATM 205 H	0	0.317 -11.732	1.467	H
HETATM 206 H	0	-0.179 -10.325	2.403	H
HETATM 207 H	0	2.310 -13.075	4.133	H
HETATM 208 H	0	2.122 -13.096	2.384	H
HETATM 209 N	0	3.459 -7.543	0.419	N
HETATM 210 C	0	4.665 -6.871	-0.088	C
HETATM 211 C	0	5.229 -5.877	0.929	C
HETATM 212 O	0	6.435 -5.831	1.114	O
HETATM 213 C	0	4.438 -6.162	-1.434	C
HETATM 214 C	0	5.711 -5.472	-1.940	C
HETATM 215 C	0	4.056 -7.113	-2.564	C
HETATM 216 H	0	2.574 -7.421	-0.064	H
HETATM 217 H	0	5.422 -7.632	-0.256	H
HETATM 218 H	0	3.648 -5.425	-1.315	H
HETATM 219 H	0	6.523 -6.197	-1.979	H
HETATM 220 H	0	5.993 -4.650	-1.284	H
HETATM 221 H	0	5.557 -5.078	-2.944	H
HETATM 222 H	0	3.757 -6.520	-3.421	H
HETATM 223 H	0	3.244 -7.773	-2.272	H
HETATM 224 H	0	4.909 -7.708	-2.875	H
HETATM 225 N	0	4.389 -5.091	1.601	N
HETATM 226 C	0	4.750 -4.173	2.692	C
HETATM 227 C	0	5.486 -4.871	3.814	C
HETATM 228 O	0	6.632 -4.544	4.129	O
HETATM 229 C	0	3.470 -3.453	3.215	C
HETATM 230 C	0	3.134 -2.280	2.283	C
HETATM 231 C	0	3.567 -2.954	4.671	C
HETATM 232 C	0	1.682 -1.789	2.345	C
HETATM 233 H	0	3.409 -5.162	1.346	H
HETATM 234 H	0	5.422 -3.408	2.306	H
HETATM 235 H	0	2.638 -4.147	3.172	H
HETATM 236 H	0	3.806 -1.455	2.504	H
HETATM 237 H	0	3.315 -2.601	1.264	H
HETATM 238 H	0	3.571 -3.789	5.371	H
HETATM 239 H	0	2.699 -2.350	4.927	H
HETATM 240 H	0	4.477 -2.372	4.806	H
HETATM 241 H	0	1.551 -0.968	1.640	H

HETATM 242 H	0	1.436	-1.434	3.343	H
HETATM 243 H	0	1.003	-2.597	2.073	H
HETATM 244 N	0	4.804	-5.851	4.394	N
HETATM 245 C	0	5.376	-6.784	5.337	C
HETATM 246 C	0	6.686	-7.366	4.742	C
HETATM 247 O	0	7.709	-7.366	5.416	O
HETATM 248 C	0	4.339	-7.872	5.617	C
HETATM 249 O	0	4.808	-8.838	6.529	O
HETATM 250 H	0	3.857	-6.014	4.062	H
HETATM 251 H	0	5.615	-6.269	6.266	H
HETATM 252 H	0	4.074	-8.370	4.684	H
HETATM 253 H	0	3.439	-7.408	6.025	H
HETATM 254 H	0	4.082	-9.496	6.598	H
HETATM 255 N	0	6.714	-7.775	3.461	N
HETATM 256 C	0	7.870	-8.316	2.727	C
HETATM 257 C	0	9.080	-7.400	2.612	C
HETATM 258 O	0	10.208	-7.859	2.801	O
HETATM 259 C	0	7.495	-8.919	1.367	C
HETATM 260 H	0	5.833	-7.768	2.963	H
HETATM 261 H	0	8.212	-9.160	3.325	H
HETATM 262 H	0	8.344	-9.483	0.980	H
HETATM 263 H	0	7.260	-8.138	0.652	H
HETATM 264 H	0	6.655	-9.605	1.473	H
HETATM 265 N	0	8.864	-6.109	2.350	N
HETATM 266 C	0	9.901	-5.079	2.417	C
HETATM 267 C	0	10.654	-5.172	3.754	C
HETATM 268 O	0	11.863	-4.981	3.784	O
HETATM 269 C	0	9.316	-3.657	2.277	C
HETATM 270 C	0	8.386	-3.432	1.072	C
HETATM 271 C	0	8.554	-2.054	0.424	C
HETATM 272 N	0	9.755	-2.034	-0.429	N
HETATM 273 C	0	9.821	-2.167	-1.739	C
HETATM 274 N	0	8.765	-2.217	-2.472	N
HETATM 275 N	0	10.964	-2.251	-2.345	N
HETATM 276 H	0	7.900	-5.845	2.162	H
HETATM 277 H	0	10.623	-5.251	1.621	H
HETATM 278 H	0	8.761	-3.401	3.180	H
HETATM 279 H	0	10.152	-2.962	2.225	H
HETATM 280 H	0	7.360	-3.512	1.416	H
HETATM 281 H	0	8.558	-4.199	0.321	H
HETATM 282 H	0	8.630	-1.292	1.200	H
HETATM 283 H	0	7.662	-1.827	-0.160	H
HETATM 284 H	0	10.649	-2.080	0.039	H
HETATM 285 H	0	8.779	-2.262	-3.475	H
HETATM 286 H	0	7.831	-2.171	-2.068	H
HETATM 287 H	0	11.799	-1.951	-1.870	H

HETATM 288 H	0	10.977	-2.352	-3.353	H
HETATM 289 N	0	9.949	-5.473	4.854	N
HETATM 290 C	0	10.441	-5.450	6.251	C
HETATM 291 C	0	10.858	-6.827	6.805	C
HETATM 292 O	0	11.833	-6.880	7.554	O
HETATM 293 C	0	9.436	-4.727	7.149	C
HETATM 294 C	0	9.088	-3.306	6.665	C
HETATM 295 C	0	8.978	-2.304	7.806	C
HETATM 296 N	0	8.075	-2.758	8.877	N
HETATM 297 C	0	6.825	-2.389	9.070	C
HETATM 298 N	0	6.151	-1.618	8.214	N
HETATM 299 N	0	6.181	-2.757	10.214	N
HETATM 300 H	0	8.960	-5.640	4.701	H
HETATM 301 H	0	11.349	-4.838	6.247	H
HETATM 302 H	0	8.522	-5.319	7.295	H
HETATM 303 H	0	9.911	-4.638	8.130	H
HETATM 304 H	0	8.166	-3.312	6.069	H
HETATM 305 H	0	9.904	-2.936	6.033	H
HETATM 306 H	0	8.624	-1.332	7.457	H
HETATM 307 H	0	9.970	-2.118	8.230	H
HETATM 308 H	0	8.411	-3.518	9.466	H
HETATM 309 H	0	5.335	-1.149	8.603	H
HETATM 310 H	0	6.585	-1.162	7.403	H
HETATM 311 H	0	6.670	-3.394	10.837	H
HETATM 312 H	0	5.191	-2.968	10.135	H
HETATM 313 N	0	10.219	-7.927	6.396	N
HETATM 314 C	0	10.712	-9.311	6.512	C
HETATM 315 C	0	12.090	-9.413	5.800	C
HETATM 316 O	0	13.098	-9.727	6.429	O
HETATM 317 C	0	9.669	-10.270	5.923	C
HETATM 318 H	0	9.364	-7.771	5.879	H
HETATM 319 H	0	10.860	-9.550	7.567	H
HETATM 320 H	0	9.996	-11.299	6.076	H
HETATM 321 H	0	9.548	-10.090	4.856	H
HETATM 322 H	0	8.709	-10.125	6.421	H
HETATM 323 N	0	12.152	-9.089	4.498	N
HETATM 324 C	0	13.317	-9.274	3.617	C
HETATM 325 H	0	12.966	-9.364	2.589	H
HETATM 326 C	0	14.394	-8.138	3.651	C
HETATM 327 O	0	15.550	-8.424	3.355	O
HETATM 328 H	0	11.293	-8.782	4.055	H
HETATM 329 H	0	13.815	-10.208	3.880	H
HETATM 330 N	0	14.068	-6.861	3.947	N
HETATM 331 C	0	14.990	-5.680	3.982	C
HETATM 332 H	0	15.973	-5.990	4.336	H
HETATM 333 C	0	15.132	-5.037	2.611	C

HETATM 334 O	0	16.200	-5.089	1.999	O
HETATM 335 H	0	13.096	-6.671	4.145	H
HETATM 336 H	0	14.580	-4.939	4.666	H
HETATM 337 N	0	14.046	-4.431	2.133	N
HETATM 338 C	0	13.883	-3.966	0.753	C
HETATM 339 C	0	13.357	-2.520	0.770	C
HETATM 340 O	0	12.156	-2.298	0.879	O
HETATM 341 C	0	13.043	-4.934	-0.097	C
HETATM 342 C	0	13.492	-4.757	-1.542	C
HETATM 343 C	0	13.245	-6.399	0.311	C
HETATM 344 H	0	13.232	-4.442	2.739	H
HETATM 345 H	0	14.877	-3.928	0.308	H
HETATM 346 H	0	11.982	-4.697	-0.024	H
HETATM 347 H	0	12.913	-5.401	-2.191	H
HETATM 348 H	0	14.549	-5.000	-1.656	H
HETATM 349 H	0	13.317	-3.733	-1.848	H
HETATM 350 H	0	14.304	-6.609	0.448	H
HETATM 351 H	0	12.859	-7.052	-0.460	H
HETATM 352 H	0	12.711	-6.606	1.239	H
HETATM 353 N	0	14.233	-1.508	0.683	N
HETATM 354 C	0	13.855	-0.072	0.631	C
HETATM 355 C	0	12.871	0.209	-0.496	C
HETATM 356 O	0	12.928	-0.461	-1.528	O
HETATM 357 C	0	15.094	0.807	0.456	C
HETATM 358 O	0	15.888	0.783	1.629	O
HETATM 359 H	0	15.215	-1.752	0.743	H
HETATM 360 H	0	13.386	0.160	1.581	H
HETATM 361 H	0	14.783	1.836	0.270	H
HETATM 362 H	0	15.677	0.458	-0.399	H
HETATM 363 H	0	16.171	-0.148	1.803	H
HETATM 364 N	0	11.942	1.157	-0.314	N
HETATM 365 C	0	10.776	1.290	-1.175	C
HETATM 366 C	0	10.982	1.318	-2.676	C
HETATM 367 O	0	10.346	0.522	-3.365	O
HETATM 368 C	0	10.015	2.525	-0.681	C
HETATM 369 C	0	10.438	2.630	0.776	C
HETATM 370 C	0	11.876	2.134	0.768	C
HETATM 371 H	0	10.133	0.439	-0.967	H
HETATM 372 H	0	10.327	3.422	-1.209	H
HETATM 373 H	0	8.938	2.394	-0.778	H
HETATM 374 H	0	9.832	1.952	1.378	H
HETATM 375 H	0	10.367	3.654	1.139	H
HETATM 376 H	0	12.112	1.711	1.743	H
HETATM 377 H	0	12.549	2.965	0.548	H
HETATM 378 N	0	11.856	2.182	-3.212	N
HETATM 379 C	0	11.933	2.327	-4.647	C

HETATM 380 C	0	12.623	1.162	-5.350	C
HETATM 381 O	0	12.741	1.154	-6.578	O
HETATM 382 C	0	12.683	3.645	-4.864	C
HETATM 383 C	0	13.640	3.694	-3.679	C
HETATM 384 C	0	12.800	3.086	-2.560	C
HETATM 385 H	0	10.939	2.416	-5.081	H
HETATM 386 H	0	13.211	3.682	-5.818	H
HETATM 387 H	0	11.978	4.472	-4.787	H
HETATM 388 H	0	13.951	4.713	-3.446	H
HETATM 389 H	0	14.503	3.058	-3.877	H
HETATM 390 H	0	12.263	3.877	-2.044	H
HETATM 391 H	0	13.457	2.561	-1.867	H
HETATM 392 N	0	13.061	0.156	-4.591	N
HETATM 393 C	0	13.489	-1.109	-5.140	C
HETATM 394 C	0	12.300	-1.826	-5.776	C
HETATM 395 O	0	11.565	-2.574	-5.132	O
HETATM 396 C	0	14.288	-1.908	-4.101	C
HETATM 397 C	0	15.469	-1.162	-3.445	C
HETATM 398 C	0	16.140	-2.071	-2.415	C
HETATM 399 C	0	16.531	-0.740	-4.462	C
HETATM 400 H	0	12.889	0.209	-3.596	H
HETATM 401 H	0	14.187	-0.891	-5.950	H
HETATM 402 H	0	13.602	-2.237	-3.329	H
HETATM 403 H	0	14.697	-2.779	-4.602	H
HETATM 404 H	0	15.113	-0.271	-2.930	H
HETATM 405 H	0	16.540	-2.960	-2.904	H
HETATM 406 H	0	15.409	-2.376	-1.671	H
HETATM 407 H	0	16.948	-1.536	-1.917	H
HETATM 408 H	0	16.885	-1.607	-5.020	H
HETATM 409 H	0	17.372	-0.279	-3.943	H
HETATM 410 H	0	16.116	-0.006	-5.151	H
HETATM 411 N	0	12.174	-1.630	-7.091	N
HETATM 412 C	0	11.453	-2.494	-8.038	C
HETATM 413 C	0	12.112	-3.882	-8.170	C
HETATM 414 O	0	12.087	-4.515	-9.227	O
HETATM 415 C	0	11.291	-1.777	-9.394	C
HETATM 416 O	0	10.522	-2.561	-10.277	O
HETATM 417 C	0	12.607	-1.434	-10.096	C
HETATM 418 H	0	12.724	-0.859	-7.452	H
HETATM 419 H	0	10.451	-2.665	-7.643	H
HETATM 420 H	0	10.753	-0.845	-9.222	H
HETATM 421 H	0	13.185	-2.336	-10.298	H
HETATM 422 H	0	13.197	-0.756	-9.480	H
HETATM 423 H	0	12.390	-0.938	-11.042	H
HETATM 424 H	0	11.047	-3.365	-10.428	H
HETATM 425 N	0	12.719	-4.366	-7.090	N

HETATM 426 C	0	13.725	-5.410	-7.075	C
HETATM 427 H	0	14.571	-5.100	-7.689	H
HETATM 428 C	0	14.248	-5.730	-5.648	C
HETATM 429 O	0	13.890	-5.022	-4.714	O
HETATM 430 H	0	12.553	-3.906	-6.201	H
HETATM 431 N	0	15.098	-6.755	-5.440	N
HETATM 432 C	0	15.742	-7.065	-4.133	C
HETATM 433 C	0	15.985	-8.557	-3.881	C
HETATM 434 O	0	16.156	-9.300	-4.847	O
HETATM 435 H	0	15.331	-7.363	-6.212	H
HETATM 436 H	0	16.703	-6.553	-4.083	H
HETATM 437 H	0	15.107	-6.676	-3.339	H
HETATM 438 N	0	15.991	-9.003	-2.605	N
HETATM 439 C	0	15.873	-10.416	-2.232	C
HETATM 440 C	0	14.766	-11.093	-3.089	C
HETATM 441 O	0	13.664	-10.545	-3.171	O
HETATM 442 C	0	15.544	-10.429	-0.734	C
HETATM 443 C	0	16.158	-9.124	-0.235	C
HETATM 444 C	0	15.938	-8.175	-1.412	C
HETATM 445 H	0	16.838	-10.894	-2.397	H
HETATM 446 H	0	14.464	-10.398	-0.581	H
HETATM 447 H	0	15.975	-11.296	-0.234	H
HETATM 448 H	0	17.228	-9.259	-0.066	H
HETATM 449 H	0	15.668	-8.765	0.670	H
HETATM 450 H	0	16.705	-7.400	-1.424	H
HETATM 451 H	0	14.948	-7.730	-1.345	H
HETATM 452 N	0	15.007	-12.229	-3.770	N
HETATM 453 C	0	14.089	-12.761	-4.794	C
HETATM 454 C	0	12.762	-13.284	-4.253	C
HETATM 455 O	0	11.794	-13.325	-5.004	O
HETATM 456 C	0	14.882	-13.860	-5.511	C
HETATM 457 C	0	15.891	-14.320	-4.459	C
HETATM 458 C	0	16.219	-13.029	-3.710	C
HETATM 459 H	0	13.860	-11.975	-5.514	H
HETATM 460 H	0	14.247	-14.680	-5.848	H
HETATM 461 H	0	15.416	-13.425	-6.357	H
HETATM 462 H	0	16.779	-14.761	-4.914	H
HETATM 463 H	0	15.415	-15.028	-3.779	H
HETATM 464 H	0	17.027	-12.502	-4.220	H
HETATM 465 H	0	16.499	-13.252	-2.680	H
HETATM 466 N	0	12.672	-13.621	-2.961	N
HETATM 467 C	0	11.377	-13.839	-2.324	C
HETATM 468 H	0	13.314	-6.325	-7.499	H
HETATM 469 H	0	11.528	-14.191	-1.305	H
HETATM 470 H	0	10.823	-14.599	-2.876	H
HETATM 471 C	0	10.547	-12.565	-2.283	C

HETATM 472 O	0	9.372 -12.592 -2.636	O
HETATM 473 N	0	11.160 -11.437 -1.903	N
HETATM 474 C	0	10.531 -10.133 -2.089	C
HETATM 475 C	0	10.155 -9.888 -3.551	C
HETATM 476 O	0	9.013 -9.542 -3.822	O
HETATM 477 C	0	11.336 -8.957 -1.511	C
HETATM 478 C	0	10.880 -7.619 -2.079	C
HETATM 479 C	0	9.834 -6.898 -1.472	C
HETATM 480 C	0	11.430 -7.154 -3.292	C
HETATM 481 C	0	9.329 -5.741 -2.092	C
HETATM 482 C	0	10.902 -6.017 -3.924	C
HETATM 483 C	0	9.847 -5.314 -3.326	C
HETATM 484 H	0	12.158 -11.486 -1.755	H
HETATM 485 H	0	9.582 -10.150 -1.550	H
HETATM 486 H	0	11.223 -8.953 -0.426	H
HETATM 487 H	0	12.394 -9.077 -1.727	H
HETATM 488 H	0	9.395 -7.246 -0.549	H
HETATM 489 H	0	12.241 -7.688 -3.765	H
HETATM 490 H	0	8.518 -5.189 -1.646	H
HETATM 491 H	0	11.301 -5.683 -4.870	H
HETATM 492 H	0	9.432 -4.451 -3.825	H
HETATM 493 N	0	11.094 -10.028 -4.485	N
HETATM 494 C	0	10.854 -9.693 -5.889	C
HETATM 495 H	0	11.781 -9.800 -6.450	H
HETATM 496 H	0	10.535 -8.654 -5.963	H
HETATM 497 C	0	9.790 -10.582 -6.553	C
HETATM 498 N	0	9.780 -11.882 -6.241	N
HETATM 499 H	0	10.538 -12.227 -5.662	H
HETATM 500 O	0	8.958 -10.090 -7.309	O
HETATM 501 H	0	12.023 -10.292 -4.173	H
HETATM 502 C	0	8.686 -12.820 -6.511	C
HETATM 503 H	0	8.596 -12.972 -7.587	H
HETATM 504 H	0	8.901 -13.777 -6.036	H
HETATM 505 C	0	7.359 -12.291 -5.979	C
HETATM 506 O	0	6.387 -12.194 -6.721	O
HETATM 507 N	0	7.323 -11.920 -4.698	N
HETATM 508 C	0	6.151 -11.340 -4.031	C
HETATM 509 C	0	5.648 -10.038 -4.651	C
HETATM 510 O	0	4.451 -9.886 -4.881	O
HETATM 511 C	0	6.362 -11.297 -2.499	C
HETATM 512 C	0	5.351 -10.447 -1.724	C
HETATM 513 C	0	6.251 -12.720 -1.929	C
HETATM 514 H	0	8.166 -12.047 -4.146	H
HETATM 515 H	0	5.329 -12.037 -4.198	H
HETATM 516 H	0	7.353 -10.906 -2.277	H
HETATM 517 H	0	4.337 -10.642 -2.075	H

HETATM 518 H	0	5.604 -9.403 -1.864	H
HETATM 519 H	0	5.414 -10.657 -0.657	H
HETATM 520 H	0	5.232 -13.092 -2.040	H
HETATM 521 H	0	6.525 -12.719 -0.874	H
HETATM 522 H	0	6.928 -13.394 -2.454	H
HETATM 523 N	0	6.554 -9.126 -4.977	N
HETATM 524 C	0	6.325 -7.938 -5.789	C
HETATM 525 C	0	5.698 -8.253 -7.108	C
HETATM 526 O	0	4.631 -7.750 -7.435	O
HETATM 527 C	0	7.669 -7.199 -5.929	C
HETATM 528 C	0	7.698 -6.006 -6.868	C
HETATM 529 C	0	7.533 -4.713 -6.347	C
HETATM 530 C	0	7.952 -6.178 -8.245	C
HETATM 531 C	0	7.604 -3.590 -7.191	C
HETATM 532 C	0	8.030 -5.057 -9.096	C
HETATM 533 C	0	7.845 -3.761 -8.571	C
HETATM 534 O	0	7.927 -2.677 -9.387	O
HETATM 535 H	0	7.509 -9.340 -4.715	H
HETATM 536 H	0	5.633 -7.281 -5.259	H
HETATM 537 H	0	7.980 -6.871 -4.936	H
HETATM 538 H	0	8.427 -7.898 -6.270	H
HETATM 539 H	0	7.367 -4.593 -5.287	H
HETATM 540 H	0	8.084 -7.172 -8.654	H
HETATM 541 H	0	7.492 -2.601 -6.773	H
HETATM 542 H	0	8.209 -5.188 -10.153	H
HETATM 543 H	0	8.712 -2.748 -9.957	H
HETATM 544 N	0	6.367 -9.096 -7.867	N
HETATM 545 C	0	5.901 -9.436 -9.175	C
HETATM 546 H	0	6.616 -10.113 -9.641	H
HETATM 547 C	0	4.539 -10.108 -9.190	C
HETATM 548 O	0	3.698 -9.762 -10.013	O
HETATM 549 H	0	7.238 -9.493 -7.526	H
HETATM 550 H	0	5.841 -8.532 -9.782	H
HETATM 551 N	0	4.315 -11.033 -8.261	N
HETATM 552 C	0	3.011 -11.603 -7.994	C
HETATM 553 C	0	1.940 -10.506 -7.696	C
HETATM 554 O	0	0.879 -10.496 -8.316	O
HETATM 555 C	0	3.129 -12.622 -6.853	C
HETATM 556 H	0	5.082 -11.294 -7.651	H
HETATM 557 H	0	2.681 -12.134 -8.888	H
HETATM 558 H	0	3.466 -12.131 -5.940	H
HETATM 559 H	0	3.842 -13.400 -7.125	H
HETATM 560 H	0	2.156 -13.080 -6.673	H
HETATM 561 N	0	2.201 -9.581 -6.758	N
HETATM 562 C	0	1.322 -8.470 -6.328	C
HETATM 563 C	0	1.032 -7.423 -7.425	C

HETATM 564 O	0	-0.119	-7.003	-7.566	O
HETATM 565 C	0	1.956	-7.842	-5.086	C
HETATM 566 C	0	1.224	-6.600	-4.551	C
HETATM 567 C	0	1.729	-5.287	-5.139	C
HETATM 568 O	0	2.903	-5.114	-5.426	O
HETATM 569 N	0	0.898	-4.281	-5.249	N
HETATM 570 H	0	3.095	-9.667	-6.284	H
HETATM 571 H	0	0.360	-8.897	-6.042	H
HETATM 572 H	0	1.966	-8.597	-4.301	H
HETATM 573 H	0	2.995	-7.598	-5.301	H
HETATM 574 H	0	1.413	-6.553	-3.487	H
HETATM 575 H	0	0.150	-6.697	-4.704	H
HETATM 576 H	0	1.261	-3.416	-5.648	H
HETATM 577 H	0	-0.011	-4.303	-4.806	H
HETATM 578 N	0	2.057	-6.943	-8.139	N
HETATM 579 C	0	1.962	-6.008	-9.280	C
HETATM 580 C	0	1.301	-6.716	-10.489	C
HETATM 581 O	0	0.464	-6.105	-11.150	O
HETATM 582 C	0	3.344	-5.432	-9.665	C
HETATM 583 C	0	3.248	-4.432	-10.826	C
HETATM 584 C	0	3.995	-4.671	-8.501	C
HETATM 585 H	0	2.975	-7.299	-7.893	H
HETATM 586 H	0	1.314	-5.178	-8.998	H
HETATM 587 H	0	4.005	-6.248	-9.962	H
HETATM 588 H	0	2.870	-4.925	-11.722	H
HETATM 589 H	0	4.233	-4.027	-11.053	H
HETATM 590 H	0	2.576	-3.615	-10.559	H
HETATM 591 H	0	3.318	-3.899	-8.143	H
HETATM 592 H	0	4.932	-4.219	-8.823	H
HETATM 593 H	0	4.212	-5.344	-7.678	H
HETATM 594 N	0	1.653	-7.981	-10.793	N
HETATM 595 C	0	1.029	-8.828	-11.824	C
HETATM 596 H	0	0.782	-9.789	-11.422	H
HETATM 597 H	0	1.669	-8.950	-12.672	H
HETATM 598 H	0	0.133	-8.326	-12.123	H
HETATM 599 H	0	2.354	-8.431	-10.213	H
HETATM 600 C	0	13.207	5.330	-9.264	C
HETATM 601 H	0	12.990	5.814	-10.193	H
HETATM 602 H	0	13.375	4.288	-9.435	H
HETATM 603 H	0	14.084	5.766	-8.831	H
HETATM 604 C	0	12.033	5.536	-8.372	C
HETATM 605 O	0	10.949	5.117	-8.752	O
HETATM 606 N	0	12.227	6.276	-7.275	N
HETATM 607 C	0	11.163	6.845	-6.440	C
HETATM 608 H	0	11.536	7.719	-5.907	H
HETATM 609 C	0	9.923	7.249	-7.233	C

HETATM 610 O	0	8.851	6.716	-6.996	O
HETATM 611 H	0	13.179	6.529	-7.041	H
HETATM 612 H	0	10.829	6.112	-5.704	H
HETATM 613 N	0	10.080	8.137	-8.217	N
HETATM 614 C	0	9.015	8.554	-9.143	C
HETATM 615 H	0	9.398	9.329	-9.807	H
HETATM 616 C	0	8.429	7.436	-10.007	C
HETATM 617 O	0	7.215	7.245	-9.989	O
HETATM 618 H	0	11.004	8.526	-8.313	H
HETATM 619 H	0	8.200	8.989	-8.563	H
HETATM 620 N	0	9.278	6.714	-10.756	N
HETATM 621 C	0	8.918	5.514	-11.535	C
HETATM 622 H	0	9.815	4.945	-11.780	H
HETATM 623 C	0	7.964	4.620	-10.741	C
HETATM 624 O	0	6.824	4.395	-11.136	O
HETATM 625 H	0	10.256	6.935	-10.668	H
HETATM 626 H	0	8.423	5.814	-12.459	H
HETATM 627 N	0	8.423	4.156	-9.580	N
HETATM 628 C	0	7.691	3.306	-8.644	C
HETATM 629 C	0	6.482	3.925	-7.985	C
HETATM 630 O	0	5.448	3.275	-7.984	O
HETATM 631 C	0	8.662	2.786	-7.564	C
HETATM 632 C	0	9.216	1.362	-7.758	C
HETATM 633 C	0	8.214	0.249	-8.125	C
HETATM 634 N	0	7.004	0.221	-7.282	N
HETATM 635 C	0	5.846	-0.350	-7.569	C
HETATM 636 N	0	5.625	-1.122	-8.586	N
HETATM 637 N	0	4.820	-0.208	-6.810	N
HETATM 638 H	0	9.357	4.457	-9.315	H
HETATM 639 H	0	7.292	2.462	-9.202	H
HETATM 640 H	0	9.503	3.470	-7.451	H
HETATM 641 H	0	8.159	2.823	-6.611	H
HETATM 642 H	0	9.716	1.073	-6.832	H
HETATM 643 H	0	9.977	1.397	-8.539	H
HETATM 644 H	0	8.730	-0.704	-8.022	H
HETATM 645 H	0	7.925	0.367	-9.170	H
HETATM 646 H	0	7.011	0.766	-6.415	H
HETATM 647 H	0	4.665	-1.447	-8.709	H
HETATM 648 H	0	6.395	-1.486	-9.126	H
HETATM 649 H	0	4.966	0.231	-5.900	H
HETATM 650 H	0	3.923	-0.575	-7.129	H
HETATM 651 N	0	6.575	5.134	-7.444	N
HETATM 652 C	0	5.412	5.853	-6.943	C
HETATM 653 C	0	4.276	5.863	-8.020	C
HETATM 654 O	0	3.124	5.587	-7.688	O
HETATM 655 C	0	5.801	7.295	-6.589	C

HETATM 656 H	0	7.478	5.592	-7.421	H
HETATM 657 H	0	5.037	5.350	-6.050	H
HETATM 658 H	0	4.947	7.796	-6.136	H
HETATM 659 H	0	6.099	7.836	-7.488	H
HETATM 660 H	0	6.633	7.309	-5.889	H
HETATM 661 N	0	4.589	6.141	-9.304	N
HETATM 662 C	0	3.715	5.998	-10.497	C
HETATM 663 H	0	4.276	6.276	-11.389	H
HETATM 664 C	0	3.207	4.567	-10.672	C
HETATM 665 O	0	1.996	4.384	-10.660	O
HETATM 666 H	0	5.558	6.392	-9.484	H
HETATM 667 H	0	2.859	6.665	-10.400	H
HETATM 668 N	0	4.086	3.558	-10.801	N
HETATM 669 C	0	3.686	2.133	-10.911	C
HETATM 670 C	0	2.755	1.718	-9.762	C
HETATM 671 O	0	1.725	1.118	-10.032	O
HETATM 672 C	0	4.859	1.155	-11.123	C
HETATM 673 C	0	4.362	-0.283	-11.339	C
HETATM 674 C	0	5.653	1.480	-12.396	C
HETATM 675 H	0	5.072	3.801	-10.831	H
HETATM 676 H	0	3.076	2.062	-11.813	H
HETATM 677 H	0	5.525	1.191	-10.261	H
HETATM 678 H	0	3.738	-0.336	-12.231	H
HETATM 679 H	0	3.770	-0.623	-10.491	H
HETATM 680 H	0	5.208	-0.958	-11.462	H
HETATM 681 H	0	5.010	1.391	-13.273	H
HETATM 682 H	0	6.492	0.793	-12.498	H
HETATM 683 H	0	6.041	2.491	-12.367	H
HETATM 684 N	0	3.032	2.095	-8.512	N
HETATM 685 C	0	2.172	1.911	-7.338	C
HETATM 686 C	0	0.819	2.587	-7.476	C
HETATM 687 O	0	-0.221	2.003	-7.200	O
HETATM 688 C	0	2.921	2.410	-6.077	C
HETATM 689 C	0	2.266	1.931	-4.791	C
HETATM 690 O	0	1.120	2.241	-4.524	O
HETATM 691 N	0	2.939	1.181	-3.959	N
HETATM 692 H	0	3.906	2.587	-8.377	H
HETATM 693 H	0	1.995	0.851	-7.211	H
HETATM 694 H	0	2.940	3.497	-6.061	H
HETATM 695 H	0	3.956	2.080	-6.087	H
HETATM 696 H	0	2.495	0.842	-3.106	H
HETATM 697 H	0	3.929	0.999	-4.097	H
HETATM 698 N	0	0.803	3.850	-7.866	N
HETATM 699 C	0	-0.461	4.517	-8.072	C
HETATM 700 C	0	-1.297	3.915	-9.218	C
HETATM 701 O	0	-2.498	3.702	-9.044	O

HETATM 702 C	0	-0.234	6.017	-8.304	C
HETATM 703 S	0	0.391	6.802	-6.792	S
HETATM 704 H	0	1.679	4.318	-8.079	H
HETATM 705 H	0	-1.076	4.403	-7.179	H
HETATM 706 H	0	-1.184	6.483	-8.574	H
HETATM 707 H	0	0.473	6.167	-9.123	H
HETATM 708 H	0	1.657	6.373	-6.943	H
HETATM 709 N	0	-0.666	3.647	-10.366	N
HETATM 710 C	0	-1.196	2.859	-11.479	C
HETATM 711 H	0	-0.413	2.688	-12.218	H
HETATM 712 C	0	-1.713	1.477	-10.968	C
HETATM 713 O	0	-2.833	1.121	-11.296	O
HETATM 714 H	0	0.319	3.880	-10.411	H
HETATM 715 H	0	-2.022	3.392	-11.950	H
HETATM 716 N	0	-0.970	0.703	-10.145	N
HETATM 717 C	0	-1.310	-0.664	-9.642	C
HETATM 718 C	0	-2.416	-0.678	-8.574	C
HETATM 719 O	0	-3.260	-1.575	-8.566	O
HETATM 720 C	0	-0.058	-1.499	-9.285	C
HETATM 721 C	0	0.355	-1.307	-7.830	C
HETATM 722 C	0	1.802	-1.627	-7.462	C
HETATM 723 O	0	2.003	-1.936	-6.273	O
HETATM 724 O	0	2.774	-1.412	-8.223	O
HETATM 725 H	0	-0.046	1.050	-9.920	H
HETATM 726 H	0	-1.756	-1.181	-10.493	H
HETATM 727 H	0	-0.283	-2.556	-9.434	H
HETATM 728 H	0	0.757	-1.240	-9.960	H
HETATM 729 H	0	-0.315	-1.899	-7.202	H
HETATM 730 H	0	0.196	-0.273	-7.576	H
HETATM 731 N	0	-2.452	0.320	-7.686	N
HETATM 732 C	0	-3.565	0.540	-6.759	C
HETATM 733 C	0	-4.829	1.061	-7.442	C
HETATM 734 O	0	-5.945	0.853	-6.964	O
HETATM 735 C	0	-3.160	1.440	-5.584	C
HETATM 736 C	0	-2.453	0.754	-4.425	C
HETATM 737 C	0	-1.158	0.230	-4.586	C
HETATM 738 C	0	-3.048	0.735	-3.146	C
HETATM 739 C	0	-0.421	-0.217	-3.474	C
HETATM 740 C	0	-2.317	0.277	-2.030	C
HETATM 741 C	0	-0.981	-0.155	-2.184	C
HETATM 742 O	0	-0.221	-0.439	-1.093	O
HETATM 743 H	0	-1.688	0.988	-7.701	H
HETATM 744 H	0	-3.843	-0.424	-6.332	H
HETATM 745 H	0	-2.531	2.252	-5.949	H
HETATM 746 H	0	-4.066	1.896	-5.184	H
HETATM 747 H	0	-0.686	0.224	-5.555	H

HETATM 748 H	0	-4.047	1.122	-3.004	H
HETATM 749 H	0	0.594	-0.563	-3.611	H
HETATM 750 H	0	-2.757	0.299	-1.044	H
HETATM 751 H	0	0.735	-0.410	-1.345	H
HETATM 752 N	0	-4.668	1.740	-8.570	N
HETATM 753 C	0	-5.743	2.337	-9.336	C
HETATM 754 H	0	-5.311	2.752	-10.247	H
HETATM 755 C	0	-6.887	1.424	-9.756	C
HETATM 756 O	0	-8.027	1.800	-9.515	O
HETATM 757 H	0	-3.719	1.887	-8.895	H
HETATM 758 H	0	-6.154	3.171	-8.772	H
HETATM 759 N	0	-6.654	0.254	-10.370	N
HETATM 760 C	0	-7.676	-0.761	-10.568	C
HETATM 761 C	0	-8.521	-1.058	-9.335	C
HETATM 762 O	0	-9.721	-1.259	-9.467	O
HETATM 763 C	0	-6.925	-2.010	-11.039	C
HETATM 764 C	0	-5.748	-1.423	-11.810	C
HETATM 765 C	0	-5.428	-0.152	-11.027	C
HETATM 766 H	0	-8.340	-0.428	-11.367	H
HETATM 767 H	0	-6.549	-2.574	-10.183	H
HETATM 768 H	0	-7.549	-2.643	-11.672	H
HETATM 769 H	0	-6.065	-1.161	-12.820	H
HETATM 770 H	0	-4.898	-2.106	-11.836	H
HETATM 771 H	0	-5.105	0.623	-11.720	H
HETATM 772 H	0	-4.661	-0.363	-10.284	H
HETATM 773 N	0	-7.925	-1.080	-8.139	N
HETATM 774 C	0	-8.660	-1.285	-6.891	C
HETATM 775 C	0	-9.470	-0.028	-6.507	C
HETATM 776 O	0	-10.606	-0.163	-6.069	O
HETATM 777 C	0	-7.717	-1.637	-5.729	C
HETATM 778 C	0	-6.605	-2.656	-6.017	C
HETATM 779 C	0	-5.993	-3.077	-4.680	C
HETATM 780 C	0	-7.097	-3.902	-6.752	C
HETATM 781 H	0	-6.937	-0.870	-8.092	H
HETATM 782 H	0	-9.356	-2.111	-7.030	H
HETATM 783 H	0	-7.240	-0.727	-5.363	H
HETATM 784 H	0	-8.339	-2.013	-4.920	H
HETATM 785 H	0	-5.837	-2.176	-6.623	H
HETATM 786 H	0	-6.727	-3.601	-4.067	H
HETATM 787 H	0	-5.636	-2.198	-4.145	H
HETATM 788 H	0	-5.142	-3.732	-4.856	H
HETATM 789 H	0	-7.825	-4.439	-6.147	H
HETATM 790 H	0	-6.238	-4.533	-6.967	H
HETATM 791 H	0	-7.549	-3.643	-7.706	H
HETATM 792 N	0	-8.913	1.185	-6.651	N
HETATM 793 C	0	-9.649	2.470	-6.603	C

HETATM 794 C	0	-10.868	2.411	-7.512	C
HETATM 795 O	0	-11.978	2.501	-7.014	O
HETATM 796 C	0	-8.675	3.631	-6.875	C
HETATM 797 C	0	-9.264	4.885	-7.490	C
HETATM 798 C	0	-9.847	5.873	-6.677	C
HETATM 799 C	0	-9.186	5.083	-8.883	C
HETATM 800 C	0	-10.327	7.062	-7.258	C
HETATM 801 C	0	-9.690	6.260	-9.462	C
HETATM 802 C	0	-10.256	7.253	-8.647	C
HETATM 803 H	0	-7.951	1.191	-6.971	H
HETATM 804 H	0	-10.039	2.606	-5.594	H
HETATM 805 H	0	-8.190	3.896	-5.936	H
HETATM 806 H	0	-7.880	3.286	-7.525	H
HETATM 807 H	0	-9.905	5.728	-5.607	H
HETATM 808 H	0	-8.742	4.331	-9.518	H
HETATM 809 H	0	-10.748	7.839	-6.643	H
HETATM 810 H	0	-9.636	6.405	-10.533	H
HETATM 811 H	0	-10.634	8.165	-9.090	H
HETATM 812 N	0	-10.670	2.150	-8.801	N
HETATM 813 C	0	-11.706	1.852	-9.780	C
HETATM 814 H	0	-11.244	1.460	-10.685	H
HETATM 815 C	0	-12.740	0.839	-9.290	C
HETATM 816 O	0	-13.927	1.148	-9.251	O
HETATM 817 H	0	-9.705	2.061	-9.093	H
HETATM 818 H	0	-12.233	2.772	-10.032	H
HETATM 819 N	0	-12.289	-0.356	-8.904	N
HETATM 820 C	0	-13.115	-1.448	-8.399	C
HETATM 821 C	0	-14.001	-1.030	-7.253	C
HETATM 822 O	0	-15.224	-1.042	-7.349	O
HETATM 823 C	0	-12.243	-2.668	-8.082	C
HETATM 824 H	0	-11.299	-0.539	-9.016	H
HETATM 825 H	0	-13.789	-1.739	-9.207	H
HETATM 826 H	0	-12.871	-3.485	-7.724	H
HETATM 827 H	0	-11.512	-2.415	-7.319	H
HETATM 828 H	0	-11.722	-2.995	-8.983	H
HETATM 829 N	0	-13.366	-0.653	-6.161	N
HETATM 830 C	0	-14.068	-0.266	-4.958	C
HETATM 831 C	0	-14.925	0.982	-5.159	C
HETATM 832 O	0	-15.983	1.064	-4.555	O
HETATM 833 C	0	-13.128	-0.034	-3.769	C
HETATM 834 O	0	-11.913	-0.729	-3.857	O
HETATM 835 C	0	-13.774	-0.573	-2.503	C
HETATM 836 H	0	-12.355	-0.634	-6.196	H
HETATM 837 H	0	-14.746	-1.081	-4.704	H
HETATM 838 H	0	-12.911	1.029	-3.663	H
HETATM 839 H	0	-14.742	-0.101	-2.338	H

HETATM 840 H	0	-13.111	-0.354	-1.674	H
HETATM 841 H	0	-13.904	-1.652	-2.578	H
HETATM 842 H	0	-11.428	-0.411	-4.640	H
HETATM 843 N	0	-14.501	1.953	-5.975	N
HETATM 844 C	0	-15.267	3.161	-6.294	C
HETATM 845 C	0	-16.518	2.871	-7.125	C
HETATM 846 O	0	-17.583	3.362	-6.777	O
HETATM 847 C	0	-14.369	4.226	-6.949	C
HETATM 848 C	0	-15.041	5.594	-7.176	C
HETATM 849 C	0	-15.433	6.275	-5.861	C
HETATM 850 C	0	-14.061	6.519	-7.899	C
HETATM 851 H	0	-13.603	1.844	-6.436	H
HETATM 852 H	0	-15.623	3.564	-5.347	H
HETATM 853 H	0	-13.499	4.385	-6.312	H
HETATM 854 H	0	-14.029	3.845	-7.913	H
HETATM 855 H	0	-15.927	5.476	-7.800	H
HETATM 856 H	0	-14.567	6.344	-5.204	H
HETATM 857 H	0	-16.221	5.701	-5.374	H
HETATM 858 H	0	-15.824	7.271	-6.069	H
HETATM 859 H	0	-13.166	6.663	-7.297	H
HETATM 860 H	0	-14.535	7.481	-8.094	H
HETATM 861 H	0	-13.778	6.074	-8.853	H
HETATM 862 N	0	-16.410	2.092	-8.202	N
HETATM 863 C	0	-17.559	1.643	-8.994	C
HETATM 864 H	0	-17.207	1.078	-9.856	H
HETATM 865 C	0	-18.511	0.761	-8.198	C
HETATM 866 O	0	-19.721	0.932	-8.294	O
HETATM 867 H	0	-15.490	1.737	-8.444	H
HETATM 868 H	0	-18.114	2.511	-9.350	H
HETATM 869 N	0	-17.968	-0.169	-7.406	N
HETATM 870 C	0	-18.755	-0.972	-6.467	C
HETATM 871 C	0	-19.467	-0.103	-5.414	C
HETATM 872 O	0	-20.646	-0.315	-5.154	O
HETATM 873 C	0	-17.938	-2.107	-5.814	C
HETATM 874 C	0	-18.729	-2.854	-4.731	C
HETATM 875 C	0	-17.547	-3.171	-6.853	C
HETATM 876 H	0	-16.960	-0.283	-7.424	H
HETATM 877 H	0	-19.558	-1.445	-7.034	H
HETATM 878 H	0	-17.036	-1.692	-5.362	H
HETATM 879 H	0	-19.659	-3.243	-5.148	H
HETATM 880 H	0	-18.979	-2.185	-3.908	H
HETATM 881 H	0	-18.142	-3.677	-4.333	H
HETATM 882 H	0	-18.440	-3.675	-7.224	H
HETATM 883 H	0	-16.878	-3.900	-6.399	H
HETATM 884 H	0	-17.041	-2.712	-7.700	H
HETATM 885 N	0	-18.766	0.840	-4.776	N

HETATM 886 C	0	-19.327	1.736	-3.761	C
HETATM 887 C	0	-20.307	2.788	-4.310	C
HETATM 888 O	0	-21.213	3.214	-3.595	O
HETATM 889 C	0	-18.195	2.432	-2.994	C
HETATM 890 H	0	-17.784	0.942	-4.995	H
HETATM 891 H	0	-19.892	1.130	-3.050	H
HETATM 892 H	0	-18.622	3.061	-2.212	H
HETATM 893 H	0	-17.617	3.056	-3.676	H
HETATM 894 H	0	-17.544	1.693	-2.530	H
HETATM 895 N	0	-20.082	3.263	-5.538	N
HETATM 896 C	0	-20.905	4.247	-6.215	C
HETATM 897 H	0	-21.910	3.879	-6.218	H
HETATM 898 H	0	-20.572	4.384	-7.223	H
HETATM 899 H	0	-20.869	5.183	-5.697	H
HETATM 900 H	0	-19.277	2.900	-6.035	H
HETATM 901 C	0	-15.470	11.722	-2.061	C
HETATM 902 H	0	-16.392	11.223	-1.848	H
HETATM 903 H	0	-15.394	11.898	-3.114	H
HETATM 904 H	0	-15.440	12.655	-1.540	H
HETATM 905 C	0	-14.289	10.863	-1.625	C
HETATM 906 O	0	-13.160	11.299	-1.791	O
HETATM 907 N	0	-14.503	9.629	-1.145	N
HETATM 908 C	0	-13.456	8.632	-0.786	C
HETATM 909 C	0	-12.441	8.454	-1.920	C
HETATM 910 O	0	-11.235	8.454	-1.697	O
HETATM 911 C	0	-14.138	7.328	-0.358	C
HETATM 912 S	0	-15.478	7.670	0.822	S
HETATM 913 H	0	-15.460	9.364	-0.958	H
HETATM 914 H	0	-12.904	9.020	0.072	H
HETATM 915 H	0	-13.399	6.676	0.111	H
HETATM 916 H	0	-14.559	6.836	-1.233	H
HETATM 917 H	0	-15.922	6.415	0.977	H
HETATM 918 N	0	-12.939	8.399	-3.154	N
HETATM 919 C	0	-12.119	8.475	-4.354	C
HETATM 920 C	0	-11.238	9.716	-4.472	C
HETATM 921 O	0	-10.049	9.604	-4.754	O
HETATM 922 H	0	-13.943	8.402	-3.247	H
HETATM 923 H	0	-11.468	7.600	-4.380	H
HETATM 924 H	0	-12.765	8.434	-5.231	H
HETATM 925 N	0	-11.815	10.895	-4.250	N
HETATM 926 C	0	-11.083	12.155	-4.146	C
HETATM 927 H	0	-11.775	12.957	-3.889	H
HETATM 928 C	0	-9.973	12.121	-3.085	C
HETATM 929 O	0	-8.868	12.595	-3.337	O
HETATM 930 H	0	-12.774	10.897	-3.939	H
HETATM 931 H	0	-10.627	12.388	-5.109	H

HETATM 932 N	0	-10.248	11.544	-1.908	N
HETATM 933 C	0	-9.251	11.320	-0.842	C
HETATM 934 C	0	-8.121	10.431	-1.296	C
HETATM 935 O	0	-6.970	10.806	-1.106	O
HETATM 936 C	0	-9.879	10.801	0.471	C
HETATM 937 C	0	-8.835	10.685	1.594	C
HETATM 938 C	0	-10.973	11.743	0.991	C
HETATM 939 H	0	-11.206	11.239	-1.771	H
HETATM 940 H	0	-8.803	12.289	-0.618	H
HETATM 941 H	0	-10.319	9.819	0.305	H
HETATM 942 H	0	-8.052	9.978	1.321	H
HETATM 943 H	0	-9.311	10.327	2.506	H
HETATM 944 H	0	-8.380	11.658	1.782	H
HETATM 945 H	0	-10.562	12.739	1.159	H
HETATM 946 H	0	-11.381	11.360	1.927	H
HETATM 947 H	0	-11.786	11.816	0.274	H
HETATM 948 N	0	-8.421	9.284	-1.904	N
HETATM 949 C	0	-7.401	8.483	-2.572	C
HETATM 950 C	0	-6.556	9.302	-3.528	C
HETATM 951 O	0	-5.332	9.236	-3.465	O
HETATM 952 C	0	-8.022	7.248	-3.244	C
HETATM 953 C	0	-7.030	6.435	-4.063	C
HETATM 954 C	0	-6.222	5.459	-3.446	C
HETATM 955 C	0	-6.895	6.684	-5.443	C
HETATM 956 C	0	-5.275	4.745	-4.208	C
HETATM 957 C	0	-5.951	5.972	-6.209	C
HETATM 958 C	0	-5.133	5.005	-5.590	C
HETATM 959 O	0	-4.183	4.348	-6.305	O
HETATM 960 H	0	-9.400	9.036	-2.007	H
HETATM 961 H	0	-6.718	8.117	-1.808	H
HETATM 962 H	0	-8.455	6.610	-2.473	H
HETATM 963 H	0	-8.835	7.558	-3.897	H
HETATM 964 H	0	-6.322	5.266	-2.385	H
HETATM 965 H	0	-7.513	7.434	-5.921	H
HETATM 966 H	0	-4.634	4.007	-3.749	H
HETATM 967 H	0	-5.852	6.177	-7.264	H
HETATM 968 H	0	-4.188	4.541	-7.247	H
HETATM 969 N	0	-7.205	10.095	-4.370	N
HETATM 970 C	0	-6.511	10.987	-5.289	C
HETATM 971 H	0	-5.557	11.286	-4.909	H
HETATM 972 H	0	-7.087	11.856	-5.531	H
HETATM 973 H	0	-8.227	10.037	-4.304	H
HETATM 974 H	0	-6.334	10.448	-6.220	H
HETATM 975 N	0	-4.549	12.263	-1.591	N
HETATM 976 O	0	-3.107	13.822	-2.258	O
HETATM 977 C	0	-4.262	13.411	-2.214	C

HETATM 978 C	0	-5.325	14.188	-2.993	C
HETATM 979 H	0	-6.303	13.756	-3.036	H
HETATM 980 H	0	-4.883	14.167	-3.967	H
HETATM 981 H	0	-5.397	15.200	-2.655	H
HETATM 982 C	0	-3.540	11.463	-0.859	C
HETATM 983 C	0	-2.469	10.827	-1.753	C
HETATM 984 O	0	-1.286	10.900	-1.426	O
HETATM 985 C	0	-4.257	10.475	0.051	C
HETATM 986 H	0	-5.510	11.933	-1.589	H
HETATM 987 H	0	-3.004	12.154	-0.206	H
HETATM 988 H	0	-3.524	9.960	0.656	H
HETATM 989 H	0	-4.819	9.761	-0.544	H
HETATM 990 H	0	-4.942	11.009	0.710	H
HETATM 991 N	0	-2.826	10.211	-2.884	N
HETATM 992 C	0	-1.836	9.676	-3.830	C
HETATM 993 C	0	-0.955	10.763	-4.489	C
HETATM 994 O	0	0.194	10.450	-4.796	O
HETATM 995 C	0	-2.442	8.684	-4.840	C
HETATM 996 C	0	-2.755	7.295	-4.241	C
HETATM 997 C	0	-1.610	6.757	-3.369	C
HETATM 998 N	0	-1.749	5.338	-3.016	N
HETATM 999 C	0	-1.084	4.347	-3.568	C
HETATM 1000 N	0	-0.416	4.476	-4.670	N
HETATM 1001 N	0	-1.052	3.187	-3.007	N
HETATM 1002 H	0	-3.820	10.112	-3.082	H
HETATM 1003 H	0	-1.117	9.137	-3.239	H
HETATM 1004 H	0	-3.344	9.106	-5.286	H
HETATM 1005 H	0	-1.720	8.537	-5.644	H
HETATM 1006 H	0	-2.925	6.607	-5.068	H
HETATM 1007 H	0	-3.661	7.342	-3.642	H
HETATM 1008 H	0	-1.574	7.323	-2.439	H
HETATM 1009 H	0	-0.666	6.918	-3.888	H
HETATM 1010 H	0	-2.194	5.101	-2.137	H
HETATM 1011 H	0	0.120	3.659	-4.943	H
HETATM 1012 H	0	-0.363	5.348	-5.161	H
HETATM 1013 H	0	-1.570	3.031	-2.151	H
HETATM 1014 H	0	-0.481	2.456	-3.422	H
HETATM 1015 N	0	-1.406	12.024	-4.620	N
HETATM 1016 C	0	-0.551	13.188	-4.934	C
HETATM 1017 H	0	-0.977	13.853	-5.655	H
HETATM 1018 H	0	0.380	12.812	-5.302	H
HETATM 1019 H	0	-0.387	13.714	-4.017	H
HETATM 1020 H	0	-2.341	12.199	-4.283	H
HETATM 1021 C	0	0.985	13.859	-1.542	C
HETATM 1022 H	0	-0.034	13.537	-1.475	H
HETATM 1023 H	0	1.189	14.192	-2.538	H

HETATM 1024	H	0	1.151	14.662	-0.855	H
HETATM 1025	C	0	1.941	12.715	-1.335	C
HETATM 1026	O	0	3.122	12.955	-1.127	O
HETATM 1027	N	0	1.469	11.483	-1.515	N
HETATM 1028	C	0	2.297	10.275	-1.582	C
HETATM 1029	C	0	3.343	10.390	-2.700	C
HETATM 1030	O	0	4.522	10.353	-2.387	O
HETATM 1031	C	0	1.432	9.027	-1.776	C
HETATM 1032	C	0	2.172	7.759	-2.167	C
HETATM 1033	C	0	2.964	7.084	-1.223	C
HETATM 1034	C	0	2.059	7.248	-3.476	C
HETATM 1035	C	0	3.610	5.878	-1.565	C
HETATM 1036	C	0	2.687	6.034	-3.818	C
HETATM 1037	C	0	3.443	5.332	-2.856	C
HETATM 1038	O	0	4.030	4.156	-3.193	O
HETATM 1039	H	0	0.467	11.381	-1.637	H
HETATM 1040	H	0	2.838	10.169	-0.641	H
HETATM 1041	H	0	0.858	8.838	-0.868	H
HETATM 1042	H	0	0.735	9.248	-2.568	H
HETATM 1043	H	0	3.059	7.497	-0.231	H
HETATM 1044	H	0	1.488	7.784	-4.222	H
HETATM 1045	H	0	4.210	5.344	-0.845	H
HETATM 1046	H	0	2.600	5.619	-4.810	H
HETATM 1047	H	0	4.442	3.702	-2.439	H
HETATM 1048	N	0	2.953	10.564	-3.973	N
HETATM 1049	C	0	3.870	10.773	-5.112	C
HETATM 1050	H	0	3.299	11.055	-5.997	H
HETATM 1051	C	0	4.920	11.870	-4.826	C
HETATM 1052	O	0	6.102	11.622	-5.020	O
HETATM 1053	H	0	1.957	10.540	-4.166	H
HETATM 1054	H	0	4.397	9.843	-5.319	H
HETATM 1055	N	0	4.514	13.054	-4.331	N
HETATM 1056	C	0	5.398	14.169	-3.904	C
HETATM 1057	H	0	4.795	14.982	-3.502	H
HETATM 1058	C	0	6.408	13.760	-2.862	C
HETATM 1059	O	0	7.620	13.841	-3.058	O
HETATM 1060	H	0	3.525	13.149	-4.170	H
HETATM 1061	H	0	5.943	14.542	-4.772	H
HETATM 1062	N	0	5.867	13.299	-1.747	N
HETATM 1063	C	0	6.635	12.795	-0.641	C
HETATM 1064	C	0	7.624	11.746	-1.010	C
HETATM 1065	O	0	8.795	11.891	-0.715	O
HETATM 1066	H	0	4.856	13.252	-1.675	H
HETATM 1067	H	0	7.173	13.624	-0.181	H
HETATM 1068	H	0	5.952	12.381	0.100	H
HETATM 1069	N	0	7.138	10.705	-1.653	N

HETATM 1070	C	0	7.920	9.581	-2.087	C
HETATM 1071	C	0	9.002	9.943	-3.086	C
HETATM 1072	O	0	10.142	9.492	-2.958	O
HETATM 1073	C	0	6.974	8.505	-2.658	C
HETATM 1074	C	0	7.518	7.108	-2.922	C
HETATM 1075	C	0	6.664	6.186	-3.554	C
HETATM 1076	C	0	8.826	6.707	-2.579	C
HETATM 1077	C	0	7.122	4.908	-3.921	C
HETATM 1078	C	0	9.298	5.442	-2.971	C
HETATM 1079	C	0	8.455	4.546	-3.653	C
HETATM 1080	O	0	8.934	3.339	-4.031	O
HETATM 1081	H	0	6.151	10.713	-1.879	H
HETATM 1082	H	0	8.426	9.169	-1.215	H
HETATM 1083	H	0	6.132	8.380	-1.984	H
HETATM 1084	H	0	6.563	8.881	-3.596	H
HETATM 1085	H	0	5.653	6.478	-3.795	H
HETATM 1086	H	0	9.502	7.347	-2.035	H
HETATM 1087	H	0	6.472	4.209	-4.427	H
HETATM 1088	H	0	10.312	5.143	-2.762	H
HETATM 1089	H	0	8.229	2.758	-4.397	H
HETATM 1090	N	0	8.662	10.776	-4.063	N
HETATM 1091	C	0	9.646	11.327	-4.962	C
HETATM 1092	C	0	10.844	11.962	-4.223	C
HETATM 1093	O	0	11.990	11.745	-4.624	O
HETATM 1094	C	0	8.990	12.304	-5.944	C
HETATM 1095	H	0	7.703	11.100	-4.144	H
HETATM 1096	H	0	10.051	10.502	-5.549	H
HETATM 1097	H	0	9.747	12.705	-6.619	H
HETATM 1098	H	0	8.525	13.130	-5.405	H
HETATM 1099	H	0	8.234	11.786	-6.534	H
HETATM 1100	N	0	10.592	12.678	-3.118	N
HETATM 1101	C	0	11.612	13.147	-2.169	C
HETATM 1102	H	0	11.190	13.941	-1.554	H
HETATM 1103	C	0	12.161	12.034	-1.232	C
HETATM 1104	O	0	13.308	11.629	-1.411	O
HETATM 1105	H	0	9.612	12.831	-2.895	H
HETATM 1106	H	0	12.462	13.553	-2.719	H
HETATM 1107	N	0	11.403	11.558	-0.226	N
HETATM 1108	C	0	11.796	10.610	0.851	C
HETATM 1109	C	0	10.827	9.439	1.169	C
HETATM 1110	O	0	9.600	9.540	1.069	O
HETATM 1111	C	0	12.163	11.375	2.138	C
HETATM 1112	O	0	11.250	11.171	3.211	O
HETATM 1113	H	0	10.443	11.876	-0.225	H
HETATM 1114	H	0	12.719	10.137	0.513	H
HETATM 1115	H	0	12.241	12.443	1.928	H

HETATM 1116	H	0	13.147	11.036	2.462	H
HETATM 1117	H	0	11.723	11.423	4.029	H
HETATM 1118	N	0	11.389	8.332	1.682	N
HETATM 1119	C	0	10.715	7.106	2.149	C
HETATM 1120	C	0	9.870	7.271	3.431	C
HETATM 1121	O	0	9.312	6.287	3.925	O
HETATM 1122	C	0	11.790	6.034	2.382	C
HETATM 1123	H	0	12.395	8.352	1.797	H
HETATM 1124	H	0	10.056	6.758	1.353	H
HETATM 1125	H	0	11.334	5.102	2.713	H
HETATM 1126	H	0	12.495	6.367	3.138	H
HETATM 1127	H	0	12.339	5.844	1.465	H
HETATM 1128	N	0	9.735	8.486	3.965	N
HETATM 1129	C	0	8.908	8.791	5.139	C
HETATM 1130	C	0	7.881	9.895	4.840	C
HETATM 1131	O	0	6.731	9.749	5.232	O
HETATM 1132	C	0	9.771	9.207	6.340	C
HETATM 1133	C	0	10.616	8.081	6.945	C
HETATM 1134	C	0	11.862	7.733	6.145	C
HETATM 1135	O	0	12.718	8.573	5.867	O
HETATM 1136	N	0	12.026	6.486	5.772	N
HETATM 1137	H	0	10.218	9.240	3.489	H
HETATM 1138	H	0	8.346	7.910	5.432	H
HETATM 1139	H	0	10.401	10.052	6.071	H
HETATM 1140	H	0	9.096	9.540	7.126	H
HETATM 1141	H	0	9.988	7.198	7.060	H
HETATM 1142	H	0	10.942	8.392	7.938	H
HETATM 1143	H	0	12.886	6.224	5.304	H
HETATM 1144	H	0	11.312	5.794	5.985	H
HETATM 1145	N	0	8.225	10.959	4.101	N
HETATM 1146	C	0	7.266	12.008	3.685	C
HETATM 1147	C	0	6.076	11.435	2.902	C
HETATM 1148	O	0	4.947	11.898	3.036	O
HETATM 1149	C	0	8.005	13.058	2.834	C
HETATM 1150	C	0	9.064	13.881	3.591	C
HETATM 1151	C	0	9.854	14.727	2.592	C
HETATM 1152	C	0	8.440	14.818	4.626	C
HETATM 1153	H	0	9.188	11.049	3.802	H
HETATM 1154	H	0	6.855	12.486	4.575	H
HETATM 1155	H	0	8.490	12.544	2.003	H
HETATM 1156	H	0	7.270	13.748	2.415	H
HETATM 1157	H	0	9.759	13.214	4.099	H
HETATM 1158	H	0	10.628	15.288	3.115	H
HETATM 1159	H	0	9.189	15.424	2.082	H
HETATM 1160	H	0	10.328	14.079	1.854	H
HETATM 1161	H	0	7.951	14.237	5.408	H

HETATM 1162	H	0	7.710	15.473	4.151	H
HETATM 1163	H	0	9.217	15.425	5.089	H
HETATM 1164	N	0	6.323	10.378	2.118	N
HETATM 1165	C	0	5.298	9.522	1.490	C
HETATM 1166	C	0	4.218	9.032	2.465	C
HETATM 1167	O	0	3.109	8.741	2.023	O
HETATM 1168	C	0	5.963	8.336	0.777	C
HETATM 1169	C	0	6.464	7.229	1.699	C
HETATM 1170	C	0	7.120	6.068	0.957	C
HETATM 1171	N	0	7.742	5.200	1.943	N
HETATM 1172	C	0	7.676	3.875	2.111	C
HETATM 1173	N	0	7.100	3.067	1.245	N
HETATM 1174	N	0	8.279	3.371	3.204	N
HETATM 1175	H	0	7.302	10.135	2.014	H
HETATM 1176	H	0	4.778	10.144	0.754	H
HETATM 1177	H	0	5.256	7.901	0.065	H
HETATM 1178	H	0	6.814	8.694	0.195	H
HETATM 1179	H	0	5.646	6.810	2.293	H
HETATM 1180	H	0	7.187	7.656	2.408	H
HETATM 1181	H	0	7.877	6.421	0.246	H
HETATM 1182	H	0	6.371	5.509	0.391	H
HETATM 1183	H	0	8.203	5.685	2.709	H
HETATM 1184	H	0	6.971	2.048	1.510	H
HETATM 1185	H	0	6.574	3.422	0.456	H
HETATM 1186	H	0	8.712	3.987	3.887	H
HETATM 1187	H	0	8.217	2.394	3.448	H
HETATM 1188	N	0	4.559	8.811	3.738	N
HETATM 1189	C	0	3.838	7.902	4.624	C
HETATM 1190	C	0	2.458	8.362	5.025	C
HETATM 1191	O	0	1.508	7.630	4.771	O
HETATM 1192	C	0	4.666	7.430	5.831	C
HETATM 1193	C	0	5.834	6.498	5.465	C
HETATM 1194	C	0	6.696	6.244	6.698	C
HETATM 1195	C	0	5.371	5.130	4.950	C
HETATM 1196	H	0	5.444	9.180	4.058	H
HETATM 1197	H	0	3.638	7.011	4.031	H
HETATM 1198	H	0	5.041	8.295	6.370	H
HETATM 1199	H	0	4.008	6.892	6.515	H
HETATM 1200	H	0	6.450	6.968	4.701	H
HETATM 1201	H	0	6.131	5.678	7.436	H
HETATM 1202	H	0	6.996	7.194	7.140	H
HETATM 1203	H	0	7.590	5.689	6.418	H
HETATM 1204	H	0	6.231	4.477	4.820	H
HETATM 1205	H	0	4.862	5.230	3.993	H
HETATM 1206	H	0	4.693	4.671	5.671	H
HETATM 1207	N	0	2.311	9.524	5.643	N

HETATM 1208	C	0	0.990	9.968	6.045	C
HETATM 1209	C	0	-0.059	10.008	4.901	C
HETATM 1210	O	0	-1.156	9.478	5.093	O
HETATM 1211	C	0	1.104	11.271	6.849	C
HETATM 1212	H	0	3.131	10.072	5.894	H
HETATM 1213	H	0	0.615	9.221	6.748	H
HETATM 1214	H	0	1.611	12.049	6.281	H
HETATM 1215	H	0	1.682	11.083	7.756	H
HETATM 1216	H	0	0.110	11.618	7.133	H
HETATM 1217	N	0	0.226	10.563	3.704	N
HETATM 1218	C	0	-0.611	10.381	2.508	C
HETATM 1219	C	0	-0.770	8.911	2.067	C
HETATM 1220	O	0	-1.847	8.536	1.608	O
HETATM 1221	C	0	0.078	11.199	1.415	C
HETATM 1222	C	0	0.976	12.189	2.147	C
HETATM 1223	C	0	1.363	11.425	3.403	C
HETATM 1224	H	0	-1.593	10.809	2.700	H
HETATM 1225	H	0	0.700	10.542	0.812	H
HETATM 1226	H	0	-0.649	11.730	0.805	H
HETATM 1227	H	0	0.402	13.075	2.419	H
HETATM 1228	H	0	1.853	12.461	1.558	H
HETATM 1229	H	0	1.567	12.136	4.199	H
HETATM 1230	H	0	2.248	10.823	3.208	H
HETATM 1231	N	0	0.250	8.048	2.176	N
HETATM 1232	C	0	0.081	6.604	1.943	C
HETATM 1233	C	0	-0.977	6.011	2.867	C
HETATM 1234	O	0	-1.945	5.430	2.388	O
HETATM 1235	C	0	1.409	5.839	2.000	C
HETATM 1236	C	0	1.254	4.378	1.539	C
HETATM 1237	C	0	0.808	4.230	0.084	C
HETATM 1238	C	0	2.591	3.673	1.691	C
HETATM 1239	H	0	1.152	8.383	2.501	H
HETATM 1240	H	0	-0.299	6.508	0.928	H
HETATM 1241	H	0	2.140	6.331	1.367	H
HETATM 1242	H	0	1.784	5.843	3.022	H
HETATM 1243	H	0	0.529	3.874	2.176	H
HETATM 1244	H	0	1.458	4.793	-0.577	H
HETATM 1245	H	0	-0.210	4.586	-0.035	H
HETATM 1246	H	0	0.841	3.179	-0.207	H
HETATM 1247	H	0	3.008	3.859	2.677	H
HETATM 1248	H	0	3.291	4.010	0.928	H
HETATM 1249	H	0	2.419	2.603	1.581	H
HETATM 1250	N	0	-0.834	6.213	4.173	N
HETATM 1251	C	0	-1.850	5.874	5.157	C
HETATM 1252	C	0	-3.215	6.488	4.843	C
HETATM 1253	O	0	-4.202	5.775	4.908	O

HETATM 1254 C	0	-1.369	6.184	6.581	C
HETATM 1255 C	0	-0.330	5.194	7.078	C
HETATM 1256 C	0	1.019	5.573	7.204	C
HETATM 1257 C	0	-0.714	3.876	7.397	C
HETATM 1258 C	0	1.989	4.633	7.600	C
HETATM 1259 C	0	0.251	2.934	7.806	C
HETATM 1260 C	0	1.610	3.306	7.889	C
HETATM 1261 O	0	2.549	2.412	8.293	O
HETATM 1262 H	0	-0.001	6.707	4.478	H
HETATM 1263 H	0	-2.006	4.798	5.107	H
HETATM 1264 H	0	-0.973	7.199	6.624	H
HETATM 1265 H	0	-2.225	6.133	7.257	H
HETATM 1266 H	0	1.317	6.590	6.995	H
HETATM 1267 H	0	-1.750	3.574	7.313	H
HETATM 1268 H	0	3.025	4.921	7.693	H
HETATM 1269 H	0	-0.043	1.920	8.032	H
HETATM 1270 H	0	2.124	1.656	8.739	H
HETATM 1271 N	0	-3.311	7.766	4.475	N
HETATM 1272 C	0	-4.570	8.404	4.085	C
HETATM 1273 C	0	-5.221	7.793	2.802	C
HETATM 1274 O	0	-6.410	7.489	2.823	O
HETATM 1275 C	0	-4.337	9.910	3.931	C
HETATM 1276 H	0	-2.460	8.318	4.491	H
HETATM 1277 H	0	-5.283	8.259	4.895	H
HETATM 1278 H	0	-3.654	10.099	3.105	H
HETATM 1279 H	0	-3.911	10.319	4.847	H
HETATM 1280 H	0	-5.285	10.407	3.722	H
HETATM 1281 N	0	-4.490	7.618	1.688	N
HETATM 1282 C	0	-4.948	6.958	0.433	C
HETATM 1283 C	0	-5.316	5.459	0.718	C
HETATM 1284 O	0	-6.378	5.017	0.286	O
HETATM 1285 C	0	-3.892	7.010	-0.679	C
HETATM 1286 O	0	-2.633	6.558	-0.227	O
HETATM 1287 H	0	-3.522	7.907	1.756	H
HETATM 1288 H	0	-5.850	7.457	0.082	H
HETATM 1289 H	0	-3.782	8.022	-1.057	H
HETATM 1290 H	0	-4.222	6.380	-1.506	H
HETATM 1291 H	0	-2.288	7.207	0.414	H
HETATM 1292 N	0	-4.500	4.674	1.462	N
HETATM 1293 C	0	-4.764	3.290	1.971	C
HETATM 1294 C	0	-6.039	3.276	2.772	C
HETATM 1295 O	0	-6.915	2.456	2.540	O
HETATM 1296 C	0	-3.577	2.828	2.806	C
HETATM 1297 H	0	-3.633	5.102	1.772	H
HETATM 1298 H	0	-4.884	2.616	1.121	H
HETATM 1299 H	0	-3.715	1.784	3.068	H

HETATM 1300	H	0	-3.504	3.421	3.716	H
HETATM 1301	H	0	-2.657	2.928	2.237	H
HETATM 1302	N	0	-6.155	4.235	3.682	N
HETATM 1303	C	0	-7.343	4.476	4.462	C
HETATM 1304	C	0	-8.590	4.789	3.642	C
HETATM 1305	O	0	-9.643	4.270	3.972	O
HETATM 1306	C	0	-7.067	5.488	5.581	C
HETATM 1307	C	0	-8.285	5.878	6.440	C
HETATM 1308	C	0	-7.921	6.254	7.890	C
HETATM 1309	N	0	-6.607	6.917	8.036	N
HETATM 1310	C	0	-6.234	8.131	7.690	C
HETATM 1311	N	0	-7.062	8.969	7.133	N
HETATM 1312	N	0	-5.014	8.532	7.897	N
HETATM 1313	H	0	-5.342	4.817	3.854	H
HETATM 1314	H	0	-7.582	3.538	4.967	H
HETATM 1315	H	0	-6.313	5.038	6.227	H
HETATM 1316	H	0	-6.658	6.402	5.156	H
HETATM 1317	H	0	-8.991	5.048	6.482	H
HETATM 1318	H	0	-8.788	6.719	5.963	H
HETATM 1319	H	0	-7.887	5.330	8.472	H
HETATM 1320	H	0	-8.713	6.873	8.316	H
HETATM 1321	H	0	-5.867	6.310	8.384	H
HETATM 1322	H	0	-6.785	9.903	6.903	H
HETATM 1323	H	0	-8.003	8.651	6.990	H
HETATM 1324	H	0	-4.379	7.932	8.423	H
HETATM 1325	H	0	-4.704	9.443	7.627	H
HETATM 1326	N	0	-8.514	5.591	2.587	N
HETATM 1327	C	0	-9.621	5.796	1.647	C
HETATM 1328	C	0	-10.009	4.533	0.890	C
HETATM 1329	O	0	-11.196	4.305	0.678	O
HETATM 1330	C	0	-9.226	6.917	0.685	C
HETATM 1331	H	0	-7.628	6.051	2.418	H
HETATM 1332	H	0	-10.490	6.139	2.206	H
HETATM 1333	H	0	-8.980	7.815	1.249	H
HETATM 1334	H	0	-10.064	7.126	0.026	H
HETATM 1335	H	0	-8.370	6.623	0.081	H
HETATM 1336	N	0	-9.034	3.702	0.519	N
HETATM 1337	C	0	-9.313	2.355	0.043	C
HETATM 1338	C	0	-10.005	1.506	1.095	C
HETATM 1339	O	0	-11.025	0.898	0.812	O
HETATM 1340	C	0	-8.034	1.709	-0.532	C
HETATM 1341	C	0	-8.277	0.392	-1.300	C
HETATM 1342	C	0	-9.020	0.594	-2.624	C
HETATM 1343	C	0	-6.936	-0.263	-1.636	C
HETATM 1344	H	0	-8.073	3.995	0.656	H
HETATM 1345	H	0	-10.024	2.460	-0.777	H

HETATM 1346	H	0	-7.545	2.418	-1.202	H
HETATM 1347	H	0	-7.348	1.502	0.286	H
HETATM 1348	H	0	-8.849	-0.293	-0.676	H
HETATM 1349	H	0	-8.431	1.203	-3.308	H
HETATM 1350	H	0	-9.993	1.052	-2.451	H
HETATM 1351	H	0	-9.195	-0.378	-3.085	H
HETATM 1352	H	0	-6.356	0.377	-2.300	H
HETATM 1353	H	0	-7.108	-1.223	-2.123	H
HETATM 1354	H	0	-6.368	-0.436	-0.722	H
HETATM 1355	N	0	-9.489	1.507	2.315	N
HETATM 1356	C	0	-10.081	0.832	3.457	C
HETATM 1357	C	0	-11.517	1.283	3.750	C
HETATM 1358	O	0	-12.377	0.484	4.115	O
HETATM 1359	C	0	-9.185	0.979	4.693	C
HETATM 1360	C	0	-8.837	-0.262	5.462	C
HETATM 1361	C	0	-7.744	-0.334	6.252	C
HETATM 1362	C	0	-9.470	-1.591	5.529	C
HETATM 1363	N	0	-7.654	-1.591	6.806	N
HETATM 1364	C	0	-8.675	-2.409	6.389	C
HETATM 1365	C	0	-10.603	-2.218	4.956	C
HETATM 1366	C	0	-8.976	-3.750	6.661	C
HETATM 1367	C	0	-10.910	-3.568	5.215	C
HETATM 1368	C	0	-10.095	-4.337	6.059	C
HETATM 1369	H	0	-8.611	1.994	2.442	H
HETATM 1370	H	0	-10.125	-0.223	3.197	H
HETATM 1371	H	0	-8.235	1.412	4.388	H
HETATM 1372	H	0	-9.633	1.695	5.379	H
HETATM 1373	H	0	-7.038	0.477	6.394	H
HETATM 1374	H	0	-6.879	-1.885	7.398	H
HETATM 1375	H	0	-11.258	-1.674	4.302	H
HETATM 1376	H	0	-8.355	-4.324	7.328	H
HETATM 1377	H	0	-11.779	-4.021	4.761	H
HETATM 1378	H	0	-10.331	-5.374	6.250	H
HETATM 1379	N	0	-11.765	2.578	3.605	N
HETATM 1380	C	0	-13.041	3.257	3.724	C
HETATM 1381	C	0	-14.003	2.881	2.613	C
HETATM 1382	O	0	-15.094	2.420	2.923	O
HETATM 1383	C	0	-12.760	4.773	3.783	C
HETATM 1384	C	0	-13.958	5.733	3.682	C
HETATM 1385	C	0	-14.932	5.605	4.848	C
HETATM 1386	C	0	-13.436	7.171	3.662	C
HETATM 1387	H	0	-10.951	3.153	3.421	H
HETATM 1388	H	0	-13.503	2.960	4.666	H
HETATM 1389	H	0	-12.220	4.983	4.707	H
HETATM 1390	H	0	-12.103	5.013	2.956	H
HETATM 1391	H	0	-14.492	5.549	2.751	H

HETATM 1392	H	0	-14.423	5.818	5.787	H
HETATM 1393	H	0	-15.340	4.599	4.871	H
HETATM 1394	H	0	-15.755	6.308	4.722	H
HETATM 1395	H	0	-12.878	7.380	4.575	H
HETATM 1396	H	0	-14.274	7.865	3.592	H
HETATM 1397	H	0	-12.790	7.318	2.798	H
HETATM 1398	N	0	-13.605	3.053	1.350	N
HETATM 1399	C	0	-14.320	2.531	0.191	C
HETATM 1400	C	0	-14.646	1.040	0.394	C
HETATM 1401	O	0	-15.796	0.685	0.227	O
HETATM 1402	C	0	-13.505	2.709	-1.107	C
HETATM 1403	C	0	-13.560	4.097	-1.753	C
HETATM 1404	C	0	-12.557	4.191	-2.902	C
HETATM 1405	C	0	-14.949	4.391	-2.331	C
HETATM 1406	H	0	-12.678	3.436	1.201	H
HETATM 1407	H	0	-15.274	3.048	0.097	H
HETATM 1408	H	0	-12.467	2.436	-0.915	H
HETATM 1409	H	0	-13.895	2.014	-1.844	H
HETATM 1410	H	0	-13.302	4.844	-1.011	H
HETATM 1411	H	0	-12.795	3.462	-3.677	H
HETATM 1412	H	0	-11.553	3.997	-2.523	H
HETATM 1413	H	0	-12.573	5.190	-3.334	H
HETATM 1414	H	0	-15.247	3.585	-3.003	H
HETATM 1415	H	0	-14.937	5.322	-2.893	H
HETATM 1416	H	0	-15.685	4.471	-1.533	H
HETATM 1417	N	0	-13.692	0.174	0.770	N
HETATM 1418	C	0	-13.896	-1.268	1.051	C
HETATM 1419	C	0	-14.961	-1.455	2.119	C
HETATM 1420	O	0	-15.909	-2.196	1.901	O
HETATM 1421	C	0	-12.574	-1.989	1.385	C
HETATM 1422	C	0	-12.778	-3.368	2.021	C
HETATM 1423	C	0	-11.755	-2.221	0.108	C
HETATM 1424	H	0	-12.751	0.543	0.845	H
HETATM 1425	H	0	-14.300	-1.727	0.150	H
HETATM 1426	H	0	-11.994	-1.380	2.075	H
HETATM 1427	H	0	-11.807	-3.831	2.185	H
HETATM 1428	H	0	-13.375	-4.004	1.367	H
HETATM 1429	H	0	-13.273	-3.278	2.987	H
HETATM 1430	H	0	-12.325	-2.819	-0.602	H
HETATM 1431	H	0	-10.831	-2.744	0.346	H
HETATM 1432	H	0	-11.496	-1.274	-0.359	H
HETATM 1433	N	0	-14.836	-0.792	3.265	N
HETATM 1434	C	0	-15.797	-0.902	4.354	C
HETATM 1435	C	0	-17.175	-0.237	4.086	C
HETATM 1436	O	0	-18.159	-0.619	4.718	O
HETATM 1437	C	0	-15.121	-0.404	5.629	C

HETATM 1438 H	0	-14.018	-0.208	3.397	H
HETATM 1439 H	0	-16.007	-1.962	4.505	H
HETATM 1440 H	0	-14.277	-1.052	5.872	H
HETATM 1441 H	0	-15.831	-0.433	6.456	H
HETATM 1442 H	0	-14.752	0.609	5.484	H
HETATM 1443 N	0	-17.273	0.748	3.183	N
HETATM 1444 C	0	-18.528	1.283	2.622	C
HETATM 1445 C	0	-19.119	0.255	1.611	C
HETATM 1446 O	0	-20.229	-0.212	1.824	O
HETATM 1447 C	0	-18.277	2.634	1.925	C
HETATM 1448 C	0	-18.027	3.812	2.882	C
HETATM 1449 C	0	-17.480	4.998	2.087	C
HETATM 1450 C	0	-19.300	4.257	3.601	C
HETATM 1451 H	0	-16.407	1.060	2.759	H
HETATM 1452 H	0	-19.265	1.410	3.414	H
HETATM 1453 H	0	-17.422	2.526	1.259	H
HETATM 1454 H	0	-19.143	2.874	1.305	H
HETATM 1455 H	0	-17.289	3.533	3.630	H
HETATM 1456 H	0	-18.202	5.298	1.326	H
HETATM 1457 H	0	-16.546	4.707	1.610	H
HETATM 1458 H	0	-17.297	5.836	2.760	H
HETATM 1459 H	0	-20.065	4.536	2.876	H
HETATM 1460 H	0	-19.083	5.113	4.241	H
HETATM 1461 H	0	-19.679	3.450	4.227	H
HETATM 1462 N	0	-18.371	-0.135	0.561	N
HETATM 1463 C	0	-18.651	-1.175	-0.460	C
HETATM 1464 C	0	-19.144	-2.488	0.158	C
HETATM 1465 O	0	-20.021	-3.153	-0.385	O
HETATM 1466 C	0	-17.411	-1.387	-1.334	C
HETATM 1467 H	0	-17.466	0.305	0.484	H
HETATM 1468 H	0	-19.457	-0.812	-1.099	H
HETATM 1469 H	0	-17.614	-2.160	-2.072	H
HETATM 1470 H	0	-16.570	-1.701	-0.716	H
HETATM 1471 H	0	-17.158	-0.464	-1.852	H
HETATM 1472 N	0	-18.541	-2.874	1.280	N
HETATM 1473 C	0	-18.898	-4.052	2.044	C
HETATM 1474 C	0	-20.137	-3.907	2.934	C
HETATM 1475 O	0	-20.771	-4.910	3.258	O
HETATM 1476 C	0	-17.708	-4.454	2.932	C
HETATM 1477 H	0	-17.746	-2.327	1.585	H
HETATM 1478 H	0	-19.106	-4.869	1.352	H
HETATM 1479 H	0	-17.952	-5.371	3.470	H
HETATM 1480 H	0	-17.505	-3.662	3.653	H
HETATM 1481 H	0	-16.816	-4.627	2.332	H
HETATM 1482 N	0	-20.431	-2.691	3.393	N
HETATM 1483 C	0	-21.666	-2.380	4.078	C

HETATM 1484 H	0	-21.835	-3.008	4.928	H
HETATM 1485 H	0	-22.440	-2.541	3.357	H
HETATM 1486 H	0	-21.672	-1.355	4.385	H
HETATM 1487 H	0	-19.900	-1.913	3.021	H
HETATM 1488 N	0	4.241	-2.756	-5.130	N
HETATM 1489 C	0	4.308	-2.227	-3.743	C
HETATM 1490 C	0	5.764	-2.349	-3.195	C
HETATM 1491 O	0	6.625	-2.701	-4.038	O
HETATM 1492 O	0	6.047	-2.131	-1.992	O
HETATM 1493 C	0	3.189	-2.882	-2.914	C
HETATM 1494 C	0	3.146	-2.505	-1.421	C
HETATM 1495 C	0	3.145	-1.013	-1.146	C
HETATM 1496 O	0	2.308	-0.313	-1.699	O
HETATM 1497 N	0	4.081	-0.546	-0.286	N
HETATM 1498 C	0	4.229	0.855	0.028	C
HETATM 1499 C	0	5.200	1.565	-0.915	C
HETATM 1500 O	0	5.205	2.794	-1.015	O
HETATM 1501 C	0	4.651	1.053	1.492	C
HETATM 1502 S	0	6.203	0.229	2.016	S
HETATM 1503 N	0	6.021	0.755	-1.600	N
HETATM 1504 C	0	6.976	1.225	-2.594	C
HETATM 1505 C	0	6.483	1.091	-4.019	C
HETATM 1506 O	0	5.509	0.364	-4.279	O
HETATM 1507 O	0	7.072	1.736	-4.899	O
HETATM 1508 H	0	5.150	-2.611	-5.551	H
HETATM 1509 H	0	3.491	-2.301	-5.652	H
HETATM 1510 H	0	4.011	-3.747	-5.159	H
HETATM 1511 H	0	4.095	-1.160	-3.761	H
HETATM 1512 H	0	2.236	-2.587	-3.358	H
HETATM 1513 H	0	3.270	-3.963	-2.996	H
HETATM 1514 H	0	3.977	-2.975	-0.899	H
HETATM 1515 H	0	2.229	-2.892	-0.995	H
HETATM 1516 H	0	4.718	-1.178	0.196	H
HETATM 1517 H	0	3.261	1.336	-0.136	H
HETATM 1518 H	0	3.827	0.715	2.130	H
HETATM 1519 H	0	4.742	2.132	1.658	H
HETATM 1520 H	0	5.976	-0.253	-1.493	H
HETATM 1521 H	0	7.213	2.271	-2.419	H
HETATM 1522 H	0	7.892	0.643	-2.518	H
HETATM 1523 O	0	10.937	-6.914	-8.058	O
HETATM 1524 H	0	10.025	-6.624	-7.969	H
HETATM 1525 H	0	11.326	-6.268	-8.661	H
HETATM 1526 O	0	22.008	-2.058	3.033	O
HETATM 1527 H	0	22.766	-2.590	2.773	H
HETATM 1528 H	0	22.364	-1.474	3.710	H
HETATM 1529 O	0	16.309	5.927	-5.219	O

HETATM 1530	H	0	15.495	6.461	-5.121	H
HETATM 1531	H	0	16.926	6.553	-5.603	H
HETATM 1532	O	0	13.851	8.628	3.268	O
HETATM 1533	H	0	13.450	8.545	4.147	H
HETATM 1534	H	0	14.657	9.153	3.452	H
HETATM 1535	O	0	4.742	10.857	6.722	O
HETATM 1536	H	0	5.114	10.685	7.595	H
HETATM 1537	H	0	5.470	10.594	6.135	H
HETATM 1538	O	0	7.957	11.910	7.407	O
HETATM 1539	H	0	7.543	11.126	7.817	H
HETATM 1540	H	0	7.496	12.639	7.823	H
HETATM 1541	O	0	4.733	8.042	9.104	O
HETATM 1542	H	0	3.766	8.176	9.059	H
HETATM 1543	H	0	4.806	7.110	9.364	H
HETATM 1544	O	0	14.293	-1.450	4.250	O
HETATM 1545	H	0	13.565	-1.898	4.739	H
HETATM 1546	H	0	15.068	-2.000	4.472	H
HETATM 1547	O	0	-2.997	-3.056	-6.311	O
HETATM 1548	H	0	-2.758	-3.972	-6.551	H
HETATM 1549	H	0	-3.120	-2.626	-7.178	H
HETATM 1550	O	0	-8.990	3.967	-3.345	O
HETATM 1551	H	0	-8.180	4.354	-3.690	H
HETATM 1552	H	0	-8.757	3.057	-3.160	H
HETATM 1553	O	0	-14.822	1.559	8.037	O
HETATM 1554	H	0	-14.194	0.931	8.447	H
HETATM 1555	H	0	-15.480	1.665	8.746	H
HETATM 1556	O	0	-16.447	-4.472	6.478	O
HETATM 1557	H	0	-16.667	-3.936	7.270	H
HETATM 1558	H	0	-17.206	-4.314	5.907	H
HETATM 1559	O	0	-16.416	2.543	6.019	O
HETATM 1560	H	0	-16.022	2.490	5.138	H
HETATM 1561	H	0	-15.773	2.075	6.589	H
HETATM 1562	O	0	-10.251	-1.388	8.946	O
HETATM 1563	H	0	-10.496	-1.076	8.059	H
HETATM 1564	H	0	-11.063	-1.841	9.236	H
HETATM 1565	O	0	-13.442	3.736	7.211	O
HETATM 1566	H	0	-14.086	4.409	7.467	H
HETATM 1567	H	0	-13.873	2.918	7.527	H
HETATM 1568	O	0	3.206	-7.669	9.335	O
HETATM 1569	H	0	3.291	-6.809	8.884	H
HETATM 1570	H	0	2.524	-8.118	8.797	H
HETATM 1571	O	0	-5.915	-4.447	6.263	O
HETATM 1572	H	0	-6.684	-4.328	5.697	H
HETATM 1573	H	0	-6.158	-5.230	6.799	H
HETATM 1574	O	0	17.160	3.866	-3.677	O
HETATM 1575	H	0	16.786	4.615	-4.189	H

HETATM 1576 H	0	17.829	3.519	-4.270	H
HETATM 1577 O	0	16.324	3.658	-1.121	O
HETATM 1578 H	0	16.636	3.736	-2.048	H
HETATM 1579 H	0	17.053	3.182	-0.688	H
HETATM 1580 O	0	16.487	-3.031	4.746	O
HETATM 1581 H	0	16.260	-3.520	5.560	H
HETATM 1582 H	0	17.288	-3.491	4.440	H
HETATM 1583 O	0	18.008	2.157	0.530	O
HETATM 1584 H	0	18.646	1.427	0.386	H
HETATM 1585 H	0	17.265	1.688	0.952	H
HETATM 1586 O	0	19.447	-2.214	2.187	O
HETATM 1587 H	0	19.188	-3.069	2.583	H
HETATM 1588 H	0	20.374	-2.120	2.494	H
HETATM 1589 O	0	18.428	-4.495	3.320	O
HETATM 1590 H	0	17.692	-4.758	2.727	H
HETATM 1591 H	0	18.854	-5.336	3.515	H
HETATM 1592 O	0	19.425	-0.149	0.360	O
HETATM 1593 H	0	19.393	-0.861	1.027	H
HETATM 1594 H	0	20.123	-0.442	-0.231	H
HETATM 1595 O	0	16.766	-1.670	2.166	O
HETATM 1596 H	0	16.549	-2.094	3.012	H
HETATM 1597 H	0	17.726	-1.832	2.090	H
HETATM 1598 O	0	-2.277	-5.686	-6.601	O
HETATM 1599 H	0	-2.091	-5.947	-5.694	H
HETATM 1600 H	0	-1.524	-6.068	-7.098	H
HETATM 1601 O	0	1.077	0.389	-12.590	O
HETATM 1602 H	0	1.292	0.547	-11.657	H
HETATM 1603 H	0	0.834	-0.538	-12.613	H
HETATM 1604 O	0	-8.257	-12.469	0.678	O
HETATM 1605 H	0	-7.914	-13.177	0.124	H
HETATM 1606 H	0	-9.061	-12.173	0.189	H
HETATM 1607 O	0	-10.510	-11.562	-0.305	O
HETATM 1608 H	0	-11.159	-11.303	0.377	H
HETATM 1609 H	0	-10.806	-11.066	-1.091	H
HETATM 1610 O	0	-6.213	-12.034	3.643	O
HETATM 1611 H	0	-6.766	-11.414	3.137	H
HETATM 1612 H	0	-5.469	-12.199	3.057	H
HETATM 1613 O	0	2.757	-10.595	6.545	O
HETATM 1614 H	0	3.272	-11.372	6.853	H
HETATM 1615 H	0	2.204	-10.955	5.827	H
HETATM 1616 O	0	4.550	-12.356	7.525	O
HETATM 1617 H	0	4.777	-13.170	7.981	H
HETATM 1618 H	0	5.203	-11.719	7.873	H
HETATM 1619 O	0	14.498	-7.066	7.130	O
HETATM 1620 H	0	13.557	-7.002	7.374	H
HETATM 1621 H	0	14.599	-8.014	6.967	H

HETATM 1622	O	0	14.976	7.221	1.151	O
HETATM 1623	H	0	14.538	7.724	1.859	H
HETATM 1624	H	0	15.909	7.230	1.430	H
HETATM 1625	O	0	15.133	8.152	7.182	O
HETATM 1626	H	0	14.297	8.413	6.756	H
HETATM 1627	H	0	15.357	8.912	7.728	H
HETATM 1628	O	0	17.883	9.634	1.924	O
HETATM 1629	H	0	17.853	8.659	1.938	H
HETATM 1630	H	0	18.484	9.828	1.200	H
HETATM 1631	O	0	13.863	10.084	-3.643	O
HETATM 1632	H	0	14.012	10.580	-2.818	H
HETATM 1633	H	0	13.288	10.700	-4.139	H
HETATM 1634	O	0	14.934	4.162	2.398	O
HETATM 1635	H	0	15.896	4.134	2.248	H
HETATM 1636	H	0	14.584	4.391	1.518	H
HETATM 1637	O	0	17.726	4.232	2.235	O
HETATM 1638	H	0	18.335	3.928	2.915	H
HETATM 1639	H	0	17.900	3.605	1.502	H
HETATM 1640	O	0	17.448	6.955	2.316	O
HETATM 1641	H	0	17.635	6.005	2.186	H
HETATM 1642	H	0	17.249	7.005	3.269	H
HETATM 1643	O	0	14.889	12.320	4.358	O
HETATM 1644	H	0	14.062	12.102	4.825	H
HETATM 1645	H	0	14.961	13.273	4.455	H
HETATM 1646	O	0	10.056	4.412	6.772	O
HETATM 1647	H	0	9.188	4.011	6.992	H
HETATM 1648	H	0	10.683	3.714	7.042	H
HETATM 1649	O	0	16.091	9.948	3.897	O
HETATM 1650	H	0	16.775	10.024	3.194	H
HETATM 1651	H	0	15.818	10.881	4.034	H
HETATM 1652	O	0	14.620	5.483	7.517	O
HETATM 1653	H	0	14.692	5.273	6.572	H
HETATM 1654	H	0	14.914	6.412	7.547	H
HETATM 1655	O	0	14.083	1.181	3.783	O
HETATM 1656	H	0	14.248	0.228	3.958	H
HETATM 1657	H	0	14.762	1.384	3.119	H
HETATM 1658	O	0	6.732	9.768	8.615	O
HETATM 1659	H	0	7.465	9.214	8.944	H
HETATM 1660	H	0	5.958	9.198	8.813	H
HETATM 1661	O	0	11.942	2.634	7.547	O
HETATM 1662	H	0	12.338	3.220	8.226	H
HETATM 1663	H	0	12.465	2.851	6.746	H
HETATM 1664	O	0	16.431	7.445	4.842	O
HETATM 1665	H	0	16.405	8.362	4.497	H
HETATM 1666	H	0	16.258	7.587	5.788	H
HETATM 1667	O	0	2.016	7.981	9.181	O

HETATM 1668	H	0	1.065	8.198	9.151	H
HETATM 1669	H	0	2.071	7.335	9.905	H
HETATM 1670	O	0	11.816	6.170	-0.974	O
HETATM 1671	H	0	12.659	5.753	-0.728	H
HETATM 1672	H	0	12.066	6.776	-1.695	H
HETATM 1673	O	0	11.396	1.008	9.801	O
HETATM 1674	H	0	11.912	0.178	9.833	H
HETATM 1675	H	0	11.691	1.408	8.966	H
HETATM 1676	O	0	14.181	7.597	-5.027	O
HETATM 1677	H	0	14.353	8.524	-4.789	H
HETATM 1678	H	0	13.470	7.368	-4.404	H
HETATM 1679	O	0	14.209	5.006	-0.176	O
HETATM 1680	H	0	14.554	5.865	0.152	H
HETATM 1681	H	0	14.993	4.594	-0.602	H
HETATM 1682	O	0	14.567	5.451	4.702	O
HETATM 1683	H	0	14.690	5.002	3.833	H
HETATM 1684	H	0	15.253	6.149	4.664	H
HETATM 1685	O	0	5.255	3.047	8.339	O
HETATM 1686	H	0	4.343	2.805	8.098	H
HETATM 1687	H	0	5.468	2.357	9.013	H
HETATM 1688	O	0	10.392	5.616	9.262	O
HETATM 1689	H	0	11.281	5.275	9.470	H
HETATM 1690	H	0	10.274	5.340	8.338	H
HETATM 1691	O	0	12.320	7.945	-2.991	O
HETATM 1692	H	0	12.935	8.699	-3.071	H
HETATM 1693	H	0	11.454	8.398	-2.982	H
HETATM 1694	O	0	12.605	11.378	5.585	O
HETATM 1695	H	0	12.691	10.423	5.751	H
HETATM 1696	H	0	12.192	11.708	6.392	H
HETATM 1697	O	0	7.862	3.011	7.496	O
HETATM 1698	H	0	6.893	3.034	7.634	H
HETATM 1699	H	0	8.128	2.222	8.020	H
HETATM 1700	O	0	11.120	-2.814	11.300	O
HETATM 1701	H	0	11.694	-2.196	10.808	H
HETATM 1702	H	0	11.384	-3.673	10.929	H
HETATM 1703	O	0	8.469	7.778	9.439	O
HETATM 1704	H	0	7.856	7.046	9.598	H
HETATM 1705	H	0	9.329	7.344	9.528	H
HETATM 1706	O	0	15.729	-4.654	6.950	O
HETATM 1707	H	0	16.311	-4.722	7.714	H
HETATM 1708	H	0	15.316	-5.547	6.925	H
HETATM 1709	O	0	2.610	6.016	11.052	O
HETATM 1710	H	0	2.860	6.093	11.979	H
HETATM 1711	H	0	3.446	5.721	10.631	H
HETATM 1712	O	0	7.711	5.053	9.755	O
HETATM 1713	H	0	8.671	5.162	9.873	H

HETATM 1714 H	0	7.658	4.301	9.150	H
HETATM 1715 O	0	12.990	3.223	5.146	O
HETATM 1716 H	0	13.518	4.022	4.972	H
HETATM 1717 H	0	13.451	2.548	4.602	H
HETATM 1718 O	0	12.930	4.468	9.290	O
HETATM 1719 H	0	13.575	4.875	8.664	H
HETATM 1720 H	0	13.463	4.326	10.079	H
HETATM 1721 O	0	-2.502	3.527	-0.611	O
HETATM 1722 H	0	-2.079	2.804	-0.096	H
HETATM 1723 H	0	-2.550	4.245	0.031	H
HETATM 1724 O	0	-9.369	-12.676	5.391	O
HETATM 1725 H	0	-9.616	-12.775	4.443	H
HETATM 1726 H	0	-9.918	-13.337	5.821	H
HETATM 1727 O	0	-18.566	3.069	8.858	O
HETATM 1728 H	0	-19.461	3.362	9.059	H
HETATM 1729 H	0	-18.710	2.409	8.151	H
HETATM 1730 O	0	-5.522	2.575	7.273	O
HETATM 1731 H	0	-5.228	3.411	7.672	H
HETATM 1732 H	0	-6.496	2.638	7.348	H
HETATM 1733 O	0	-8.194	2.737	7.679	O
HETATM 1734 H	0	-8.333	2.732	8.644	H
HETATM 1735 H	0	-9.113	2.728	7.351	H
HETATM 1736 O	0	-4.857	4.805	8.863	O
HETATM 1737 H	0	-5.432	4.376	9.539	H
HETATM 1738 H	0	-3.978	4.767	9.284	H
HETATM 1739 O	0	-8.035	-0.002	9.607	O
HETATM 1740 H	0	-8.865	-0.500	9.451	H
HETATM 1741 H	0	-7.661	0.052	8.720	H
HETATM 1742 O	0	-5.533	-3.302	10.503	O
HETATM 1743 H	0	-4.761	-3.886	10.364	H
HETATM 1744 H	0	-6.279	-3.922	10.390	H
HETATM 1745 O	0	-11.255	-4.063	11.723	O
HETATM 1746 H	0	-10.405	-3.573	11.648	H
HETATM 1747 H	0	-11.346	-4.195	12.672	H
HETATM 1748 O	0	-2.860	-2.395	-3.719	O
HETATM 1749 H	0	-2.985	-2.639	-4.663	H
HETATM 1750 H	0	-2.678	-1.449	-3.765	H
HETATM 1751 O	0	-12.715	-4.874	8.120	O
HETATM 1752 H	0	-13.058	-5.745	8.401	H
HETATM 1753 H	0	-13.022	-4.824	7.196	H
HETATM 1754 O	0	-12.996	-0.000	9.260	O
HETATM 1755 H	0	-12.518	-0.059	8.405	H
HETATM 1756 H	0	-12.984	-0.921	9.575	H
HETATM 1757 O	0	-7.831	-10.300	2.222	O
HETATM 1758 H	0	-7.613	-9.598	1.584	H
HETATM 1759 H	0	-8.015	-11.065	1.637	H

HETATM 1760	O	0	-13.511	-7.436	8.728	O
HETATM 1761	H	0	-14.309	-7.391	8.152	H
HETATM 1762	H	0	-13.842	-7.906	9.499	H
HETATM 1763	O	0	-11.963	-7.327	5.417	O
HETATM 1764	H	0	-12.534	-6.547	5.507	H
HETATM 1765	H	0	-11.532	-7.393	6.289	H
HETATM 1766	O	0	-18.675	1.223	6.760	O
HETATM 1767	H	0	-18.854	0.582	6.049	H
HETATM 1768	H	0	-17.948	1.756	6.384	H
HETATM 1769	O	0	-8.324	-8.516	7.001	O
HETATM 1770	H	0	-9.220	-8.302	7.321	H
HETATM 1771	H	0	-8.508	-8.992	6.165	H
HETATM 1772	O	0	-17.242	-3.091	8.668	O
HETATM 1773	H	0	-16.494	-2.877	9.275	H
HETATM 1774	H	0	-17.891	-3.475	9.265	H
HETATM 1775	O	0	-5.829	-0.561	11.230	O
HETATM 1776	H	0	-5.788	-1.534	11.266	H
HETATM 1777	H	0	-6.659	-0.404	10.739	H
HETATM 1778	O	0	-15.303	-7.448	4.468	O
HETATM 1779	H	0	-15.992	-7.433	3.796	H
HETATM 1780	H	0	-14.857	-8.304	4.296	H
HETATM 1781	O	0	-14.181	-9.894	4.044	O
HETATM 1782	H	0	-13.211	-9.800	4.133	H
HETATM 1783	H	0	-14.381	-10.643	4.612	H
HETATM 1784	O	0	-15.295	-2.456	10.347	O
HETATM 1785	H	0	-15.376	-1.684	10.946	H
HETATM 1786	H	0	-14.337	-2.531	10.225	H
HETATM 1787	O	0	-12.088	-10.937	1.831	O
HETATM 1788	H	0	-13.044	-10.930	1.951	H
HETATM 1789	H	0	-11.779	-10.404	2.593	H
HETATM 1790	O	0	-11.719	0.144	6.931	O
HETATM 1791	H	0	-12.010	0.070	6.008	H
HETATM 1792	H	0	-11.357	1.050	6.975	H
HETATM 1793	O	0	-15.694	-7.119	7.209	O
HETATM 1794	H	0	-15.635	-7.401	6.280	H
HETATM 1795	H	0	-16.099	-6.240	7.131	H
HETATM 1796	O	0	-10.355	-5.421	9.477	O
HETATM 1797	H	0	-11.038	-5.079	8.872	H
HETATM 1798	H	0	-10.681	-5.123	10.346	H
HETATM 1799	O	0	-16.126	4.344	8.168	O
HETATM 1800	H	0	-16.268	3.917	7.307	H
HETATM 1801	H	0	-16.990	4.219	8.591	H
HETATM 1802	O	0	-17.596	-0.309	8.796	O
HETATM 1803	H	0	-17.550	-1.260	8.601	H
HETATM 1804	H	0	-18.106	0.051	8.049	H
HETATM 1805	O	0	-11.761	2.345	10.062	O

HETATM 1806	H	0	-12.174	1.465	9.972	H
HETATM 1807	H	0	-12.534	2.903	10.279	H
HETATM 1808	O	0	-10.948	2.741	7.482	O
HETATM 1809	H	0	-11.128	2.654	8.439	H
HETATM 1810	H	0	-11.736	3.238	7.183	H
HETATM 1811	O	0	-11.496	-9.590	4.113	O
HETATM 1812	H	0	-10.571	-9.770	4.376	H
HETATM 1813	H	0	-11.650	-8.709	4.527	H
HETATM 1814	O	0	-8.901	-10.012	4.764	O
HETATM 1815	H	0	-8.938	-10.945	5.052	H
HETATM 1816	H	0	-8.463	-10.072	3.892	H
HETATM 1817	O	0	-12.566	-2.708	9.755	O
HETATM 1818	H	0	-12.697	-3.434	9.107	H
HETATM 1819	H	0	-12.212	-3.186	10.533	H
HETATM 1820	O	0	-16.570	1.681	10.198	O
HETATM 1821	H	0	-16.935	0.856	9.796	H
HETATM 1822	H	0	-17.277	2.318	9.985	H
HETATM 1823	O	0	-8.932	2.517	10.313	O
HETATM 1824	H	0	-8.716	1.566	10.291	H
HETATM 1825	H	0	-9.902	2.517	10.426	H
HETATM 1826	O	0	-14.316	3.481	10.316	O
HETATM 1827	H	0	-14.791	4.031	9.676	H
HETATM 1828	H	0	-14.997	2.848	10.588	H
HETATM 1829	O	0	-15.441	-0.226	11.876	O
HETATM 1830	H	0	-15.800	0.508	11.347	H
HETATM 1831	H	0	-15.562	0.073	12.780	H
HETATM 1832	O	0	-13.948	-5.316	5.612	O
HETATM 1833	H	0	-14.747	-4.836	5.902	H
HETATM 1834	H	0	-14.338	-6.039	5.084	H
HETATM 1835	O	0	-10.843	-7.621	7.909	O
HETATM 1836	H	0	-10.494	-6.953	8.529	H
HETATM 1837	H	0	-11.742	-7.773	8.254	H
HETATM 1838	O	0	-6.581	-6.548	7.826	O
HETATM 1839	H	0	-5.701	-6.961	7.944	H
HETATM 1840	H	0	-7.137	-7.297	7.527	H
HETATM 1841	O	0	-5.306	-1.658	8.389	O
HETATM 1842	H	0	-5.448	-2.126	9.237	H
HETATM 1843	H	0	-4.719	-2.285	7.917	H
HETATM 1844	O	0	-0.459	-7.945	10.354	O
HETATM 1845	H	0	-0.768	-8.571	9.681	H
HETATM 1846	H	0	-0.778	-7.086	10.030	H
HETATM 1847	O	0	9.138	-5.199	10.431	O
HETATM 1848	H	0	10.097	-5.213	10.266	H
HETATM 1849	H	0	8.840	-6.059	10.067	H
HETATM 1850	O	0	0.821	-6.022	7.277	O
HETATM 1851	H	0	1.052	-6.971	7.360	H

HETATM 1852	H	0	1.689	-5.591	7.379	H
HETATM 1853	O	0	-1.920	-1.420	7.431	O
HETATM 1854	H	0	-2.538	-0.665	7.391	H
HETATM 1855	H	0	-2.519	-2.189	7.305	H
HETATM 1856	O	0	-1.681	-7.151	6.703	O
HETATM 1857	H	0	-0.853	-6.654	6.805	H
HETATM 1858	H	0	-1.399	-7.942	6.209	H
HETATM 1859	O	0	3.416	-5.214	8.121	O
HETATM 1860	H	0	3.304	-4.491	8.758	H
HETATM 1861	H	0	4.389	-5.318	8.107	H
HETATM 1862	O	0	7.880	0.032	11.355	O
HETATM 1863	H	0	8.088	-0.791	11.834	H
HETATM 1864	H	0	8.550	0.648	11.723	H
HETATM 1865	O	0	-6.421	3.620	10.666	O
HETATM 1866	H	0	-6.053	3.041	11.359	H
HETATM 1867	H	0	-7.353	3.335	10.626	H
HETATM 1868	O	0	-6.140	-10.068	7.772	O
HETATM 1869	H	0	-6.933	-9.534	7.592	H
HETATM 1870	H	0	-6.333	-10.893	7.275	H
HETATM 1871	O	0	5.648	-8.356	10.231	O
HETATM 1872	H	0	5.680	-7.675	10.927	H
HETATM 1873	H	0	4.738	-8.234	9.886	H
HETATM 1874	O	0	1.803	-7.072	11.607	O
HETATM 1875	H	0	0.923	-7.431	11.378	H
HETATM 1876	H	0	2.354	-7.414	10.881	H
HETATM 1877	O	0	-7.643	-4.916	9.746	O
HETATM 1878	H	0	-8.572	-5.208	9.664	H
HETATM 1879	H	0	-7.188	-5.517	9.122	H
HETATM 1880	O	0	3.208	-5.032	12.526	O
HETATM 1881	H	0	2.929	-4.904	13.439	H
HETATM 1882	H	0	2.639	-5.785	12.234	H
HETATM 1883	O	0	-1.168	1.557	0.676	O
HETATM 1884	H	0	-0.765	0.852	0.141	H
HETATM 1885	H	0	-0.990	1.280	1.580	H
HETATM 1886	O	0	-3.883	0.491	7.681	O
HETATM 1887	H	0	-4.425	1.279	7.453	H
HETATM 1888	H	0	-4.563	-0.194	7.848	H
HETATM 1889	O	0	6.208	-10.317	8.410	O
HETATM 1890	H	0	5.936	-9.748	7.667	H
HETATM 1891	H	0	5.987	-9.758	9.182	H
HETATM 1892	O	0	5.575	-5.909	11.476	O
HETATM 1893	H	0	6.252	-5.393	11.960	H
HETATM 1894	H	0	4.748	-5.643	11.925	H
HETATM 1895	O	0	7.509	-4.219	12.286	O
HETATM 1896	H	0	8.219	-4.649	11.763	H
HETATM 1897	H	0	7.974	-3.454	12.677	H

HETATM 1898	O	0	-3.757	-9.955	8.931	O
HETATM 1899	H	0	-4.621	-10.043	8.459	H
HETATM 1900	H	0	-3.931	-10.413	9.759	H
HETATM 1901	O	0	6.036	-5.574	8.784	O
HETATM 1902	H	0	5.852	-5.723	9.732	H
HETATM 1903	H	0	6.797	-6.154	8.628	H
HETATM 1904	O	0	-3.952	-7.316	8.172	O
HETATM 1905	H	0	-3.173	-7.221	7.582	H
HETATM 1906	H	0	-3.866	-8.238	8.481	H
HETATM 1907	O	0	1.322	-8.641	7.680	O
HETATM 1908	H	0	1.813	-9.381	7.264	H
HETATM 1909	H	0	0.498	-9.076	7.979	H
HETATM 1910	O	0	-1.008	-9.514	5.373	O
HETATM 1911	H	0	-0.206	-10.031	5.165	H
HETATM 1912	H	0	-1.501	-9.551	4.546	H
HETATM 1913	O	0	-3.537	-4.992	9.514	O
HETATM 1914	H	0	-3.798	-5.867	9.162	H
HETATM 1915	H	0	-2.571	-5.101	9.626	H
HETATM 1916	O	0	-3.294	0.215	10.341	O
HETATM 1917	H	0	-4.141	-0.141	10.673	H
HETATM 1918	H	0	-3.481	0.364	9.394	H
HETATM 1919	O	0	-10.083	-12.733	2.822	O
HETATM 1920	H	0	-10.812	-12.272	2.379	H
HETATM 1921	H	0	-9.404	-12.788	2.130	H
HETATM 1922	O	0	-1.144	-9.713	8.195	O
HETATM 1923	H	0	-1.241	-9.761	7.229	H
HETATM 1924	H	0	-2.054	-9.891	8.505	H
HETATM 1925	O	0	-6.814	-12.168	6.258	O
HETATM 1926	H	0	-7.728	-12.473	6.121	H
HETATM 1927	H	0	-6.463	-12.180	5.344	H
HETATM 1928	O	0	3.349	-3.419	10.338	O
HETATM 1929	H	0	3.347	-3.953	11.161	H
HETATM 1930	H	0	2.384	-3.327	10.159	H
HETATM 1931	O	0	-2.492	4.906	10.233	O
HETATM 1932	H	0	-2.642	4.087	10.754	H
HETATM 1933	H	0	-1.513	4.975	10.248	H
HETATM 1934	O	0	-0.656	8.591	9.268	O
HETATM 1935	H	0	-0.775	9.425	9.727	H
HETATM 1936	H	0	-1.511	8.145	9.383	H
HETATM 1937	O	0	11.873	-4.993	9.684	O
HETATM 1938	H	0	12.005	-5.868	9.290	H
HETATM 1939	H	0	12.350	-4.420	9.048	H
HETATM 1940	O	0	9.058	-2.039	12.788	O
HETATM 1941	H	0	9.820	-2.324	12.229	H
HETATM 1942	H	0	9.491	-1.743	13.595	H
HETATM 1943	O	0	-0.041	2.452	11.211	O

HETATM 1944 H	0	-0.957	2.448	11.534	H
HETATM 1945 H	0	0.094	3.381	10.956	H
HETATM 1946 O	0	-3.663	-3.438	7.289	O
HETATM 1947 H	0	-3.551	-4.066	8.032	H
HETATM 1948 H	0	-4.365	-3.871	6.755	H
HETATM 1949 O	0	1.385	0.541	9.936	O
HETATM 1950 H	0	1.009	1.241	10.514	H
HETATM 1951 H	0	0.635	-0.087	9.890	H
HETATM 1952 O	0	5.740	1.111	10.067	O
HETATM 1953 H	0	6.421	0.727	10.655	H
HETATM 1954 H	0	5.025	0.447	10.101	H
HETATM 1955 O	0	0.431	-2.771	7.045	O
HETATM 1956 H	0	0.250	-3.464	6.402	H
HETATM 1957 H	0	-0.380	-2.228	7.027	H
HETATM 1958 O	0	10.003	1.523	12.067	O
HETATM 1959 H	0	10.575	1.372	11.288	H
HETATM 1960 H	0	10.555	2.045	12.652	H
HETATM 1961 O	0	-3.182	7.471	9.840	O
HETATM 1962 H	0	-3.448	7.659	10.747	H
HETATM 1963 H	0	-2.925	6.524	9.896	H
HETATM 1964 O	0	8.105	-7.467	9.349	O
HETATM 1965 H	0	8.613	-8.291	9.206	H
HETATM 1966 H	0	7.267	-7.821	9.700	H
HETATM 1967 O	0	12.723	-1.416	9.617	O
HETATM 1968 H	0	12.221	-1.270	8.768	H
HETATM 1969 H	0	13.341	-2.108	9.349	H
HETATM 1970 O	0	0.807	-3.113	9.673	O
HETATM 1971 H	0	0.778	-3.012	8.695	H
HETATM 1972 H	0	0.225	-2.384	9.965	H
HETATM 1973 O	0	-0.852	-0.981	9.864	O
HETATM 1974 H	0	-1.194	-1.157	8.964	H
HETATM 1975 H	0	-1.631	-0.588	10.301	H
HETATM 1976 O	0	4.967	5.348	9.863	O
HETATM 1977 H	0	5.917	5.377	10.087	H
HETATM 1978 H	0	4.927	4.537	9.322	H
HETATM 1979 O	0	-8.998	-2.849	10.987	O
HETATM 1980 H	0	-8.373	-3.485	10.600	H
HETATM 1981 H	0	-9.262	-2.306	10.227	H
HETATM 1982 O	0	0.206	5.033	10.266	O
HETATM 1983 H	0	1.034	5.398	10.642	H
HETATM 1984 H	0	0.414	4.981	9.321	H
HETATM 1985 O	0	13.226	-3.597	7.741	O
HETATM 1986 H	0	12.823	-3.088	7.002	H
HETATM 1987 H	0	14.069	-3.895	7.361	H
HETATM 1988 O	0	3.777	-0.742	9.687	O
HETATM 1989 H	0	2.933	-0.252	9.768	H

HETATM 1990	H	0	3.531	-1.632	9.991	H
HETATM 1991	O	0	8.775	0.917	8.893	O
HETATM 1992	H	0	9.696	0.878	9.211	H
HETATM 1993	H	0	8.285	0.564	9.660	H
HETATM 1994	O	0	8.828	-10.094	9.215	O
HETATM 1995	H	0	7.953	-10.344	8.868	H
HETATM 1996	H	0	9.109	-10.873	9.700	H
HETATM 1997	O	0	-2.853	2.578	11.557	O
HETATM 1998	H	0	-3.665	2.531	12.090	H
HETATM 1999	H	0	-2.880	1.714	11.095	H
HETATM 2000	O	0	-0.824	-5.350	9.383	O
HETATM 2001	H	0	-0.320	-5.577	8.579	H
HETATM 2002	H	0	-0.286	-4.630	9.757	H
HETATM 2003	O	0	-5.400	1.820	12.499	O
HETATM 2004	H	0	-5.669	1.661	13.409	H
HETATM 2005	H	0	-5.537	0.946	12.077	H
HETATM 2006	C	0	11.752	-1.133	6.220	C
HETATM 2007	O	0	11.534	-0.975	7.450	O
HETATM 2008	C	0	11.466	0.114	5.325	C
HETATM 2009	C	0	10.084	0.724	5.542	C
HETATM 2010	C	0	8.979	-0.007	4.770	C
HETATM 2011	C	0	7.616	0.562	5.064	C
HETATM 2012	O	0	12.243	-2.157	5.683	O
HETATM 2013	C	0	6.337	0.054	4.563	C
HETATM 2014	C	0	5.198	0.999	4.510	C
HETATM 2015	O	0	6.798	-0.057	6.034	O
HETATM 2016	C	0	3.935	0.707	4.831	C
HETATM 2017	C	0	2.854	1.670	4.731	C
HETATM 2018	C	0	1.559	1.338	4.759	C
HETATM 2019	C	0	0.554	2.257	4.582	C
HETATM 2020	C	0	-0.773	1.984	4.604	C
HETATM 2021	C	0	-1.382	0.626	4.896	C
HETATM 2022	C	0	-1.676	-0.153	3.623	C
HETATM 2023	C	0	-2.861	-0.774	3.374	C
HETATM 2024	C	0	-4.012	-0.784	4.371	C
HETATM 2025	C	0	-5.107	-1.786	4.004	C
HETATM 2026	C	0	-6.038	-1.336	2.870	C
HETATM 2027	C	0	-7.163	-2.372	2.737	C
HETATM 2028	C	0	-8.079	-2.071	1.553	C
HETATM 2029	H	0	12.222	0.849	5.613	H
HETATM 2030	H	0	11.624	-0.130	4.268	H
HETATM 2031	H	0	9.884	0.704	6.617	H
HETATM 2032	H	0	10.074	1.786	5.236	H
HETATM 2033	H	0	8.979	-1.076	5.008	H
HETATM 2034	H	0	9.176	0.070	3.692	H
HETATM 2035	H	0	7.640	1.652	5.219	H

HETATM 2036	H	0	6.271	-0.951	4.177	H
HETATM 2037	H	0	5.457	2.028	4.260	H
HETATM 2038	H	0	3.674	-0.299	5.145	H
HETATM 2039	H	0	3.169	2.706	4.605	H
HETATM 2040	H	0	1.320	0.291	4.920	H
HETATM 2041	H	0	0.843	3.295	4.421	H
HETATM 2042	H	0	-1.451	2.814	4.460	H
HETATM 2043	H	0	-2.296	0.811	5.456	H
HETATM 2044	H	0	-0.732	0.038	5.541	H
HETATM 2045	H	0	-0.881	-0.238	2.886	H
HETATM 2046	H	0	-2.973	-1.322	2.438	H
HETATM 2047	H	0	-4.449	0.210	4.473	H
HETATM 2048	H	0	-3.620	-1.083	5.341	H
HETATM 2049	H	0	-5.706	-1.964	4.896	H
HETATM 2050	H	0	-4.637	-2.725	3.722	H
HETATM 2051	H	0	-6.468	-0.360	3.104	H
HETATM 2052	H	0	-5.477	-1.269	1.937	H
HETATM 2053	H	0	-7.759	-2.376	3.648	H
HETATM 2054	H	0	-6.738	-3.369	2.619	H
HETATM 2055	H	0	-8.523	-1.084	1.666	H
HETATM 2056	H	0	-7.513	-2.110	0.623	H
HETATM 2057	H	0	-8.870	-2.819	1.518	H

PC (Head-to-tail orientation)

E = -2163.36940119 hartrees

HETATM 1	C	0	-14.993	-7.287	-7.595	C
HETATM 2	H	0	-15.522	-8.195	-7.394	H
HETATM 3	H	0	-14.201	-7.481	-8.288	H
HETATM 4	H	0	-15.665	-6.567	-8.013	H
HETATM 5	C	0	-14.369	-6.905	-6.253	C
HETATM 6	O	0	-13.157	-6.992	-6.089	O
HETATM 7	N	0	-15.189	-6.603	-5.243	N
HETATM 8	C	0	-14.790	-6.245	-3.861	C
HETATM 9	C	0	-13.957	-7.279	-3.124	C
HETATM 10	O	0	-12.892	-6.968	-2.592	O
HETATM 11	C	0	-16.075	-5.909	-3.091	C
HETATM 12	C	0	-15.848	-5.492	-1.631	C
HETATM 13	C	0	-15.016	-4.216	-1.516	C
HETATM 14	C	0	-17.209	-5.261	-0.995	C
HETATM 15	H	0	-16.170	-6.550	-5.476	H
HETATM 16	H	0	-14.182	-5.340	-3.922	H
HETATM 17	H	0	-16.585	-5.098	-3.609	H
HETATM 18	H	0	-16.733	-6.780	-3.104	H
HETATM 19	H	0	-15.351	-6.291	-1.082	H
HETATM 20	H	0	-15.020	-3.873	-0.482	H

HETATM	21	H	0	-15.436	-3.438	-2.152	H
HETATM	22	H	0	-13.986	-4.412	-1.812	H
HETATM	23	H	0	-17.064	-4.945	0.031	H
HETATM	24	H	0	-17.792	-6.182	-0.998	H
HETATM	25	H	0	-17.760	-4.491	-1.535	H
HETATM	26	N	0	-14.449	-8.514	-3.088	N
HETATM	27	C	0	-13.686	-9.630	-2.551	C
HETATM	28	H	0	-14.211	-10.565	-2.745	H
HETATM	29	C	0	-12.272	-9.723	-3.169	C
HETATM	30	O	0	-11.316	-10.071	-2.480	O
HETATM	31	H	0	-15.349	-8.676	-3.513	H
HETATM	32	H	0	-13.576	-9.510	-1.472	H
HETATM	33	N	0	-12.124	-9.363	-4.450	N
HETATM	34	C	0	-10.852	-9.263	-5.171	C
HETATM	35	C	0	-9.993	-8.080	-4.787	C
HETATM	36	O	0	-8.797	-8.251	-4.625	O
HETATM	37	H	0	-12.942	-9.023	-4.934	H
HETATM	38	H	0	-10.276	-10.174	-5.006	H
HETATM	39	H	0	-11.056	-9.189	-6.240	H
HETATM	40	N	0	-10.566	-6.897	-4.587	N
HETATM	41	C	0	-9.836	-5.779	-3.970	C
HETATM	42	C	0	-9.178	-6.180	-2.676	C
HETATM	43	O	0	-8.016	-5.872	-2.467	O
HETATM	44	C	0	-10.750	-4.558	-3.736	C
HETATM	45	C	0	-10.064	-3.469	-2.899	C
HETATM	46	C	0	-11.179	-3.959	-5.077	C
HETATM	47	H	0	-11.555	-6.807	-4.799	H
HETATM	48	H	0	-9.036	-5.477	-4.644	H
HETATM	49	H	0	-11.645	-4.867	-3.201	H
HETATM	50	H	0	-9.105	-3.201	-3.336	H
HETATM	51	H	0	-9.902	-3.817	-1.880	H
HETATM	52	H	0	-10.698	-2.591	-2.839	H
HETATM	53	H	0	-11.694	-4.706	-5.680	H
HETATM	54	H	0	-10.306	-3.600	-5.619	H
HETATM	55	H	0	-11.865	-3.131	-4.905	H
HETATM	56	N	0	-9.906	-6.868	-1.810	N
HETATM	57	C	0	-9.338	-7.394	-0.584	C
HETATM	58	C	0	-8.256	-8.472	-0.801	C
HETATM	59	O	0	-7.319	-8.527	-0.005	O
HETATM	60	C	0	-10.490	-7.920	0.293	C
HETATM	61	C	0	-11.181	-6.789	1.079	C
HETATM	62	C	0	-12.593	-7.204	1.491	C
HETATM	63	C	0	-10.370	-6.441	2.332	C
HETATM	64	H	0	-10.878	-7.045	-2.043	H
HETATM	65	H	0	-8.843	-6.579	-0.056	H
HETATM	66	H	0	-11.219	-8.425	-0.341	H
HETATM	67	H	0	-10.109	-8.658	1.000	H
HETATM	68	H	0	-11.266	-5.900	0.453	H
HETATM	69	H	0	-12.557	-8.111	2.089	H

HETATM	70	H	0	-13.196	-7.378	0.600	H
HETATM	71	H	0	-13.055	-6.411	2.078	H
HETATM	72	H	0	-10.908	-5.718	2.941	H
HETATM	73	H	0	-9.407	-6.015	2.054	H
HETATM	74	H	0	-10.205	-7.334	2.934	H
HETATM	75	N	0	-8.351	-9.316	-1.839	N
HETATM	76	C	0	-7.250	-10.189	-2.290	C
HETATM	77	C	0	-6.027	-9.331	-2.740	C
HETATM	78	O	0	-4.907	-9.557	-2.290	O
HETATM	79	C	0	-7.741	-11.161	-3.378	C
HETATM	80	C	0	-6.672	-12.175	-3.826	C
HETATM	81	C	0	-6.275	-13.138	-2.703	C
HETATM	82	C	0	-7.212	-13.003	-4.992	C
HETATM	83	H	0	-9.172	-9.242	-2.424	H
HETATM	84	H	0	-6.926	-10.773	-1.428	H
HETATM	85	H	0	-8.612	-11.702	-3.006	H
HETATM	86	H	0	-8.044	-10.590	-4.252	H
HETATM	87	H	0	-5.790	-11.641	-4.169	H
HETATM	88	H	0	-7.157	-13.644	-2.313	H
HETATM	89	H	0	-5.770	-12.592	-1.907	H
HETATM	90	H	0	-5.579	-13.880	-3.092	H
HETATM	91	H	0	-8.103	-13.553	-4.689	H
HETATM	92	H	0	-6.449	-13.704	-5.329	H
HETATM	93	H	0	-7.458	-12.342	-5.824	H
HETATM	94	N	0	-6.228	-8.314	-3.588	N
HETATM	95	C	0	-5.191	-7.403	-4.102	C
HETATM	96	C	0	-4.529	-6.525	-3.009	C
HETATM	97	O	0	-3.302	-6.438	-2.950	O
HETATM	98	C	0	-5.704	-6.583	-5.287	C
HETATM	99	C	0	-6.102	-7.421	-6.519	C
HETATM	100	C	0	-5.028	-8.386	-7.009	C
HETATM	101	N	0	-3.850	-7.928	-7.373	N
HETATM	102	O	0	-5.233	-9.584	-7.075	O
HETATM	103	H	0	-7.174	-8.199	-3.930	H
HETATM	104	H	0	-4.383	-8.032	-4.476	H
HETATM	105	H	0	-6.565	-6.000	-4.961	H
HETATM	106	H	0	-4.913	-5.897	-5.588	H
HETATM	107	H	0	-6.359	-6.754	-7.340	H
HETATM	108	H	0	-6.990	-8.003	-6.290	H
HETATM	109	H	0	-3.235	-8.633	-7.742	H
HETATM	110	H	0	-3.576	-6.954	-7.317	H
HETATM	111	N	0	-5.313	-5.912	-2.116	N
HETATM	112	C	0	-4.882	-5.235	-0.884	C
HETATM	113	C	0	-4.085	-6.183	0.000	C
HETATM	114	O	0	-3.003	-5.817	0.461	O
HETATM	115	C	0	-6.098	-4.644	-0.171	C
HETATM	116	H	0	-6.309	-6.001	-2.268	H
HETATM	117	H	0	-4.220	-4.415	-1.165	H
HETATM	118	H	0	-5.751	-4.065	0.682	H

HETATM 119	H	0	-6.763	-5.438	0.170	H
HETATM 120	H	0	-6.639	-3.985	-0.852	H
HETATM 121	N	0	-4.586	-7.410	0.192	N
HETATM 122	C	0	-3.815	-8.460	0.834	C
HETATM 123	C	0	-2.410	-8.636	0.222	C
HETATM 124	O	0	-1.431	-8.671	0.967	O
HETATM 125	C	0	-4.582	-9.774	0.996	C
HETATM 126	C	0	-3.734	-10.890	1.575	C
HETATM 127	C	0	-3.474	-10.932	2.959	C
HETATM 128	C	0	-3.178	-11.863	0.722	C
HETATM 129	C	0	-2.675	-11.960	3.497	C
HETATM 130	C	0	-2.367	-12.883	1.255	C
HETATM 131	C	0	-2.117	-12.935	2.642	C
HETATM 132	O	0	-1.326	-13.915	3.147	O
HETATM 133	H	0	-5.491	-7.647	-0.198	H
HETATM 134	H	0	-3.625	-8.115	1.850	H
HETATM 135	H	0	-5.414	-9.590	1.670	H
HETATM 136	H	0	-4.992	-10.101	0.047	H
HETATM 137	H	0	-3.910	-10.186	3.612	H
HETATM 138	H	0	-3.370	-11.821	-0.344	H
HETATM 139	H	0	-2.495	-12.006	4.561	H
HETATM 140	H	0	-1.935	-13.637	0.614	H
HETATM 141	H	0	-1.395	-13.970	4.102	H
HETATM 142	N	0	-2.267	-8.691	-1.105	N
HETATM 143	C	0	-0.952	-8.749	-1.759	C
HETATM 144	C	0	-0.033	-7.563	-1.459	C
HETATM 145	O	0	1.101	-7.774	-1.047	O
HETATM 146	C	0	-1.098	-9.036	-3.259	C
HETATM 147	C	0	-1.815	-10.324	-3.639	C
HETATM 148	C	0	-2.590	-10.357	-4.813	C
HETATM 149	C	0	-1.668	-11.506	-2.880	C
HETATM 150	C	0	-3.219	-11.546	-5.220	C
HETATM 151	C	0	-2.304	-12.694	-3.283	C
HETATM 152	C	0	-3.077	-12.715	-4.455	C
HETATM 153	H	0	-3.106	-8.715	-1.676	H
HETATM 154	H	0	-0.429	-9.602	-1.329	H
HETATM 155	H	0	-1.600	-8.194	-3.735	H
HETATM 156	H	0	-0.098	-9.102	-3.681	H
HETATM 157	H	0	-2.698	-9.471	-5.419	H
HETATM 158	H	0	-1.061	-11.525	-1.989	H
HETATM 159	H	0	-3.812	-11.558	-6.125	H
HETATM 160	H	0	-2.188	-13.597	-2.701	H
HETATM 161	H	0	-3.560	-13.627	-4.775	H
HETATM 162	N	0	-0.473	-6.320	-1.635	N
HETATM 163	C	0	0.322	-5.120	-1.298	C
HETATM 164	C	0	0.709	-5.099	0.187	C
HETATM 165	O	0	1.863	-4.826	0.499	O
HETATM 166	C	0	-0.514	-3.890	-1.661	C
HETATM 167	O	0	-0.856	-3.968	-3.031	O

HETATM 168 H	0	-1.406	-6.194	-2.019	H
HETATM 169 H	0	1.237	-5.102	-1.886	H
HETATM 170 H	0	0.056	-2.981	-1.476	H
HETATM 171 H	0	-1.425	-3.872	-1.060	H
HETATM 172 H	0	-1.621	-3.366	-3.196	H
HETATM 173 N	0	-0.204	-5.435	1.107	N
HETATM 174 C	0	0.083	-5.653	2.537	C
HETATM 175 C	0	1.166	-6.702	2.776	C
HETATM 176 O	0	2.068	-6.506	3.591	O
HETATM 177 C	0	-1.202	-6.070	3.271	C
HETATM 178 C	0	-2.223	-4.946	3.506	C
HETATM 179 C	0	-3.541	-5.579	3.954	C
HETATM 180 C	0	-1.744	-3.981	4.593	C
HETATM 181 H	0	-1.143	-5.646	0.778	H
HETATM 182 H	0	0.447	-4.723	2.968	H
HETATM 183 H	0	-1.681	-6.867	2.707	H
HETATM 184 H	0	-0.926	-6.485	4.240	H
HETATM 185 H	0	-2.392	-4.386	2.588	H
HETATM 186 H	0	-3.388	-6.191	4.842	H
HETATM 187 H	0	-3.944	-6.196	3.153	H
HETATM 188 H	0	-4.265	-4.808	4.190	H
HETATM 189 H	0	-2.511	-3.227	4.764	H
HETATM 190 H	0	-0.836	-3.477	4.269	H
HETATM 191 H	0	-1.571	-4.528	5.520	H
HETATM 192 N	0	1.086	-7.822	2.068	N
HETATM 193 C	0	2.148	-8.808	2.074	C
HETATM 194 C	0	3.463	-8.277	1.522	C
HETATM 195 O	0	4.484	-8.549	2.132	O
HETATM 196 C	0	1.726	-10.091	1.332	C
HETATM 197 C	0	0.687	-10.939	2.085	C
HETATM 198 C	0	1.255	-11.608	3.331	C
HETATM 199 N	0	1.962	-12.708	3.197	N
HETATM 200 O	0	1.075	-11.153	4.453	O
HETATM 201 H	0	0.286	-7.952	1.456	H
HETATM 202 H	0	2.347	-9.078	3.112	H
HETATM 203 H	0	1.319	-9.833	0.357	H
HETATM 204 H	0	2.609	-10.709	1.162	H
HETATM 205 H	0	0.319	-11.712	1.412	H
HETATM 206 H	0	-0.159	-10.321	2.378	H
HETATM 207 H	0	2.292	-13.140	4.040	H
HETATM 208 H	0	2.085	-13.131	2.293	H
HETATM 209 N	0	3.477	-7.522	0.421	N
HETATM 210 C	0	4.690	-6.854	-0.078	C
HETATM 211 C	0	5.263	-5.872	0.944	C
HETATM 212 O	0	6.467	-5.840	1.140	O
HETATM 213 C	0	4.478	-6.140	-1.425	C
HETATM 214 C	0	5.761	-5.463	-1.920	C
HETATM 215 C	0	4.093	-7.082	-2.562	C
HETATM 216 H	0	2.595	-7.394	-0.066	H

HETATM 217 H	0	5.440	-7.621	-0.246	H
HETATM 218 H	0	3.694	-5.396	-1.310	H
HETATM 219 H	0	6.566	-6.197	-1.957	H
HETATM 220 H	0	6.048	-4.647	-1.258	H
HETATM 221 H	0	5.619	-5.062	-2.922	H
HETATM 222 H	0	3.801	-6.482	-3.417	H
HETATM 223 H	0	3.275	-7.736	-2.277	H
HETATM 224 H	0	4.942	-7.682	-2.873	H
HETATM 225 N	0	4.426	-5.081	1.608	N
HETATM 226 C	0	4.755	-4.172	2.717	C
HETATM 227 C	0	5.477	-4.868	3.848	C
HETATM 228 O	0	6.613	-4.526	4.183	O
HETATM 229 C	0	3.420	-3.518	3.200	C
HETATM 230 C	0	3.098	-2.319	2.299	C
HETATM 231 C	0	3.354	-3.129	4.695	C
HETATM 232 C	0	1.633	-1.858	2.296	C
HETATM 233 H	0	3.451	-5.148	1.333	H
HETATM 234 H	0	5.410	-3.379	2.358	H
HETATM 235 H	0	2.620	-4.231	3.045	H
HETATM 236 H	0	3.733	-1.496	2.599	H
HETATM 237 H	0	3.349	-2.584	1.278	H
HETATM 238 H	0	3.303	-4.017	5.323	H
HETATM 239 H	0	2.448	-2.566	4.907	H
HETATM 240 H	0	4.225	-2.546	4.984	H
HETATM 241 H	0	1.528	-1.008	1.621	H
HETATM 242 H	0	1.320	-1.552	3.291	H
HETATM 243 H	0	0.988	-2.662	1.948	H
HETATM 244 N	0	4.800	-5.866	4.403	N
HETATM 245 C	0	5.363	-6.798	5.351	C
HETATM 246 C	0	6.681	-7.367	4.762	C
HETATM 247 O	0	7.706	-7.348	5.434	O
HETATM 248 C	0	4.330	-7.893	5.617	C
HETATM 249 O	0	4.793	-8.848	6.546	O
HETATM 250 H	0	3.859	-6.035	4.059	H
HETATM 251 H	0	5.592	-6.284	6.283	H
HETATM 252 H	0	4.089	-8.400	4.682	H
HETATM 253 H	0	3.419	-7.436	6.005	H
HETATM 254 H	0	4.076	-9.517	6.599	H
HETATM 255 N	0	6.715	-7.780	3.482	N
HETATM 256 C	0	7.876	-8.314	2.750	C
HETATM 257 C	0	9.087	-7.398	2.650	C
HETATM 258 O	0	10.215	-7.856	2.847	O
HETATM 259 C	0	7.510	-8.915	1.386	C
HETATM 260 H	0	5.835	-7.783	2.983	H
HETATM 261 H	0	8.214	-9.161	3.346	H
HETATM 262 H	0	8.363	-9.478	1.004	H
HETATM 263 H	0	7.280	-8.135	0.669	H
HETATM 264 H	0	6.670	-9.601	1.485	H
HETATM 265 N	0	8.873	-6.106	2.401	N

HETATM 266 C	0	9.907	-5.074	2.472	C
HETATM 267 C	0	10.656	-5.147	3.812	C
HETATM 268 O	0	11.840	-4.839	3.862	O
HETATM 269 C	0	9.313	-3.656	2.319	C
HETATM 270 C	0	8.391	-3.439	1.107	C
HETATM 271 C	0	8.557	-2.065	0.450	C
HETATM 272 N	0	9.772	-2.036	-0.383	N
HETATM 273 C	0	9.856	-2.154	-1.693	C
HETATM 274 N	0	8.812	-2.206	-2.444	N
HETATM 275 N	0	11.009	-2.223	-2.281	N
HETATM 276 H	0	7.910	-5.844	2.204	H
HETATM 277 H	0	10.635	-5.246	1.681	H
HETATM 278 H	0	8.748	-3.404	3.217	H
HETATM 279 H	0	10.143	-2.956	2.272	H
HETATM 280 H	0	7.362	-3.519	1.444	H
HETATM 281 H	0	8.569	-4.210	0.361	H
HETATM 282 H	0	8.611	-1.294	1.220	H
HETATM 283 H	0	7.672	-1.852	-0.151	H
HETATM 284 H	0	10.661	-2.077	0.096	H
HETATM 285 H	0	8.843	-2.227	-3.447	H
HETATM 286 H	0	7.871	-2.166	-2.055	H
HETATM 287 H	0	11.834	-1.915	-1.793	H
HETATM 288 H	0	11.037	-2.315	-3.289	H
HETATM 289 N	0	9.975	-5.535	4.899	N
HETATM 290 C	0	10.454	-5.483	6.301	C
HETATM 291 C	0	10.836	-6.857	6.877	C
HETATM 292 O	0	11.791	-6.918	7.650	O
HETATM 293 C	0	9.462	-4.716	7.175	C
HETATM 294 C	0	9.117	-3.317	6.639	C
HETATM 295 C	0	8.950	-2.287	7.751	C
HETATM 296 N	0	7.988	-2.663	8.772	N
HETATM 297 C	0	6.673	-2.353	8.721	C
HETATM 298 N	0	6.115	-1.796	7.684	N
HETATM 299 N	0	5.986	-2.578	9.916	N
HETATM 300 H	0	9.004	-5.782	4.741	H
HETATM 301 H	0	11.380	-4.899	6.293	H
HETATM 302 H	0	8.545	-5.294	7.349	H
HETATM 303 H	0	9.939	-4.588	8.149	H
HETATM 304 H	0	8.204	-3.363	6.032	H
HETATM 305 H	0	9.938	-2.959	6.006	H
HETATM 306 H	0	8.621	-1.327	7.355	H
HETATM 307 H	0	9.913	-2.098	8.229	H
HETATM 308 H	0	8.255	-3.397	9.420	H
HETATM 309 H	0	5.191	-1.460	7.987	H
HETATM 310 H	0	6.645	-0.443	6.635	H
HETATM 311 H	0	6.511	-3.090	10.624	H
HETATM 312 H	0	5.064	-2.985	9.792	H
HETATM 313 N	0	10.197	-7.949	6.449	N
HETATM 314 C	0	10.693	-9.329	6.549	C

HETATM 315 C	0	12.075	-9.422	5.844	C
HETATM 316 O	0	13.081	-9.731	6.479	O
HETATM 317 C	0	9.654	-10.284	5.946	C
HETATM 318 H	0	9.352	-7.786	5.917	H
HETATM 319 H	0	10.836	-9.580	7.601	H
HETATM 320 H	0	9.985	-11.314	6.086	H
HETATM 321 H	0	9.533	-10.092	4.882	H
HETATM 322 H	0	8.693	-10.151	6.446	H
HETATM 323 N	0	12.145	-9.096	4.544	N
HETATM 324 C	0	13.317	-9.275	3.671	C
HETATM 325 H	0	12.974	-9.369	2.641	H
HETATM 326 C	0	14.387	-8.132	3.709	C
HETATM 327 O	0	15.541	-8.409	3.396	O
HETATM 328 H	0	11.286	-8.797	4.094	H
HETATM 329 H	0	13.820	-10.205	3.939	H
HETATM 330 N	0	14.060	-6.860	4.029	N
HETATM 331 C	0	14.986	-5.682	4.068	C
HETATM 332 H	0	15.967	-5.997	4.426	H
HETATM 333 C	0	15.138	-5.041	2.697	C
HETATM 334 O	0	16.202	-5.112	2.082	O
HETATM 335 H	0	13.092	-6.681	4.252	H
HETATM 336 H	0	14.579	-4.939	4.751	H
HETATM 337 N	0	14.059	-4.422	2.219	N
HETATM 338 C	0	13.900	-3.950	0.842	C
HETATM 339 C	0	13.366	-2.506	0.864	C
HETATM 340 O	0	12.163	-2.288	0.965	O
HETATM 341 C	0	13.067	-4.916	-0.018	C
HETATM 342 C	0	13.527	-4.732	-1.459	C
HETATM 343 C	0	13.265	-6.383	0.384	C
HETATM 344 H	0	13.249	-4.404	2.831	H
HETATM 345 H	0	14.897	-3.905	0.403	H
HETATM 346 H	0	12.006	-4.680	0.048	H
HETATM 347 H	0	12.951	-5.371	-2.116	H
HETATM 348 H	0	14.584	-4.976	-1.567	H
HETATM 349 H	0	13.355	-3.706	-1.761	H
HETATM 350 H	0	14.324	-6.594	0.525	H
HETATM 351 H	0	12.883	-7.032	-0.392	H
HETATM 352 H	0	12.727	-6.593	1.308	H
HETATM 353 N	0	14.242	-1.494	0.787	N
HETATM 354 C	0	13.871	-0.056	0.742	C
HETATM 355 C	0	12.891	0.235	-0.386	C
HETATM 356 O	0	12.954	-0.427	-1.423	O
HETATM 357 C	0	15.116	0.816	0.565	C
HETATM 358 O	0	15.938	0.757	1.717	O
HETATM 359 H	0	15.223	-1.741	0.853	H
HETATM 360 H	0	13.404	0.178	1.692	H
HETATM 361 H	0	14.811	1.852	0.410	H
HETATM 362 H	0	15.677	0.483	-0.310	H
HETATM 363 H	0	16.210	-0.181	1.870	H

HETATM 364 N	0	11.957	1.178	-0.201	N
HETATM 365 C	0	10.804	1.316	-1.077	C
HETATM 366 C	0	11.024	1.353	-2.576	C
HETATM 367 O	0	10.405	0.552	-3.276	O
HETATM 368 C	0	10.024	2.539	-0.575	C
HETATM 369 C	0	10.425	2.637	0.890	C
HETATM 370 C	0	11.863	2.133	0.901	C
HETATM 371 H	0	10.164	0.458	-0.885	H
HETATM 372 H	0	10.334	3.445	-1.091	H
HETATM 373 H	0	8.948	2.402	-0.680	H
HETATM 374 H	0	9.801	1.968	1.484	H
HETATM 375 H	0	10.356	3.661	1.253	H
HETATM 376 H	0	12.076	1.688	1.871	H
HETATM 377 H	0	12.544	2.966	0.716	H
HETATM 378 N	0	11.895	2.225	-3.101	N
HETATM 379 C	0	11.984	2.373	-4.536	C
HETATM 380 C	0	12.681	1.213	-5.240	C
HETATM 381 O	0	12.806	1.212	-6.466	O
HETATM 382 C	0	12.732	3.694	-4.742	C
HETATM 383 C	0	13.673	3.747	-3.543	C
HETATM 384 C	0	12.821	3.136	-2.435	C
HETATM 385 H	0	10.993	2.462	-4.976	H
HETATM 386 H	0	13.273	3.733	-5.688	H
HETATM 387 H	0	12.024	4.518	-4.674	H
HETATM 388 H	0	13.977	4.768	-3.307	H
HETATM 389 H	0	14.542	3.115	-3.729	H
HETATM 390 H	0	12.269	3.925	-1.930	H
HETATM 391 H	0	13.470	2.617	-1.731	H
HETATM 392 N	0	13.114	0.203	-4.484	N
HETATM 393 C	0	13.545	-1.059	-5.037	C
HETATM 394 C	0	12.361	-1.772	-5.688	C
HETATM 395 O	0	11.621	-2.525	-5.055	O
HETATM 396 C	0	14.336	-1.865	-3.998	C
HETATM 397 C	0	15.512	-1.123	-3.328	C
HETATM 398 C	0	16.175	-2.038	-2.299	C
HETATM 399 C	0	16.582	-0.693	-4.334	C
HETATM 400 H	0	12.936	0.250	-3.489	H
HETATM 401 H	0	14.248	-0.837	-5.841	H
HETATM 402 H	0	13.645	-2.199	-3.233	H
HETATM 403 H	0	14.750	-2.732	-4.501	H
HETATM 404 H	0	15.151	-0.235	-2.809	H
HETATM 405 H	0	16.579	-2.924	-2.791	H
HETATM 406 H	0	15.440	-2.348	-1.561	H
HETATM 407 H	0	16.981	-1.506	-1.792	H
HETATM 408 H	0	16.940	-1.556	-4.895	H
HETATM 409 H	0	17.418	-0.235	-3.806	H
HETATM 410 H	0	16.171	0.045	-5.021	H
HETATM 411 N	0	12.244	-1.569	-7.002	N
HETATM 412 C	0	11.529	-2.429	-7.957	C

HETATM 413 C	0	12.187	-3.817	-8.092	C
HETATM 414 O	0	12.164	-4.446	-9.151	O
HETATM 415 C	0	11.376	-1.706	-9.311	C
HETATM 416 O	0	10.609	-2.484	-10.201	O
HETATM 417 C	0	12.696	-1.364	-10.005	C
HETATM 418 H	0	12.797	-0.797	-7.356	H
HETATM 419 H	0	10.525	-2.600	-7.569	H
HETATM 420 H	0	10.840	-0.773	-9.138	H
HETATM 421 H	0	13.271	-2.267	-10.209	H
HETATM 422 H	0	13.286	-0.692	-9.383	H
HETATM 423 H	0	12.484	-0.863	-10.950	H
HETATM 424 H	0	11.132	-3.288	-10.352	H
HETATM 425 N	0	12.792	-4.304	-7.011	N
HETATM 426 C	0	13.796	-5.349	-6.996	C
HETATM 427 H	0	14.645	-5.037	-7.604	H
HETATM 428 C	0	14.310	-5.676	-5.567	C
HETATM 429 O	0	13.946	-4.973	-4.631	O
HETATM 430 H	0	12.622	-3.847	-6.122	H
HETATM 431 N	0	15.159	-6.702	-5.359	N
HETATM 432 C	0	15.794	-7.020	-4.050	C
HETATM 433 C	0	16.033	-8.514	-3.806	C
HETATM 434 O	0	16.208	-9.252	-4.775	O
HETATM 435 H	0	15.397	-7.306	-6.133	H
HETATM 436 H	0	16.754	-6.509	-3.990	H
HETATM 437 H	0	15.153	-6.635	-3.258	H
HETATM 438 N	0	16.034	-8.967	-2.531	N
HETATM 439 C	0	15.913	-10.382	-2.167	C
HETATM 440 C	0	14.811	-11.055	-3.034	C
HETATM 441 O	0	13.709	-10.508	-3.119	O
HETATM 442 C	0	15.575	-10.403	-0.672	C
HETATM 443 C	0	16.188	-9.101	-0.162	C
HETATM 444 C	0	15.976	-8.146	-1.335	C
HETATM 445 H	0	16.879	-10.859	-2.328	H
HETATM 446 H	0	14.494	-10.372	-0.524	H
HETATM 447 H	0	16.003	-11.273	-0.173	H
HETATM 448 H	0	17.257	-9.238	0.012	H
HETATM 449 H	0	15.693	-8.746	0.741	H
HETATM 450 H	0	16.744	-7.371	-1.339	H
HETATM 451 H	0	14.986	-7.699	-1.270	H
HETATM 452 N	0	15.058	-12.186	-3.721	N
HETATM 453 C	0	14.147	-12.713	-4.754	C
HETATM 454 C	0	12.818	-13.239	-4.225	C
HETATM 455 O	0	11.854	-13.276	-4.983	O
HETATM 456 C	0	14.946	-13.807	-5.472	C
HETATM 457 C	0	15.949	-14.272	-4.417	C
HETATM 458 C	0	16.271	-12.986	-3.659	C
HETATM 459 H	0	13.923	-11.923	-5.471	H
HETATM 460 H	0	14.314	-14.626	-5.818	H
HETATM 461 H	0	15.485	-13.367	-6.313	H

HETATM 462 H	0	16.840 -14.709 -4.869	H
HETATM 463 H	0	15.470 -14.985 -3.744	H
HETATM 464 H	0	17.081 -12.454 -4.161	H
HETATM 465 H	0	16.546 -13.214 -2.628	H
HETATM 466 N	0	12.719 -13.583 -2.936	N
HETATM 467 C	0	11.419 -13.806 -2.309	C
HETATM 468 H	0	13.385 -6.262 -7.426	H
HETATM 469 H	0	11.564 -14.165 -1.291	H
HETATM 470 H	0	10.869 -14.563 -2.870	H
HETATM 471 C	0	10.588 -12.533 -2.264	C
HETATM 472 O	0	9.414 -12.559 -2.623	O
HETATM 473 N	0	11.199 -11.407 -1.875	N
HETATM 474 C	0	10.570 -10.102 -2.059	C
HETATM 475 C	0	10.204 -9.850 -3.521	C
HETATM 476 O	0	9.064 -9.502 -3.799	O
HETATM 477 C	0	11.370 -8.929 -1.468	C
HETATM 478 C	0	10.923 -7.589 -2.038	C
HETATM 479 C	0	9.870 -6.868 -1.443	C
HETATM 480 C	0	11.488 -7.123 -3.244	C
HETATM 481 C	0	9.374 -5.710 -2.069	C
HETATM 482 C	0	10.967 -5.986 -3.882	C
HETATM 483 C	0	9.906 -5.283 -3.296	C
HETATM 484 H	0	12.196 -11.456 -1.724	H
HETATM 485 H	0	9.618 -10.123 -1.527	H
HETATM 486 H	0	11.244 -8.927 -0.384	H
HETATM 487 H	0	12.430 -9.051 -1.672	H
HETATM 488 H	0	9.419 -7.217 -0.526	H
HETATM 489 H	0	12.305 -7.657 -3.708	H
HETATM 490 H	0	8.557 -5.157 -1.632	H
HETATM 491 H	0	11.376 -5.653 -4.824	H
HETATM 492 H	0	9.500 -4.419 -3.800	H
HETATM 493 N	0	11.149 -9.985 -4.451	N
HETATM 494 C	0	10.918 -9.641 -5.854	C
HETATM 495 H	0	11.850 -9.742 -6.409	H
HETATM 496 H	0	10.599 -8.601 -5.923	H
HETATM 497 C	0	9.860 -10.526 -6.531	C
HETATM 498 N	0	9.849 -11.827 -6.226	N
HETATM 499 H	0	10.602 -12.176 -5.644	H
HETATM 500 O	0	9.033 -10.031 -7.291	O
HETATM 501 H	0	12.076 -10.250 -4.134	H
HETATM 502 C	0	8.757 -12.764 -6.509	C
HETATM 503 H	0	8.673 -12.910 -7.586	H
HETATM 504 H	0	8.968 -13.724 -6.037	H
HETATM 505 C	0	7.426 -12.239 -5.982	C
HETATM 506 O	0	6.459 -12.136 -6.731	O
HETATM 507 N	0	7.381 -11.876 -4.700	N
HETATM 508 C	0	6.204 -11.300 -4.037	C
HETATM 509 C	0	5.705 -9.994 -4.652	C
HETATM 510 O	0	4.509 -9.841 -4.889	O

HETATM 511 C	0	6.406 -11.265 -2.503	C
HETATM 512 C	0	5.394 -10.415 -1.730	C
HETATM 513 C	0	6.288 -12.691 -1.942	C
HETATM 514 H	0	8.219 -12.007 -4.142	H
HETATM 515 H	0	5.384 -11.996 -4.213	H
HETATM 516 H	0	7.397 -10.879 -2.274	H
HETATM 517 H	0	4.381 -10.602 -2.089	H
HETATM 518 H	0	5.653 -9.371 -1.861	H
HETATM 519 H	0	5.449 -10.632 -0.663	H
HETATM 520 H	0	5.269 -13.059 -2.061	H
HETATM 521 H	0	6.555 -12.696 -0.885	H
HETATM 522 H	0	6.966 -13.363 -2.466	H
HETATM 523 N	0	6.612 -9.080 -4.966	N
HETATM 524 C	0	6.388 -7.887 -5.774	C
HETATM 525 C	0	5.768 -8.197 -7.098	C
HETATM 526 O	0	4.705 -7.691 -7.429	O
HETATM 527 C	0	7.735 -7.152 -5.908	C
HETATM 528 C	0	7.770 -5.956 -6.842	C
HETATM 529 C	0	7.614 -4.665 -6.314	C
HETATM 530 C	0	8.020 -6.120 -8.221	C
HETATM 531 C	0	7.686 -3.536 -7.151	C
HETATM 532 C	0	8.100 -4.995 -9.065	C
HETATM 533 C	0	7.921 -3.700 -8.533	C
HETATM 534 O	0	8.002 -2.611 -9.343	O
HETATM 535 H	0	7.566 -9.295 -4.700	H
HETATM 536 H	0	5.695 -7.232 -5.246	H
HETATM 537 H	0	8.043 -6.829 -4.912	H
HETATM 538 H	0	8.492 -7.850 -6.249	H
HETATM 539 H	0	7.455 -4.551 -5.252	H
HETATM 540 H	0	8.150 -7.112 -8.636	H
HETATM 541 H	0	7.581 -2.550 -6.726	H
HETATM 542 H	0	8.276 -5.119 -10.124	H
HETATM 543 H	0	8.795 -2.674 -9.903	H
HETATM 544 N	0	6.443 -9.036 -7.857	N
HETATM 545 C	0	5.988 -9.366 -9.171	C
HETATM 546 H	0	6.707 -10.039 -9.637	H
HETATM 547 C	0	4.627 -10.039 -9.201	C
HETATM 548 O	0	3.791 -9.688 -10.028	O
HETATM 549 H	0	7.311 -9.436 -7.513	H
HETATM 550 H	0	5.932 -8.458 -9.772	H
HETATM 551 N	0	4.397 -10.970 -8.279	N
HETATM 552 C	0	3.091 -11.541 -8.022	C
HETATM 553 C	0	2.018 -10.446 -7.727	C
HETATM 554 O	0	0.962 -10.433 -8.354	O
HETATM 555 C	0	3.202 -12.565 -6.886	C
HETATM 556 H	0	5.160 -11.235 -7.665	H
HETATM 557 H	0	2.766 -12.068 -8.921	H
HETATM 558 H	0	3.533 -12.079 -5.968	H
HETATM 559 H	0	3.917 -13.343 -7.157	H

HETATM 560	H	0	2.228	-13.025	-6.714	H
HETATM 561	N	0	2.273	-9.526	-6.781	N
HETATM 562	C	0	1.390	-8.419	-6.350	C
HETATM 563	C	0	1.108	-7.363	-7.442	C
HETATM 564	O	0	-0.041	-6.941	-7.586	O
HETATM 565	C	0	2.009	-7.806	-5.094	C
HETATM 566	C	0	1.268	-6.572	-4.558	C
HETATM 567	C	0	1.759	-5.259	-5.152	C
HETATM 568	O	0	2.927	-5.088	-5.463	O
HETATM 569	N	0	0.926	-4.254	-5.245	N
HETATM 570	H	0	3.163	-9.615	-6.302	H
HETATM 571	H	0	0.425	-8.849	-6.079	H
HETATM 572	H	0	2.010	-8.570	-4.317	H
HETATM 573	H	0	3.050	-7.560	-5.295	H
HETATM 574	H	0	1.462	-6.521	-3.495	H
HETATM 575	H	0	0.194	-6.679	-4.707	H
HETATM 576	H	0	1.286	-3.386	-5.641	H
HETATM 577	H	0	0.024	-4.275	-4.785	H
HETATM 578	N	0	2.137	-6.880	-8.147	N
HETATM 579	C	0	2.048	-5.940	-9.284	C
HETATM 580	C	0	1.393	-6.642	-10.499	C
HETATM 581	O	0	0.557	-6.029	-11.158	O
HETATM 582	C	0	3.432	-5.363	-9.661	C
HETATM 583	C	0	3.340	-4.360	-10.821	C
HETATM 584	C	0	4.079	-4.604	-8.494	C
HETATM 585	H	0	3.053	-7.238	-7.898	H
HETATM 586	H	0	1.399	-5.111	-9.000	H
HETATM 587	H	0	4.094	-6.178	-9.958	H
HETATM 588	H	0	2.968	-4.851	-11.719	H
HETATM 589	H	0	4.327	-3.954	-11.043	H
HETATM 590	H	0	2.667	-3.544	-10.555	H
HETATM 591	H	0	3.400	-3.835	-8.137	H
HETATM 592	H	0	5.016	-4.151	-8.813	H
HETATM 593	H	0	4.295	-5.281	-7.674	H
HETATM 594	N	0	1.750	-7.904	-10.810	N
HETATM 595	C	0	1.134	-8.745	-11.850	C
HETATM 596	H	0	0.885	-9.708	-11.455	H
HETATM 597	H	0	1.780	-8.862	-12.695	H
HETATM 598	H	0	0.239	-8.241	-12.152	H
HETATM 599	H	0	2.449	-8.356	-10.230	H
HETATM 600	C	0	13.288	5.403	-9.126	C
HETATM 601	H	0	13.077	5.892	-10.054	H
HETATM 602	H	0	13.457	4.362	-9.302	H
HETATM 603	H	0	14.161	5.837	-8.685	H
HETATM 604	C	0	12.107	5.603	-8.241	C
HETATM 605	O	0	11.026	5.187	-8.631	O
HETATM 606	N	0	12.293	6.336	-7.138	N
HETATM 607	C	0	11.223	6.900	-6.307	C
HETATM 608	H	0	11.592	7.772	-5.768	H

HETATM 609 C	0	9.989	7.308	-7.107	C
HETATM 610 O	0	8.916	6.772	-6.882	O
HETATM 611 H	0	13.244	6.589	-6.897	H
HETATM 612 H	0	10.885	6.165	-5.577	H
HETATM 613 N	0	10.152	8.203	-8.084	N
HETATM 614 C	0	9.094	8.624	-9.016	C
HETATM 615 H	0	9.481	9.403	-9.672	H
HETATM 616 C	0	8.513	7.511	-9.890	C
HETATM 617 O	0	7.300	7.320	-9.882	O
HETATM 618 H	0	11.077	8.594	-8.169	H
HETATM 619 H	0	8.274	9.056	-8.438	H
HETATM 620 N	0	9.368	6.794	-10.637	N
HETATM 621 C	0	9.014	5.599	-11.425	C
HETATM 622 H	0	9.912	5.031	-11.667	H
HETATM 623 C	0	8.054	4.699	-10.644	C
HETATM 624 O	0	6.919	4.472	-11.051	O
HETATM 625 H	0	10.346	7.014	-10.540	H
HETATM 626 H	0	8.525	5.904	-12.351	H
HETATM 627 N	0	8.504	4.232	-9.480	N
HETATM 628 C	0	7.768	3.373	-8.555	C
HETATM 629 C	0	6.556	3.985	-7.896	C
HETATM 630 O	0	5.523	3.333	-7.903	O
HETATM 631 C	0	8.739	2.842	-7.480	C
HETATM 632 C	0	9.297	1.422	-7.693	C
HETATM 633 C	0	8.293	0.312	-8.064	C
HETATM 634 N	0	7.086	0.281	-7.218	N
HETATM 635 C	0	5.926	-0.287	-7.501	C
HETATM 636 N	0	5.701	-1.057	-8.519	N
HETATM 637 N	0	4.904	-0.142	-6.737	N
HETATM 638 H	0	9.435	4.535	-9.206	H
HETATM 639 H	0	7.372	2.535	-9.123	H
HETATM 640 H	0	9.577	3.527	-7.356	H
HETATM 641 H	0	8.234	2.864	-6.528	H
HETATM 642 H	0	9.803	1.126	-6.773	H
HETATM 643 H	0	10.052	1.468	-8.479	H
HETATM 644 H	0	8.809	-0.643	-7.969	H
HETATM 645 H	0	8.001	0.437	-9.108	H
HETATM 646 H	0	7.091	0.831	-6.354	H
HETATM 647 H	0	4.739	-1.374	-8.644	H
HETATM 648 H	0	6.468	-1.418	-9.065	H
HETATM 649 H	0	5.054	0.295	-5.827	H
HETATM 650 H	0	4.004	-0.498	-7.058	H
HETATM 651 N	0	6.643	5.193	-7.349	N
HETATM 652 C	0	5.477	5.910	-6.855	C
HETATM 653 C	0	4.349	5.922	-7.941	C
HETATM 654 O	0	3.196	5.639	-7.619	O
HETATM 655 C	0	5.863	7.350	-6.494	C
HETATM 656 H	0	7.547	5.651	-7.319	H
HETATM 657 H	0	5.095	5.404	-5.967	H

HETATM 658 H	0	5.005	7.850	-6.046	H
HETATM 659 H	0	6.168	7.894	-7.389	H
HETATM 660 H	0	6.689	7.363	-5.788	H
HETATM 661 N	0	4.670	6.210	-9.220	N
HETATM 662 C	0	3.804	6.074	-10.420	C
HETATM 663 H	0	4.370	6.358	-11.307	H
HETATM 664 C	0	3.298	4.644	-10.606	C
HETATM 665 O	0	2.087	4.460	-10.604	O
HETATM 666 H	0	5.639	6.466	-9.392	H
HETATM 667 H	0	2.946	6.740	-10.324	H
HETATM 668 N	0	4.178	3.636	-10.735	N
HETATM 669 C	0	3.780	2.211	-10.856	C
HETATM 670 C	0	2.841	1.790	-9.715	C
HETATM 671 O	0	1.816	1.187	-9.994	O
HETATM 672 C	0	4.955	1.236	-11.062	C
HETATM 673 C	0	4.462	-0.204	-11.281	C
HETATM 674 C	0	5.756	1.564	-12.331	C
HETATM 675 H	0	5.164	3.880	-10.759	H
HETATM 676 H	0	3.176	2.144	-11.762	H
HETATM 677 H	0	5.616	1.272	-10.196	H
HETATM 678 H	0	3.842	-0.258	-12.177	H
HETATM 679 H	0	3.868	-0.546	-10.436	H
HETATM 680 H	0	5.311	-0.877	-11.402	H
HETATM 681 H	0	5.118	1.472	-13.211	H
HETATM 682 H	0	6.598	0.880	-12.427	H
HETATM 683 H	0	6.139	2.577	-12.299	H
HETATM 684 N	0	3.110	2.161	-8.462	N
HETATM 685 C	0	2.241	1.969	-7.295	C
HETATM 686 C	0	0.888	2.645	-7.437	C
HETATM 687 O	0	-0.153	2.062	-7.164	O
HETATM 688 C	0	2.979	2.461	-6.023	C
HETATM 689 C	0	2.313	1.975	-4.744	C
HETATM 690 O	0	1.167	2.289	-4.483	O
HETATM 691 N	0	2.977	1.216	-3.914	N
HETATM 692 H	0	3.981	2.655	-8.318	H
HETATM 693 H	0	2.066	0.908	-7.176	H
HETATM 694 H	0	2.997	3.548	-6.002	H
HETATM 695 H	0	4.015	2.133	-6.026	H
HETATM 696 H	0	2.529	0.869	-3.067	H
HETATM 697 H	0	3.969	1.036	-4.042	H
HETATM 698 N	0	0.875	3.908	-7.825	N
HETATM 699 C	0	-0.388	4.578	-8.031	C
HETATM 700 C	0	-1.216	3.986	-9.189	C
HETATM 701 O	0	-2.419	3.775	-9.025	O
HETATM 702 C	0	-0.159	6.080	-8.242	C
HETATM 703 S	0	0.460	6.842	-6.715	S
HETATM 704 H	0	1.752	4.376	-8.032	H
HETATM 705 H	0	-1.009	4.454	-7.144	H
HETATM 706 H	0	-1.106	6.551	-8.511	H

HETATM 707 H	0	0.553	6.241	-9.056	H
HETATM 708 H	0	1.725	6.406	-6.861	H
HETATM 709 N	0	-0.578	3.723	-10.333	N
HETATM 710 C	0	-1.099	2.939	-11.453	C
HETATM 711 H	0	-0.310	2.770	-12.186	H
HETATM 712 C	0	-1.620	1.556	-10.949	C
HETATM 713 O	0	-2.742	1.206	-11.277	O
HETATM 714 H	0	0.408	3.956	-10.370	H
HETATM 715 H	0	-1.921	3.473	-11.929	H
HETATM 716 N	0	-0.880	0.774	-10.132	N
HETATM 717 C	0	-1.224	-0.595	-9.637	C
HETATM 718 C	0	-2.338	-0.614	-8.578	C
HETATM 719 O	0	-3.182	-1.511	-8.581	O
HETATM 720 C	0	0.027	-1.431	-9.271	C
HETATM 721 C	0	0.429	-1.237	-7.812	C
HETATM 722 C	0	1.867	-1.571	-7.425	C
HETATM 723 O	0	2.046	-1.910	-6.240	O
HETATM 724 O	0	2.856	-1.343	-8.161	O
HETATM 725 H	0	0.045	1.118	-9.904	H
HETATM 726 H	0	-1.662	-1.109	-10.494	H
HETATM 727 H	0	-0.198	-2.488	-9.421	H
HETATM 728 H	0	0.847	-1.172	-9.938	H
HETATM 729 H	0	-0.255	-1.817	-7.189	H
HETATM 730 H	0	0.278	-0.201	-7.566	H
HETATM 731 N	0	-2.380	0.378	-7.684	N
HETATM 732 C	0	-3.499	0.592	-6.762	C
HETATM 733 C	0	-4.758	1.118	-7.450	C
HETATM 734 O	0	-5.878	0.909	-6.979	O
HETATM 735 C	0	-3.101	1.484	-5.578	C
HETATM 736 C	0	-2.396	0.793	-4.419	C
HETATM 737 C	0	-1.103	0.264	-4.581	C
HETATM 738 C	0	-2.990	0.773	-3.140	C
HETATM 739 C	0	-0.369	-0.194	-3.472	C
HETATM 740 C	0	-2.262	0.308	-2.025	C
HETATM 741 C	0	-0.930	-0.135	-2.181	C
HETATM 742 O	0	-0.173	-0.433	-1.091	O
HETATM 743 H	0	-1.615	1.046	-7.689	H
HETATM 744 H	0	-3.780	-0.375	-6.344	H
HETATM 745 H	0	-2.474	2.301	-5.934	H
HETATM 746 H	0	-4.010	1.934	-5.179	H
HETATM 747 H	0	-0.631	0.259	-5.550	H
HETATM 748 H	0	-3.987	1.164	-2.996	H
HETATM 749 H	0	0.644	-0.546	-3.609	H
HETATM 750 H	0	-2.700	0.329	-1.038	H
HETATM 751 H	0	0.784	-0.414	-1.339	H
HETATM 752 N	0	-4.590	1.801	-8.574	N
HETATM 753 C	0	-5.660	2.403	-9.344	C
HETATM 754 H	0	-5.222	2.823	-10.250	H
HETATM 755 C	0	-6.800	1.492	-9.777	C

HETATM 756 O	0	-7.942	1.865	-9.541	O
HETATM 757 H	0	-3.640	1.947	-8.895	H
HETATM 758 H	0	-6.076	3.233	-8.778	H
HETATM 759 N	0	-6.564	0.325	-10.396	N
HETATM 760 C	0	-7.583	-0.689	-10.607	C
HETATM 761 C	0	-8.437	-0.994	-9.381	C
HETATM 762 O	0	-9.636	-1.193	-9.522	O
HETATM 763 C	0	-6.829	-1.936	-11.080	C
HETATM 764 C	0	-5.648	-1.344	-11.840	C
HETATM 765 C	0	-5.333	-0.077	-11.048	C
HETATM 766 H	0	-8.242	-0.352	-11.408	H
HETATM 767 H	0	-6.458	-2.504	-10.224	H
HETATM 768 H	0	-7.449	-2.566	-11.720	H
HETATM 769 H	0	-5.959	-1.076	-12.851	H
HETATM 770 H	0	-4.797	-2.026	-11.865	H
HETATM 771 H	0	-5.006	0.702	-11.735	H
HETATM 772 H	0	-4.571	-0.292	-10.302	H
HETATM 773 N	0	-7.849	-1.022	-8.182	N
HETATM 774 C	0	-8.592	-1.234	-6.940	C
HETATM 775 C	0	-9.405	0.020	-6.553	C
HETATM 776 O	0	-10.543	-0.118	-6.120	O
HETATM 777 C	0	-7.656	-1.592	-5.773	C
HETATM 778 C	0	-6.543	-2.610	-6.059	C
HETATM 779 C	0	-5.941	-3.040	-4.721	C
HETATM 780 C	0	-7.030	-3.853	-6.805	C
HETATM 781 H	0	-6.861	-0.812	-8.127	H
HETATM 782 H	0	-9.287	-2.060	-7.088	H
HETATM 783 H	0	-7.180	-0.684	-5.401	H
HETATM 784 H	0	-8.283	-1.972	-4.971	H
HETATM 785 H	0	-5.770	-2.128	-6.658	H
HETATM 786 H	0	-6.678	-3.569	-4.117	H
HETATM 787 H	0	-5.589	-2.164	-4.176	H
HETATM 788 H	0	-5.088	-3.692	-4.894	H
HETATM 789 H	0	-7.762	-4.392	-6.209	H
HETATM 790 H	0	-6.170	-4.482	-7.018	H
HETATM 791 H	0	-7.475	-3.587	-7.761	H
HETATM 792 N	0	-8.848	1.234	-6.687	N
HETATM 793 C	0	-9.584	2.519	-6.637	C
HETATM 794 C	0	-10.797	2.464	-7.554	C
HETATM 795 O	0	-11.911	2.550	-7.063	O
HETATM 796 C	0	-8.609	3.681	-6.895	C
HETATM 797 C	0	-9.195	4.938	-7.508	C
HETATM 798 C	0	-9.783	5.922	-6.692	C
HETATM 799 C	0	-9.109	5.144	-8.899	C
HETATM 800 C	0	-10.260	7.114	-7.269	C
HETATM 801 C	0	-9.609	6.324	-9.474	C
HETATM 802 C	0	-10.181	7.313	-8.657	C
HETATM 803 H	0	-7.884	1.242	-7.001	H
HETATM 804 H	0	-9.982	2.648	-5.629	H

HETATM 805 H	0	-8.131	3.941	-5.952	H
HETATM 806 H	0	-7.810	3.340	-7.542	H
HETATM 807 H	0	-9.848	5.771	-5.623	H
HETATM 808 H	0	-8.661	4.395	-9.535	H
HETATM 809 H	0	-10.685	7.888	-6.653	H
HETATM 810 H	0	-9.549	6.475	-10.544	H
HETATM 811 H	0	-10.557	8.226	-9.097	H
HETATM 812 N	0	-10.591	2.211	-8.844	N
HETATM 813 C	0	-11.620	1.917	-9.830	C
HETATM 814 H	0	-11.151	1.531	-10.735	H
HETATM 815 C	0	-12.657	0.902	-9.353	C
HETATM 816 O	0	-13.844	1.210	-9.321	O
HETATM 817 H	0	-9.624	2.123	-9.129	H
HETATM 818 H	0	-12.146	2.839	-10.081	H
HETATM 819 N	0	-12.208	-0.296	-8.972	N
HETATM 820 C	0	-13.036	-1.391	-8.479	C
HETATM 821 C	0	-13.930	-0.980	-7.335	C
HETATM 822 O	0	-15.152	-0.993	-7.439	O
HETATM 823 C	0	-12.166	-2.612	-8.163	C
HETATM 824 H	0	-11.217	-0.478	-9.079	H
HETATM 825 H	0	-13.705	-1.677	-9.292	H
HETATM 826 H	0	-12.796	-3.431	-7.814	H
HETATM 827 H	0	-11.441	-2.363	-7.394	H
HETATM 828 H	0	-11.639	-2.933	-9.063	H
HETATM 829 N	0	-13.302	-0.609	-6.237	N
HETATM 830 C	0	-14.013	-0.229	-5.037	C
HETATM 831 C	0	-14.871	1.018	-5.238	C
HETATM 832 O	0	-15.934	1.095	-4.643	O
HETATM 833 C	0	-13.083	0.001	-3.841	C
HETATM 834 O	0	-11.867	-0.695	-3.919	O
HETATM 835 C	0	-13.743	-0.538	-2.582	C
HETATM 836 H	0	-12.291	-0.589	-6.265	H
HETATM 837 H	0	-14.692	-1.046	-4.792	H
HETATM 838 H	0	-12.866	1.064	-3.732	H
HETATM 839 H	0	-14.714	-0.067	-2.429	H
HETATM 840 H	0	-13.090	-0.316	-1.746	H
HETATM 841 H	0	-13.871	-1.617	-2.658	H
HETATM 842 H	0	-11.376	-0.375	-4.697	H
HETATM 843 N	0	-14.440	1.996	-6.045	N
HETATM 844 C	0	-15.205	3.205	-6.361	C
HETATM 845 C	0	-16.450	2.920	-7.203	C
HETATM 846 O	0	-17.517	3.409	-6.859	O
HETATM 847 C	0	-14.303	4.275	-7.004	C
HETATM 848 C	0	-14.974	5.643	-7.228	C
HETATM 849 C	0	-15.374	6.317	-5.912	C
HETATM 850 C	0	-13.989	6.573	-7.939	C
HETATM 851 H	0	-13.538	1.890	-6.499	H
HETATM 852 H	0	-15.568	3.602	-5.414	H
HETATM 853 H	0	-13.437	4.429	-6.360	H

HETATM	854	H	0	-13.956	3.899	-7.968	H
HETATM	855	H	0	-15.855	5.529	-7.858	H
HETATM	856	H	0	-14.513	6.382	-5.249	H
HETATM	857	H	0	-16.166	5.740	-5.433	H
HETATM	858	H	0	-15.765	7.313	-6.116	H
HETATM	859	H	0	-13.098	6.714	-7.330	H
HETATM	860	H	0	-14.462	7.536	-8.132	H
HETATM	861	H	0	-13.699	6.133	-8.894	H
HETATM	862	N	0	-16.334	2.146	-8.283	N
HETATM	863	C	0	-17.478	1.702	-9.086	C
HETATM	864	H	0	-17.119	1.142	-9.949	H
HETATM	865	C	0	-18.435	0.815	-8.302	C
HETATM	866	O	0	-19.644	0.986	-8.405	O
HETATM	867	H	0	-15.412	1.793	-8.521	H
HETATM	868	H	0	-18.031	2.572	-9.441	H
HETATM	869	N	0	-17.896	-0.119	-7.511	N
HETATM	870	C	0	-18.690	-0.929	-6.581	C
HETATM	871	C	0	-19.410	-0.066	-5.529	C
HETATM	872	O	0	-20.591	-0.281	-5.278	O
HETATM	873	C	0	-17.876	-2.066	-5.930	C
HETATM	874	C	0	-18.675	-2.820	-4.855	C
HETATM	875	C	0	-17.478	-3.124	-6.971	C
HETATM	876	H	0	-16.888	-0.233	-7.523	H
HETATM	877	H	0	-19.488	-1.398	-7.157	H
HETATM	878	H	0	-16.978	-1.653	-5.470	H
HETATM	879	H	0	-19.602	-3.207	-5.281	H
HETATM	880	H	0	-18.930	-2.155	-4.031	H
HETATM	881	H	0	-18.089	-3.645	-4.458	H
HETATM	882	H	0	-18.369	-3.627	-7.351	H
HETATM	883	H	0	-16.811	-3.856	-6.517	H
HETATM	884	H	0	-16.967	-2.661	-7.813	H
HETATM	885	N	0	-18.714	0.874	-4.881	N
HETATM	886	C	0	-19.282	1.764	-3.864	C
HETATM	887	C	0	-20.258	2.818	-4.414	C
HETATM	888	O	0	-21.168	3.241	-3.702	O
HETATM	889	C	0	-18.154	2.456	-3.086	C
HETATM	890	H	0	-17.731	0.977	-5.093	H
HETATM	891	H	0	-19.851	1.154	-3.161	H
HETATM	892	H	0	-18.586	3.079	-2.303	H
HETATM	893	H	0	-17.572	3.083	-3.761	H
HETATM	894	H	0	-17.506	1.714	-2.623	H
HETATM	895	N	0	-20.025	3.301	-5.637	N
HETATM	896	C	0	-20.844	4.288	-6.314	C
HETATM	897	H	0	-21.849	3.920	-6.326	H
HETATM	898	H	0	-20.505	4.432	-7.319	H
HETATM	899	H	0	-20.812	5.221	-5.791	H
HETATM	900	H	0	-19.216	2.940	-6.131	H
HETATM	901	C	0	-15.440	11.741	-2.081	C
HETATM	902	H	0	-16.364	11.241	-1.877	H

HETATM 903 H	0	-15.358	11.924	-3.132	H
HETATM 904 H	0	-15.414	12.672	-1.554	H
HETATM 905 C	0	-14.262	10.880	-1.642	C
HETATM 906 O	0	-13.132	11.318	-1.798	O
HETATM 907 N	0	-14.479	9.644	-1.171	N
HETATM 908 C	0	-13.433	8.645	-0.810	C
HETATM 909 C	0	-12.412	8.474	-1.938	C
HETATM 910 O	0	-11.206	8.472	-1.707	O
HETATM 911 C	0	-14.118	7.339	-0.393	C
HETATM 912 S	0	-15.466	7.674	0.780	S
HETATM 913 H	0	-15.436	9.377	-0.991	H
HETATM 914 H	0	-12.888	9.028	0.054	H
HETATM 915 H	0	-13.382	6.684	0.077	H
HETATM 916 H	0	-14.533	6.851	-1.274	H
HETATM 917 H	0	-15.910	6.418	0.927	H
HETATM 918 N	0	-12.901	8.426	-3.176	N
HETATM 919 C	0	-12.073	8.509	-4.370	C
HETATM 920 C	0	-11.191	9.751	-4.475	C
HETATM 921 O	0	-10.000	9.641	-4.749	O
HETATM 922 H	0	-13.905	8.430	-3.276	H
HETATM 923 H	0	-11.421	7.635	-4.396	H
HETATM 924 H	0	-12.712	8.473	-5.252	H
HETATM 925 N	0	-11.770	10.929	-4.250	N
HETATM 926 C	0	-11.040	12.188	-4.134	C
HETATM 927 H	0	-11.734	12.988	-3.877	H
HETATM 928 C	0	-9.936	12.149	-3.066	C
HETATM 929 O	0	-8.831	12.624	-3.308	O
HETATM 930 H	0	-12.731	10.928	-3.946	H
HETATM 931 H	0	-10.578	12.427	-5.092	H
HETATM 932 N	0	-10.220	11.565	-1.893	N
HETATM 933 C	0	-9.230	11.335	-0.822	C
HETATM 934 C	0	-8.096	10.450	-1.274	C
HETATM 935 O	0	-6.947	10.824	-1.075	O
HETATM 936 C	0	-9.866	10.807	0.483	C
HETATM 937 C	0	-8.830	10.685	1.612	C
HETATM 938 C	0	-10.964	11.746	1.002	C
HETATM 939 H	0	-11.179	11.259	-1.764	H
HETATM 940 H	0	-8.784	12.303	-0.589	H
HETATM 941 H	0	-10.304	9.827	0.308	H
HETATM 942 H	0	-8.044	9.981	1.340	H
HETATM 943 H	0	-9.312	10.322	2.520	H
HETATM 944 H	0	-8.377	11.658	1.809	H
HETATM 945 H	0	-10.555	12.741	1.178	H
HETATM 946 H	0	-11.379	11.358	1.932	H
HETATM 947 H	0	-11.773	11.822	0.279	H
HETATM 948 N	0	-8.392	9.305	-1.890	N
HETATM 949 C	0	-7.367	8.508	-2.556	C
HETATM 950 C	0	-6.516	9.333	-3.502	C
HETATM 951 O	0	-5.292	9.266	-3.432	O

HETATM 952 C	0	-7.982	7.277	-3.239	C
HETATM 953 C	0	-6.985	6.469	-4.056	C
HETATM 954 C	0	-6.181	5.490	-3.439	C
HETATM 955 C	0	-6.840	6.727	-5.434	C
HETATM 956 C	0	-5.228	4.781	-4.199	C
HETATM 957 C	0	-5.891	6.020	-6.197	C
HETATM 958 C	0	-5.076	5.050	-5.578	C
HETATM 959 O	0	-4.120	4.397	-6.291	O
HETATM 960 H	0	-9.370	9.057	-2.001	H
HETATM 961 H	0	-6.689	8.139	-1.789	H
HETATM 962 H	0	-8.420	6.634	-2.474	H
HETATM 963 H	0	-8.792	7.590	-3.896	H
HETATM 964 H	0	-6.288	5.290	-2.380	H
HETATM 965 H	0	-7.455	7.480	-5.911	H
HETATM 966 H	0	-4.590	4.040	-3.740	H
HETATM 967 H	0	-5.784	6.232	-7.250	H
HETATM 968 H	0	-4.121	4.595	-7.232	H
HETATM 969 N	0	-7.159	10.131	-4.343	N
HETATM 970 C	0	-6.460	11.029	-5.252	C
HETATM 971 H	0	-5.508	11.326	-4.864	H
HETATM 972 H	0	-7.034	11.899	-5.494	H
HETATM 973 H	0	-8.182	10.073	-4.285	H
HETATM 974 H	0	-6.276	10.496	-6.186	H
HETATM 975 N	0	-4.523	12.284	-1.535	N
HETATM 976 O	0	-3.077	13.847	-2.184	O
HETATM 977 C	0	-4.232	13.436	-2.149	C
HETATM 978 C	0	-5.291	14.217	-2.930	C
HETATM 979 H	0	-6.268	13.785	-2.982	H
HETATM 980 H	0	-4.842	14.202	-3.901	H
HETATM 981 H	0	-5.365	15.227	-2.587	H
HETATM 982 C	0	-3.518	11.481	-0.800	C
HETATM 983 C	0	-2.442	10.847	-1.689	C
HETATM 984 O	0	-1.262	10.914	-1.351	O
HETATM 985 C	0	-4.242	10.490	0.102	C
HETATM 986 H	0	-5.484	11.953	-1.541	H
HETATM 987 H	0	-2.987	12.169	-0.141	H
HETATM 988 H	0	-3.513	9.973	0.711	H
HETATM 989 H	0	-4.800	9.778	-0.499	H
HETATM 990 H	0	-4.932	11.022	0.758	H
HETATM 991 N	0	-2.792	10.240	-2.828	N
HETATM 992 C	0	-1.794	9.712	-3.769	C
HETATM 993 C	0	-0.911	10.802	-4.419	C
HETATM 994 O	0	0.240	10.492	-4.722	O
HETATM 995 C	0	-2.389	8.718	-4.784	C
HETATM 996 C	0	-2.702	7.328	-4.187	C
HETATM 997 C	0	-1.560	6.792	-3.309	C
HETATM 998 N	0	-1.699	5.374	-2.951	N
HETATM 999 C	0	-1.047	4.380	-3.512	C
HETATM 1000 N	0	-0.397	4.505	-4.626	N

HETATM 1001	N	0	-1.006	3.220	-2.949	N
HETATM 1002	H	0	-3.783	10.145	-3.035	H
HETATM 1003	H	0	-1.075	9.176	-3.174	H
HETATM 1004	H	0	-3.289	9.136	-5.236	H
HETATM 1005	H	0	-1.661	8.573	-5.583	H
HETATM 1006	H	0	-2.867	6.639	-5.014	H
HETATM 1007	H	0	-3.612	7.374	-3.592	H
HETATM 1008	H	0	-1.527	7.361	-2.381	H
HETATM 1009	H	0	-0.614	6.951	-3.826	H
HETATM 1010	H	0	-2.130	5.144	-2.064	H
HETATM 1011	H	0	0.132	3.686	-4.908	H
HETATM 1012	H	0	-0.352	5.375	-5.119	H
HETATM 1013	H	0	-1.511	3.064	-2.085	H
HETATM 1014	H	0	-0.440	2.490	-3.372	H
HETATM 1015	N	0	-1.360	12.065	-4.544	N
HETATM 1016	C	0	-0.503	13.230	-4.844	C
HETATM 1017	H	0	-0.925	13.900	-5.565	H
HETATM 1018	H	0	0.431	12.857	-5.208	H
HETATM 1019	H	0	-0.345	13.751	-3.923	H
HETATM 1020	H	0	-2.297	12.238	-4.209	H
HETATM 1021	C	0	1.010	13.882	-1.438	C
HETATM 1022	H	0	-0.009	13.560	-1.380	H
HETATM 1023	H	0	1.220	14.221	-2.431	H
HETATM 1024	H	0	1.171	14.682	-0.746	H
HETATM 1025	C	0	1.963	12.736	-1.234	C
HETATM 1026	O	0	3.142	12.975	-1.016	O
HETATM 1027	N	0	1.491	11.505	-1.426	N
HETATM 1028	C	0	2.324	10.300	-1.490	C
HETATM 1029	C	0	3.378	10.422	-2.599	C
HETATM 1030	O	0	4.555	10.387	-2.279	O
HETATM 1031	C	0	1.470	9.043	-1.700	C
HETATM 1032	C	0	2.229	7.770	-2.047	C
HETATM 1033	C	0	3.023	7.134	-1.078	C
HETATM 1034	C	0	2.129	7.210	-3.337	C
HETATM 1035	C	0	3.685	5.924	-1.374	C
HETATM 1036	C	0	2.768	5.990	-3.632	C
HETATM 1037	C	0	3.530	5.330	-2.644	C
HETATM 1038	O	0	4.130	4.146	-2.934	O
HETATM 1039	H	0	0.490	11.402	-1.554	H
HETATM 1040	H	0	2.857	10.193	-0.544	H
HETATM 1041	H	0	0.866	8.863	-0.811	H
HETATM 1042	H	0	0.800	9.250	-2.520	H
HETATM 1043	H	0	3.108	7.579	-0.100	H
HETATM 1044	H	0	1.556	7.713	-4.104	H
HETATM 1045	H	0	4.288	5.424	-0.633	H
HETATM 1046	H	0	2.687	5.539	-4.609	H
HETATM 1047	H	0	4.586	3.742	-2.182	H
HETATM 1048	N	0	2.997	10.600	-3.875	N
HETATM 1049	C	0	3.920	10.818	-5.007	C

HETATM 1050	H	0	3.354	11.105	-5.893	H
HETATM 1051	C	0	4.967	11.915	-4.708	C
HETATM 1052	O	0	6.150	11.670	-4.899	O
HETATM 1053	H	0	2.001	10.574	-4.075	H
HETATM 1054	H	0	4.450	9.890	-5.217	H
HETATM 1055	N	0	4.557	13.095	-4.207	N
HETATM 1056	C	0	5.439	14.208	-3.769	C
HETATM 1057	H	0	4.833	15.019	-3.366	H
HETATM 1058	C	0	6.441	13.792	-2.723	C
HETATM 1059	O	0	7.654	13.875	-2.910	O
HETATM 1060	H	0	3.567	13.188	-4.048	H
HETATM 1061	H	0	5.989	14.586	-4.631	H
HETATM 1062	N	0	5.893	13.324	-1.614	N
HETATM 1063	C	0	6.654	12.815	-0.505	C
HETATM 1064	C	0	7.647	11.769	-0.872	C
HETATM 1065	O	0	8.816	11.915	-0.572	O
HETATM 1066	H	0	4.882	13.275	-1.550	H
HETATM 1067	H	0	7.188	13.643	-0.038	H
HETATM 1068	H	0	5.966	12.397	0.229	H
HETATM 1069	N	0	7.165	10.729	-1.519	N
HETATM 1070	C	0	7.950	9.610	-1.961	C
HETATM 1071	C	0	9.036	9.979	-2.952	C
HETATM 1072	O	0	10.175	9.527	-2.823	O
HETATM 1073	C	0	7.005	8.538	-2.537	C
HETATM 1074	C	0	7.548	7.144	-2.817	C
HETATM 1075	C	0	6.694	6.229	-3.459	C
HETATM 1076	C	0	8.856	6.739	-2.477	C
HETATM 1077	C	0	7.155	4.957	-3.842	C
HETATM 1078	C	0	9.330	5.479	-2.884	C
HETATM 1079	C	0	8.488	4.593	-3.580	C
HETATM 1080	O	0	8.967	3.392	-3.978	O
HETATM 1081	H	0	6.179	10.737	-1.748	H
HETATM 1082	H	0	8.454	9.194	-1.090	H
HETATM 1083	H	0	6.165	8.408	-1.859	H
HETATM 1084	H	0	6.589	8.922	-3.470	H
HETATM 1085	H	0	5.683	6.524	-3.696	H
HETATM 1086	H	0	9.531	7.373	-1.924	H
HETATM 1087	H	0	6.503	4.264	-4.355	H
HETATM 1088	H	0	10.343	5.178	-2.675	H
HETATM 1089	H	0	8.257	2.818	-4.343	H
HETATM 1090	N	0	8.703	10.820	-3.925	N
HETATM 1091	C	0	9.695	11.374	-4.814	C
HETATM 1092	C	0	10.887	12.007	-4.065	C
HETATM 1093	O	0	12.035	11.799	-4.462	O
HETATM 1094	C	0	9.046	12.354	-5.798	C
HETATM 1095	H	0	7.745	11.146	-4.011	H
HETATM 1096	H	0	10.105	10.551	-5.401	H
HETATM 1097	H	0	9.808	12.758	-6.466	H
HETATM 1098	H	0	8.577	13.178	-5.259	H

HETATM 1099	H	0	8.295	11.838	-6.396	H
HETATM 1100	N	0	10.627	12.715	-2.956	N
HETATM 1101	C	0	11.641	13.178	-1.998	C
HETATM 1102	H	0	11.215	13.968	-1.380	H
HETATM 1103	C	0	12.183	12.059	-1.064	C
HETATM 1104	O	0	13.329	11.651	-1.242	O
HETATM 1105	H	0	9.646	12.862	-2.736	H
HETATM 1106	H	0	12.495	13.587	-2.540	H
HETATM 1107	N	0	11.419	11.580	-0.064	N
HETATM 1108	C	0	11.806	10.624	1.010	C
HETATM 1109	C	0	10.838	9.448	1.314	C
HETATM 1110	O	0	9.611	9.552	1.218	O
HETATM 1111	C	0	12.166	11.379	2.304	C
HETATM 1112	O	0	11.241	11.177	3.367	O
HETATM 1113	H	0	10.460	11.900	-0.065	H
HETATM 1114	H	0	12.731	10.155	0.673	H
HETATM 1115	H	0	12.255	12.448	2.101	H
HETATM 1116	H	0	13.143	11.030	2.636	H
HETATM 1117	H	0	11.713	11.410	4.192	H
HETATM 1118	N	0	11.400	8.334	1.812	N
HETATM 1119	C	0	10.718	7.112	2.280	C
HETATM 1120	C	0	9.895	7.295	3.572	C
HETATM 1121	O	0	9.358	6.313	4.082	O
HETATM 1122	C	0	11.779	6.021	2.483	C
HETATM 1123	H	0	12.407	8.348	1.924	H
HETATM 1124	H	0	10.044	6.786	1.487	H
HETATM 1125	H	0	11.321	5.102	2.845	H
HETATM 1126	H	0	12.522	6.351	3.204	H
HETATM 1127	H	0	12.286	5.807	1.547	H
HETATM 1128	N	0	9.731	8.508	4.094	N
HETATM 1129	C	0	8.890	8.780	5.267	C
HETATM 1130	C	0	7.864	9.889	4.981	C
HETATM 1131	O	0	6.711	9.739	5.365	O
HETATM 1132	C	0	9.746	9.191	6.476	C
HETATM 1133	C	0	10.608	8.076	7.078	C
HETATM 1134	C	0	11.862	7.751	6.279	C
HETATM 1135	O	0	12.739	8.587	6.068	O
HETATM 1136	N	0	12.010	6.529	5.830	N
HETATM 1137	H	0	10.192	9.275	3.618	H
HETATM 1138	H	0	8.329	7.893	5.546	H
HETATM 1139	H	0	10.366	10.047	6.217	H
HETATM 1140	H	0	9.066	9.507	7.264	H
HETATM 1141	H	0	9.993	7.185	7.191	H
HETATM 1142	H	0	10.926	8.388	8.073	H
HETATM 1143	H	0	12.871	6.256	5.371	H
HETATM 1144	H	0	11.264	5.854	5.985	H
HETATM 1145	N	0	8.214	10.964	4.259	N
HETATM 1146	C	0	7.256	12.004	3.821	C
HETATM 1147	C	0	6.096	11.407	3.005	C

HETATM 1148 O	0	4.960	11.861	3.103	O
HETATM 1149 C	0	8.004	13.062	2.987	C
HETATM 1150 C	0	9.048	13.884	3.765	C
HETATM 1151 C	0	9.842	14.747	2.784	C
HETATM 1152 C	0	8.405	14.804	4.804	C
HETATM 1153 H	0	9.181	11.058	3.972	H
HETATM 1154 H	0	6.815	12.477	4.699	H
HETATM 1155 H	0	8.504	12.554	2.161	H
HETATM 1156 H	0	7.272	13.750	2.561	H
HETATM 1157 H	0	9.743	13.217	4.273	H
HETATM 1158 H	0	10.606	15.310	3.321	H
HETATM 1159 H	0	9.177	15.444	2.273	H
HETATM 1160 H	0	10.330	14.111	2.045	H
HETATM 1161 H	0	7.916	14.210	5.575	H
HETATM 1162 H	0	7.673	15.457	4.329	H
HETATM 1163 H	0	9.172	15.413	5.281	H
HETATM 1164 N	0	6.373	10.342	2.237	N
HETATM 1165 C	0	5.367	9.463	1.600	C
HETATM 1166 C	0	4.259	9.001	2.558	C
HETATM 1167 O	0	3.150	8.733	2.102	O
HETATM 1168 C	0	6.041	8.261	0.914	C
HETATM 1169 C	0	6.509	7.138	1.841	C
HETATM 1170 C	0	7.165	5.973	1.088	C
HETATM 1171 N	0	7.973	5.180	2.012	N
HETATM 1172 C	0	7.760	3.985	2.574	C
HETATM 1173 N	0	6.929	3.104	2.035	N
HETATM 1174 N	0	8.494	3.671	3.654	N
HETATM 1175 H	0	7.356	10.109	2.152	H
HETATM 1176 H	0	4.867	10.068	0.838	H
HETATM 1177 H	0	5.348	7.836	0.184	H
HETATM 1178 H	0	6.911	8.608	0.352	H
HETATM 1179 H	0	5.677	6.734	2.427	H
HETATM 1180 H	0	7.230	7.550	2.560	H
HETATM 1181 H	0	7.832	6.339	0.301	H
HETATM 1182 H	0	6.419	5.337	0.607	H
HETATM 1183 H	0	8.572	5.749	2.602	H
HETATM 1184 H	0	6.935	2.145	2.388	H
HETATM 1185 H	0	6.535	3.251	1.113	H
HETATM 1186 H	0	8.958	4.439	4.147	H
HETATM 1187 H	0	8.259	2.914	4.296	H
HETATM 1188 N	0	4.572	8.787	3.838	N
HETATM 1189 C	0	3.823	7.892	4.713	C
HETATM 1190 C	0	2.442	8.362	5.095	C
HETATM 1191 O	0	1.490	7.639	4.824	O
HETATM 1192 C	0	4.626	7.420	5.935	C
HETATM 1193 C	0	5.793	6.489	5.573	C
HETATM 1194 C	0	6.657	6.248	6.804	C
HETATM 1195 C	0	5.315	5.127	5.056	C
HETATM 1196 H	0	5.458	9.143	4.171	H

HETATM 1197	H	0	3.624	7.002	4.119	H
HETATM 1198	H	0	4.998	8.282	6.480	H
HETATM 1199	H	0	3.959	6.883	6.609	H
HETATM 1200	H	0	6.410	6.957	4.809	H
HETATM 1201	H	0	6.111	5.657	7.536	H
HETATM 1202	H	0	6.934	7.199	7.257	H
HETATM 1203	H	0	7.564	5.728	6.515	H
HETATM 1204	H	0	6.167	4.469	4.917	H
HETATM 1205	H	0	4.806	5.230	4.100	H
HETATM 1206	H	0	4.635	4.671	5.777	H
HETATM 1207	N	0	2.293	9.514	5.729	N
HETATM 1208	C	0	0.965	9.948	6.127	C
HETATM 1209	C	0	-0.077	9.997	4.975	C
HETATM 1210	O	0	-1.178	9.473	5.161	O
HETATM 1211	C	0	1.068	11.245	6.942	C
HETATM 1212	H	0	3.111	10.053	6.002	H
HETATM 1213	H	0	0.588	9.193	6.819	H
HETATM 1214	H	0	1.559	12.035	6.377	H
HETATM 1215	H	0	1.654	11.058	7.843	H
HETATM 1216	H	0	0.071	11.576	7.234	H
HETATM 1217	N	0	0.219	10.553	3.782	N
HETATM 1218	C	0	-0.612	10.380	2.580	C
HETATM 1219	C	0	-0.770	8.914	2.128	C
HETATM 1220	O	0	-1.846	8.540	1.664	O
HETATM 1221	C	0	0.082	11.206	1.497	C
HETATM 1222	C	0	0.985	12.183	2.238	C
HETATM 1223	C	0	1.366	11.404	3.486	C
HETATM 1224	H	0	-1.595	10.808	2.771	H
HETATM 1225	H	0	0.701	10.551	0.887	H
HETATM 1226	H	0	-0.641	11.746	0.890	H
HETATM 1227	H	0	0.415	13.070	2.520	H
HETATM 1228	H	0	1.864	12.457	1.654	H
HETATM 1229	H	0	1.582	12.104	4.289	H
HETATM 1230	H	0	2.242	10.792	3.282	H
HETATM 1231	N	0	0.250	8.052	2.235	N
HETATM 1232	C	0	0.085	6.607	1.999	C
HETATM 1233	C	0	-0.979	6.007	2.911	C
HETATM 1234	O	0	-1.939	5.422	2.421	O
HETATM 1235	C	0	1.422	5.850	2.089	C
HETATM 1236	C	0	1.307	4.375	1.664	C
HETATM 1237	C	0	0.886	4.202	0.203	C
HETATM 1238	C	0	2.656	3.696	1.843	C
HETATM 1239	H	0	1.149	8.385	2.568	H
HETATM 1240	H	0	-0.276	6.503	0.977	H
HETATM 1241	H	0	2.155	6.340	1.455	H
HETATM 1242	H	0	1.786	5.879	3.112	H
HETATM 1243	H	0	0.585	3.868	2.303	H
HETATM 1244	H	0	1.533	4.773	-0.453	H
HETATM 1245	H	0	-0.138	4.537	0.067	H

HETATM 1246	H	0	0.946	3.150	-0.079	H
HETATM 1247	H	0	3.027	3.853	2.854	H
HETATM 1248	H	0	3.378	4.079	1.124	H
HETATM 1249	H	0	2.521	2.627	1.683	H
HETATM 1250	N	0	-0.847	6.207	4.219	N
HETATM 1251	C	0	-1.867	5.857	5.195	C
HETATM 1252	C	0	-3.230	6.471	4.873	C
HETATM 1253	O	0	-4.217	5.758	4.931	O
HETATM 1254	C	0	-1.405	6.181	6.625	C
HETATM 1255	C	0	-0.364	5.205	7.144	C
HETATM 1256	C	0	0.985	5.586	7.257	C
HETATM 1257	C	0	-0.747	3.894	7.489	C
HETATM 1258	C	0	1.959	4.650	7.651	C
HETATM 1259	C	0	0.223	2.955	7.891	C
HETATM 1260	C	0	1.584	3.324	7.949	C
HETATM 1261	O	0	2.529	2.428	8.331	O
HETATM 1262	H	0	-0.018	6.704	4.530	H
HETATM 1263	H	0	-2.012	4.780	5.142	H
HETATM 1264	H	0	-1.018	7.199	6.665	H
HETATM 1265	H	0	-2.268	6.129	7.290	H
HETATM 1266	H	0	1.280	6.602	7.039	H
HETATM 1267	H	0	-1.784	3.592	7.421	H
HETATM 1268	H	0	2.996	4.938	7.735	H
HETATM 1269	H	0	-0.072	1.942	8.123	H
HETATM 1270	H	0	2.103	1.656	8.746	H
HETATM 1271	N	0	-3.324	7.751	4.512	N
HETATM 1272	C	0	-4.580	8.392	4.119	C
HETATM 1273	C	0	-5.223	7.788	2.830	C
HETATM 1274	O	0	-6.412	7.480	2.843	O
HETATM 1275	C	0	-4.347	9.900	3.975	C
HETATM 1276	H	0	-2.473	8.304	4.534	H
HETATM 1277	H	0	-5.298	8.243	4.925	H
HETATM 1278	H	0	-3.659	10.093	3.155	H
HETATM 1279	H	0	-3.928	10.305	4.896	H
HETATM 1280	H	0	-5.294	10.398	3.762	H
HETATM 1281	N	0	-4.486	7.620	1.720	N
HETATM 1282	C	0	-4.934	6.968	0.457	C
HETATM 1283	C	0	-5.301	5.466	0.727	C
HETATM 1284	O	0	-6.363	5.028	0.288	O
HETATM 1285	C	0	-3.870	7.029	-0.647	C
HETATM 1286	O	0	-2.612	6.578	-0.190	O
HETATM 1287	H	0	-3.519	7.911	1.794	H
HETATM 1288	H	0	-5.834	7.468	0.103	H
HETATM 1289	H	0	-3.760	8.044	-1.018	H
HETATM 1290	H	0	-4.193	6.403	-1.480	H
HETATM 1291	H	0	-2.274	7.223	0.458	H
HETATM 1292	N	0	-4.487	4.675	1.466	N
HETATM 1293	C	0	-4.758	3.291	1.975	C
HETATM 1294	C	0	-6.042	3.279	2.762	C

HETATM 1295	O	0	-6.918	2.463	2.519	O
HETATM 1296	C	0	-3.585	2.838	2.832	C
HETATM 1297	H	0	-3.623	5.100	1.782	H
HETATM 1298	H	0	-4.867	2.610	1.130	H
HETATM 1299	H	0	-3.784	1.837	3.207	H
HETATM 1300	H	0	-3.466	3.517	3.673	H
HETATM 1301	H	0	-2.669	2.827	2.247	H
HETATM 1302	N	0	-6.163	4.232	3.677	N
HETATM 1303	C	0	-7.355	4.461	4.455	C
HETATM 1304	C	0	-8.599	4.785	3.634	C
HETATM 1305	O	0	-9.656	4.270	3.960	O
HETATM 1306	C	0	-7.079	5.456	5.590	C
HETATM 1307	C	0	-8.293	5.835	6.457	C
HETATM 1308	C	0	-7.928	6.198	7.911	C
HETATM 1309	N	0	-6.602	6.835	8.069	N
HETATM 1310	C	0	-6.203	8.044	7.734	C
HETATM 1311	N	0	-7.012	8.902	7.177	N
HETATM 1312	N	0	-4.977	8.421	7.952	N
HETATM 1313	H	0	-5.351	4.812	3.858	H
HETATM 1314	H	0	-7.596	3.516	4.945	H
HETATM 1315	H	0	-6.326	4.992	6.229	H
HETATM 1316	H	0	-6.668	6.375	5.179	H
HETATM 1317	H	0	-8.999	5.005	6.491	H
HETATM 1318	H	0	-8.799	6.681	5.990	H
HETATM 1319	H	0	-7.914	5.271	8.489	H
HETATM 1320	H	0	-8.710	6.829	8.337	H
HETATM 1321	H	0	-5.877	6.216	8.427	H
HETATM 1322	H	0	-6.717	9.832	6.958	H
HETATM 1323	H	0	-7.958	8.602	7.026	H
HETATM 1324	H	0	-4.351	7.808	8.473	H
HETATM 1325	H	0	-4.651	9.329	7.689	H
HETATM 1326	N	0	-8.514	5.588	2.580	N
HETATM 1327	C	0	-9.614	5.797	1.633	C
HETATM 1328	C	0	-9.996	4.537	0.867	C
HETATM 1329	O	0	-11.181	4.309	0.647	O
HETATM 1330	C	0	-9.212	6.923	0.679	C
HETATM 1331	H	0	-7.625	6.043	2.416	H
HETATM 1332	H	0	-10.487	6.136	2.186	H
HETATM 1333	H	0	-8.970	7.817	1.249	H
HETATM 1334	H	0	-10.046	7.135	0.015	H
HETATM 1335	H	0	-8.352	6.632	0.079	H
HETATM 1336	N	0	-9.018	3.709	0.497	N
HETATM 1337	C	0	-9.294	2.365	0.010	C
HETATM 1338	C	0	-9.994	1.509	1.051	C
HETATM 1339	O	0	-11.009	0.897	0.757	O
HETATM 1340	C	0	-8.010	1.717	-0.553	C
HETATM 1341	C	0	-8.253	0.400	-1.320	C
HETATM 1342	C	0	-8.949	0.613	-2.667	C
HETATM 1343	C	0	-6.916	-0.287	-1.608	C

HETATM 1344	H	0	-8.057	4.001	0.641	H
HETATM 1345	H	0	-9.996	2.473	-0.816	H
HETATM 1346	H	0	-7.513	2.424	-1.218	H
HETATM 1347	H	0	-7.332	1.507	0.272	H
HETATM 1348	H	0	-8.858	-0.271	-0.712	H
HETATM 1349	H	0	-8.324	1.202	-3.335	H
HETATM 1350	H	0	-9.915	1.097	-2.525	H
HETATM 1351	H	0	-9.136	-0.357	-3.128	H
HETATM 1352	H	0	-6.293	0.345	-2.240	H
HETATM 1353	H	0	-7.092	-1.238	-2.111	H
HETATM 1354	H	0	-6.393	-0.484	-0.672	H
HETATM 1355	N	0	-9.487	1.502	2.275	N
HETATM 1356	C	0	-10.084	0.822	3.411	C
HETATM 1357	C	0	-11.522	1.270	3.697	C
HETATM 1358	O	0	-12.384	0.466	4.047	O
HETATM 1359	C	0	-9.195	0.972	4.652	C
HETATM 1360	C	0	-8.887	-0.259	5.451	C
HETATM 1361	C	0	-7.836	-0.316	6.296	C
HETATM 1362	C	0	-9.515	-1.591	5.500	C
HETATM 1363	N	0	-7.767	-1.566	6.867	N
HETATM 1364	C	0	-8.756	-2.396	6.403	C
HETATM 1365	C	0	-10.618	-2.232	4.883	C
HETATM 1366	C	0	-9.057	-3.737	6.672	C
HETATM 1367	C	0	-10.925	-3.582	5.139	C
HETATM 1368	C	0	-10.143	-4.339	6.025	C
HETATM 1369	H	0	-8.610	1.991	2.410	H
HETATM 1370	H	0	-10.121	-0.231	3.147	H
HETATM 1371	H	0	-8.230	1.368	4.344	H
HETATM 1372	H	0	-9.629	1.718	5.318	H
HETATM 1373	H	0	-7.141	0.500	6.463	H
HETATM 1374	H	0	-7.023	-1.853	7.500	H
HETATM 1375	H	0	-11.249	-1.699	4.196	H
HETATM 1376	H	0	-8.461	-4.298	7.373	H
HETATM 1377	H	0	-11.770	-4.046	4.651	H
HETATM 1378	H	0	-10.380	-5.376	6.213	H
HETATM 1379	N	0	-11.769	2.566	3.560	N
HETATM 1380	C	0	-13.047	3.244	3.671	C
HETATM 1381	C	0	-14.001	2.875	2.552	C
HETATM 1382	O	0	-15.093	2.412	2.852	O
HETATM 1383	C	0	-12.768	4.760	3.742	C
HETATM 1384	C	0	-13.967	5.719	3.640	C
HETATM 1385	C	0	-14.947	5.581	4.799	C
HETATM 1386	C	0	-13.448	7.158	3.633	C
HETATM 1387	H	0	-10.954	3.143	3.388	H
HETATM 1388	H	0	-13.516	2.942	4.608	H
HETATM 1389	H	0	-12.234	4.965	4.672	H
HETATM 1390	H	0	-12.106	5.006	2.921	H
HETATM 1391	H	0	-14.495	5.540	2.705	H
HETATM 1392	H	0	-14.445	5.790	5.742	H

HETATM 1393	H	0	-15.353	4.574	4.815	H
HETATM 1394	H	0	-15.772	6.283	4.672	H
HETATM 1395	H	0	-12.895	7.362	4.551	H
HETATM 1396	H	0	-14.287	7.851	3.563	H
HETATM 1397	H	0	-12.796	7.312	2.774	H
HETATM 1398	N	0	-13.595	3.055	1.292	N
HETATM 1399	C	0	-14.301	2.538	0.126	C
HETATM 1400	C	0	-14.627	1.046	0.321	C
HETATM 1401	O	0	-15.776	0.690	0.144	O
HETATM 1402	C	0	-13.477	2.724	-1.164	C
HETATM 1403	C	0	-13.526	4.117	-1.802	C
HETATM 1404	C	0	-12.512	4.218	-2.941	C
HETATM 1405	C	0	-14.909	4.415	-2.390	C
HETATM 1406	H	0	-12.668	3.440	1.152	H
HETATM 1407	H	0	-15.255	3.054	0.027	H
HETATM 1408	H	0	-12.441	2.448	-0.968	H
HETATM 1409	H	0	-13.863	2.036	-1.910	H
HETATM 1410	H	0	-13.275	4.859	-1.052	H
HETATM 1411	H	0	-12.743	3.495	-3.723	H
HETATM 1412	H	0	-11.512	4.022	-2.554	H
HETATM 1413	H	0	-12.524	5.221	-3.366	H
HETATM 1414	H	0	-15.202	3.614	-3.070	H
HETATM 1415	H	0	-14.892	5.350	-2.946	H
HETATM 1416	H	0	-15.652	4.490	-1.598	H
HETATM 1417	N	0	-13.675	0.179	0.701	N
HETATM 1418	C	0	-13.882	-1.265	0.967	C
HETATM 1419	C	0	-14.948	-1.466	2.032	C
HETATM 1420	O	0	-15.890	-2.212	1.807	O
HETATM 1421	C	0	-12.563	-2.000	1.273	C
HETATM 1422	C	0	-12.766	-3.382	1.901	C
HETATM 1423	C	0	-11.783	-2.221	-0.030	C
HETATM 1424	H	0	-12.735	0.547	0.784	H
HETATM 1425	H	0	-14.295	-1.707	0.062	H
HETATM 1426	H	0	-11.961	-1.402	1.956	H
HETATM 1427	H	0	-11.795	-3.851	2.049	H
HETATM 1428	H	0	-13.374	-4.009	1.249	H
HETATM 1429	H	0	-13.249	-3.296	2.873	H
HETATM 1430	H	0	-12.398	-2.757	-0.753	H
HETATM 1431	H	0	-10.889	-2.806	0.159	H
HETATM 1432	H	0	-11.481	-1.269	-0.460	H
HETATM 1433	N	0	-14.834	-0.804	3.179	N
HETATM 1434	C	0	-15.805	-0.919	4.259	C
HETATM 1435	C	0	-17.182	-0.256	3.982	C
HETATM 1436	O	0	-18.172	-0.647	4.599	O
HETATM 1437	C	0	-15.141	-0.425	5.542	C
HETATM 1438	H	0	-14.020	-0.216	3.318	H
HETATM 1439	H	0	-16.014	-1.980	4.405	H
HETATM 1440	H	0	-14.299	-1.073	5.790	H
HETATM 1441	H	0	-15.859	-0.459	6.362	H

HETATM 1442	H	0	-14.773	0.590	5.404	H
HETATM 1443	N	0	-17.274	0.737	3.088	N
HETATM 1444	C	0	-18.525	1.274	2.521	C
HETATM 1445	C	0	-19.109	0.253	1.500	C
HETATM 1446	O	0	-20.220	-0.216	1.703	O
HETATM 1447	C	0	-18.271	2.630	1.834	C
HETATM 1448	C	0	-18.027	3.802	2.799	C
HETATM 1449	C	0	-17.477	4.994	2.014	C
HETATM 1450	C	0	-19.305	4.242	3.514	C
HETATM 1451	H	0	-16.405	1.055	2.674	H
HETATM 1452	H	0	-19.268	1.396	3.309	H
HETATM 1453	H	0	-17.411	2.526	1.173	H
HETATM 1454	H	0	-19.133	2.873	1.210	H
HETATM 1455	H	0	-17.293	3.520	3.550	H
HETATM 1456	H	0	-18.194	5.297	1.251	H
HETATM 1457	H	0	-16.539	4.706	1.541	H
HETATM 1458	H	0	-17.298	5.827	2.693	H
HETATM 1459	H	0	-20.066	4.524	2.785	H
HETATM 1460	H	0	-19.092	5.094	4.159	H
HETATM 1461	H	0	-19.686	3.431	4.132	H
HETATM 1462	N	0	-18.354	-0.131	0.453	N
HETATM 1463	C	0	-18.626	-1.166	-0.575	C
HETATM 1464	C	0	-19.122	-2.482	0.033	C
HETATM 1465	O	0	-19.996	-3.144	-0.519	O
HETATM 1466	C	0	-17.380	-1.373	-1.442	C
HETATM 1467	H	0	-17.448	0.310	0.384	H
HETATM 1468	H	0	-19.428	-0.800	-1.218	H
HETATM 1469	H	0	-17.577	-2.141	-2.186	H
HETATM 1470	H	0	-16.544	-1.689	-0.820	H
HETATM 1471	H	0	-17.124	-0.447	-1.954	H
HETATM 1472	N	0	-18.525	-2.875	1.155	N
HETATM 1473	C	0	-18.889	-4.057	1.910	C
HETATM 1474	C	0	-20.134	-3.918	2.791	C
HETATM 1475	O	0	-20.772	-4.923	3.102	O
HETATM 1476	C	0	-17.706	-4.467	2.804	C
HETATM 1477	H	0	-17.731	-2.331	1.469	H
HETATM 1478	H	0	-19.093	-4.870	1.211	H
HETATM 1479	H	0	-17.956	-5.385	3.336	H
HETATM 1480	H	0	-17.506	-3.678	3.530	H
HETATM 1481	H	0	-16.811	-4.639	2.209	H
HETATM 1482	N	0	-20.431	-2.704	3.257	N
HETATM 1483	C	0	-21.672	-2.398	3.935	C
HETATM 1484	H	0	-21.846	-3.031	4.780	H
HETATM 1485	H	0	-22.440	-2.555	3.208	H
HETATM 1486	H	0	-21.680	-1.375	4.248	H
HETATM 1487	H	0	-19.897	-1.925	2.896	H
HETATM 1488	N	0	4.316	-2.763	-5.186	N
HETATM 1489	C	0	4.368	-2.234	-3.798	C
HETATM 1490	C	0	5.822	-2.337	-3.241	C

HETATM 1491 O	0	6.702	-2.625	-4.088	O
HETATM 1492 O	0	6.087	-2.169	-2.026	O
HETATM 1493 C	0	3.246	-2.899	-2.976	C
HETATM 1494 C	0	3.180	-2.544	-1.479	C
HETATM 1495 C	0	3.203	-1.059	-1.182	C
HETATM 1496 O	0	2.356	-0.332	-1.673	O
HETATM 1497 N	0	4.193	-0.631	-0.351	N
HETATM 1498 C	0	4.353	0.746	0.036	C
HETATM 1499 C	0	5.419	1.495	-0.768	C
HETATM 1500 O	0	5.508	2.719	-0.692	O
HETATM 1501 C	0	4.603	0.895	1.533	C
HETATM 1502 S	0	6.097	-0.009	2.119	S
HETATM 1503 N	0	6.199	0.717	-1.535	N
HETATM 1504 C	0	7.097	1.244	-2.552	C
HETATM 1505 C	0	6.536	1.137	-3.955	C
HETATM 1506 O	0	5.555	0.407	-4.183	O
HETATM 1507 O	0	7.079	1.803	-4.848	O
HETATM 1508 H	0	5.227	-2.614	-5.601	H
HETATM 1509 H	0	3.564	-2.310	-5.708	H
HETATM 1510 H	0	4.081	-3.753	-5.216	H
HETATM 1511 H	0	4.144	-1.169	-3.820	H
HETATM 1512 H	0	2.296	-2.602	-3.425	H
HETATM 1513 H	0	3.330	-3.979	-3.067	H
HETATM 1514 H	0	3.995	-3.034	-0.949	H
HETATM 1515 H	0	2.252	-2.924	-1.072	H
HETATM 1516 H	0	4.808	-1.315	0.079	H
HETATM 1517 H	0	3.412	1.256	-0.193	H
HETATM 1518 H	0	3.731	0.546	2.080	H
HETATM 1519 H	0	4.715	1.957	1.760	H
HETATM 1520 H	0	6.005	-0.276	-1.629	H
HETATM 1521 H	0	7.312	2.292	-2.357	H
HETATM 1522 H	0	8.027	0.683	-2.535	H
HETATM 1523 O	0	11.006	-6.844	-7.996	O
HETATM 1524 H	0	10.092	-6.559	-7.922	H
HETATM 1525 H	0	11.402	-6.197	-8.594	H
HETATM 1526 O	0	21.936	-1.988	3.406	O
HETATM 1527 H	0	22.740	-2.472	3.196	H
HETATM 1528 H	0	22.205	-1.400	4.118	H
HETATM 1529 O	0	16.367	5.973	-5.078	O
HETATM 1530 H	0	15.556	6.514	-4.992	H
HETATM 1531 H	0	16.995	6.595	-5.453	H
HETATM 1532 O	0	13.849	8.631	3.462	O
HETATM 1533 H	0	13.439	8.540	4.335	H
HETATM 1534 H	0	14.669	9.126	3.667	H
HETATM 1535 O	0	4.729	10.790	6.922	O
HETATM 1536 H	0	5.095	10.558	7.783	H
HETATM 1537 H	0	5.459	10.562	6.322	H
HETATM 1538 O	0	7.858	11.822	7.615	O
HETATM 1539 H	0	7.505	11.005	8.017	H

HETATM 1540	H	0	7.334	12.510	8.026	H
HETATM 1541	O	0	4.907	7.736	9.321	O
HETATM 1542	H	0	3.936	7.848	9.290	H
HETATM 1543	H	0	5.008	6.791	9.525	H
HETATM 1544	O	0	14.393	-1.548	4.320	O
HETATM 1545	H	0	13.668	-1.816	4.933	H
HETATM 1546	H	0	15.141	-2.098	4.617	H
HETATM 1547	O	0	-2.932	-3.002	-6.331	O
HETATM 1548	H	0	-2.692	-3.917	-6.575	H
HETATM 1549	H	0	-3.051	-2.568	-7.195	H
HETATM 1550	O	0	-8.938	3.977	-3.362	O
HETATM 1551	H	0	-8.128	4.371	-3.699	H
HETATM 1552	H	0	-8.711	3.058	-3.219	H
HETATM 1553	O	0	-14.882	1.516	7.972	O
HETATM 1554	H	0	-14.259	0.886	8.386	H
HETATM 1555	H	0	-15.548	1.618	8.674	H
HETATM 1556	O	0	-16.458	-4.485	6.342	O
HETATM 1557	H	0	-16.691	-3.960	7.137	H
HETATM 1558	H	0	-17.207	-4.316	5.760	H
HETATM 1559	O	0	-16.451	2.512	5.939	O
HETATM 1560	H	0	-16.044	2.467	5.064	H
HETATM 1561	H	0	-15.815	2.040	6.514	H
HETATM 1562	O	0	-10.309	-1.425	8.965	O
HETATM 1563	H	0	-10.529	-1.126	8.067	H
HETATM 1564	H	0	-11.130	-1.871	9.240	H
HETATM 1565	O	0	-13.492	3.692	7.163	O
HETATM 1566	H	0	-14.135	4.367	7.416	H
HETATM 1567	H	0	-13.929	2.874	7.473	H
HETATM 1568	O	0	3.193	-7.670	9.336	O
HETATM 1569	H	0	3.274	-6.845	8.822	H
HETATM 1570	H	0	2.518	-8.162	8.826	H
HETATM 1571	O	0	-6.120	-4.675	6.104	O
HETATM 1572	H	0	-6.933	-4.541	5.606	H
HETATM 1573	H	0	-6.338	-5.433	6.682	H
HETATM 1574	O	0	17.195	3.918	-3.516	O
HETATM 1575	H	0	16.826	4.664	-4.034	H
HETATM 1576	H	0	17.875	3.572	-4.096	H
HETATM 1577	O	0	16.370	3.712	-0.954	O
HETATM 1578	H	0	16.676	3.790	-1.883	H
HETATM 1579	H	0	17.089	3.213	-0.532	H
HETATM 1580	O	0	16.552	-3.117	4.901	O
HETATM 1581	H	0	16.333	-3.626	5.705	H
HETATM 1582	H	0	17.347	-3.570	4.569	H
HETATM 1583	O	0	18.051	2.146	0.640	O
HETATM 1584	H	0	18.698	1.420	0.516	H
HETATM 1585	H	0	17.305	1.675	1.055	H
HETATM 1586	O	0	19.461	-2.234	2.350	O
HETATM 1587	H	0	19.208	-3.107	2.711	H
HETATM 1588	H	0	20.356	-2.108	2.732	H

HETATM 1589	O	0	18.452	-4.563	3.393	O
HETATM 1590	H	0	17.704	-4.801	2.804	H
HETATM 1591	H	0	18.874	-5.414	3.553	H
HETATM 1592	O	0	19.492	-0.154	0.534	O
HETATM 1593	H	0	19.435	-0.870	1.195	H
HETATM 1594	H	0	20.211	-0.444	-0.032	H
HETATM 1595	O	0	16.780	-1.715	2.225	O
HETATM 1596	H	0	16.525	-2.114	3.071	H
HETATM 1597	H	0	17.743	-1.879	2.196	H
HETATM 1598	O	0	-2.212	-5.631	-6.635	O
HETATM 1599	H	0	-2.029	-5.892	-5.728	H
HETATM 1600	H	0	-1.454	-6.008	-7.128	H
HETATM 1601	O	0	1.185	0.475	-12.562	O
HETATM 1602	H	0	1.394	0.626	-11.627	H
HETATM 1603	H	0	0.939	-0.451	-12.595	H
HETATM 1604	O	0	-8.235	-12.459	0.562	O
HETATM 1605	H	0	-7.886	-13.160	0.003	H
HETATM 1606	H	0	-9.036	-12.159	0.070	H
HETATM 1607	O	0	-10.483	-11.547	-0.426	O
HETATM 1608	H	0	-11.137	-11.292	0.253	H
HETATM 1609	H	0	-10.773	-11.046	-1.211	H
HETATM 1610	O	0	-6.214	-12.065	3.539	O
HETATM 1611	H	0	-6.763	-11.435	3.041	H
HETATM 1612	H	0	-5.463	-12.216	2.957	H
HETATM 1613	O	0	2.768	-10.634	6.530	O
HETATM 1614	H	0	3.290	-11.399	6.857	H
HETATM 1615	H	0	2.238	-11.009	5.802	H
HETATM 1616	O	0	4.586	-12.317	7.608	O
HETATM 1617	H	0	4.820	-13.120	8.080	H
HETATM 1618	H	0	5.206	-11.658	7.972	H
HETATM 1619	O	0	14.452	-7.152	7.214	O
HETATM 1620	H	0	13.518	-7.077	7.477	H
HETATM 1621	H	0	14.536	-8.098	7.034	H
HETATM 1622	O	0	14.976	7.254	1.326	O
HETATM 1623	H	0	14.537	7.743	2.043	H
HETATM 1624	H	0	15.903	7.230	1.623	H
HETATM 1625	O	0	15.036	7.781	7.425	O
HETATM 1626	H	0	14.249	8.159	6.995	H
HETATM 1627	H	0	15.244	8.418	8.116	H
HETATM 1628	O	0	17.912	9.595	2.214	O
HETATM 1629	H	0	17.857	8.620	2.203	H
HETATM 1630	H	0	18.520	9.793	1.498	H
HETATM 1631	O	0	13.916	10.140	-3.494	O
HETATM 1632	H	0	14.055	10.619	-2.658	H
HETATM 1633	H	0	13.342	10.762	-3.983	H
HETATM 1634	O	0	14.972	4.161	2.441	O
HETATM 1635	H	0	15.934	4.123	2.295	H
HETATM 1636	H	0	14.626	4.405	1.565	H
HETATM 1637	O	0	17.771	4.213	2.358	O

HETATM 1638	H	0	18.343	3.883	3.058	H
HETATM 1639	H	0	17.956	3.591	1.624	H
HETATM 1640	O	0	17.423	6.920	2.523	O
HETATM 1641	H	0	17.634	5.978	2.373	H
HETATM 1642	H	0	17.213	6.944	3.475	H
HETATM 1643	O	0	14.919	12.268	4.564	O
HETATM 1644	H	0	14.075	12.063	5.006	H
HETATM 1645	H	0	15.000	13.220	4.656	H
HETATM 1646	O	0	9.885	4.589	6.495	O
HETATM 1647	H	0	8.988	4.201	6.539	H
HETATM 1648	H	0	10.449	3.790	6.581	H
HETATM 1649	O	0	16.112	9.877	4.184	O
HETATM 1650	H	0	16.806	9.951	3.491	H
HETATM 1651	H	0	15.837	10.811	4.311	H
HETATM 1652	O	0	14.334	5.094	7.526	O
HETATM 1653	H	0	14.448	4.980	6.568	H
HETATM 1654	H	0	14.676	5.994	7.666	H
HETATM 1655	O	0	14.165	1.078	3.881	O
HETATM 1656	H	0	14.296	0.128	4.092	H
HETATM 1657	H	0	14.867	1.239	3.229	H
HETATM 1658	O	0	6.788	9.567	8.773	O
HETATM 1659	H	0	7.541	9.022	9.064	H
HETATM 1660	H	0	6.036	8.970	8.976	H
HETATM 1661	O	0	11.331	2.419	6.768	O
HETATM 1662	H	0	11.776	2.635	7.607	H
HETATM 1663	H	0	11.989	2.692	6.090	H
HETATM 1664	O	0	16.401	7.336	5.059	O
HETATM 1665	H	0	16.391	8.275	4.777	H
HETATM 1666	H	0	16.184	7.408	6.005	H
HETATM 1667	O	0	2.198	7.697	9.372	O
HETATM 1668	H	0	1.250	7.918	9.319	H
HETATM 1669	H	0	2.226	6.997	10.045	H
HETATM 1670	O	0	11.842	6.249	-0.889	O
HETATM 1671	H	0	12.682	5.826	-0.639	H
HETATM 1672	H	0	12.097	6.841	-1.619	H
HETATM 1673	O	0	10.794	0.682	9.627	O
HETATM 1674	H	0	11.368	0.076	10.117	H
HETATM 1675	H	0	10.992	0.409	8.701	H
HETATM 1676	O	0	14.251	7.663	-4.922	O
HETATM 1677	H	0	14.431	8.586	-4.675	H
HETATM 1678	H	0	13.530	7.438	-4.309	H
HETATM 1679	O	0	14.228	5.089	-0.101	O
HETATM 1680	H	0	14.567	5.933	0.269	H
HETATM 1681	H	0	15.027	4.677	-0.496	H
HETATM 1682	O	0	14.515	5.393	4.749	O
HETATM 1683	H	0	14.696	4.970	3.878	H
HETATM 1684	H	0	15.217	6.074	4.792	H
HETATM 1685	O	0	5.251	2.966	8.004	O
HETATM 1686	H	0	4.301	2.778	7.909	H

HETATM 1687 H	0	5.544	2.217	8.566	H
HETATM 1688 O	0	10.102	5.258	9.132	O
HETATM 1689 H	0	10.947	4.793	9.275	H
HETATM 1690 H	0	9.972	5.141	8.173	H
HETATM 1691 O	0	12.357	7.993	-2.925	O
HETATM 1692 H	0	12.971	8.751	-2.980	H
HETATM 1693 H	0	11.490	8.444	-2.894	H
HETATM 1694 O	0	12.596	11.365	5.743	O
HETATM 1695 H	0	12.719	10.414	5.920	H
HETATM 1696 H	0	12.213	11.694	6.565	H
HETATM 1697 O	0	7.697	3.046	6.556	O
HETATM 1698 H	0	6.792	3.236	6.869	H
HETATM 1699 H	0	7.996	2.406	7.242	H
HETATM 1700 O	0	11.221	-2.759	11.357	O
HETATM 1701 H	0	11.787	-2.218	10.772	H
HETATM 1702 H	0	11.432	-3.659	11.059	H
HETATM 1703 O	0	8.494	7.518	9.644	O
HETATM 1704 H	0	7.889	7.079	10.251	H
HETATM 1705 H	0	9.175	6.842	9.496	H
HETATM 1706 O	0	15.719	-4.754	7.073	O
HETATM 1707 H	0	16.291	-4.833	7.843	H
HETATM 1708 H	0	15.299	-5.644	7.036	H
HETATM 1709 O	0	2.773	5.574	11.084	O
HETATM 1710 H	0	3.018	5.569	12.015	H
HETATM 1711 H	0	3.606	5.297	10.647	H
HETATM 1712 O	0	7.826	4.464	10.462	O
HETATM 1713 H	0	8.619	4.759	9.979	H
HETATM 1714 H	0	8.140	3.644	10.879	H
HETATM 1715 O	0	12.779	3.188	4.710	O
HETATM 1716 H	0	13.363	3.960	4.631	H
HETATM 1717 H	0	13.342	2.462	4.360	H
HETATM 1718 O	0	12.480	3.787	8.932	O
HETATM 1719 H	0	13.156	4.298	8.430	H
HETATM 1720 H	0	13.014	3.309	9.574	H
HETATM 1721 O	0	-2.422	3.496	-0.528	O
HETATM 1722 H	0	-1.992	2.769	-0.028	H
HETATM 1723 H	0	-2.506	4.189	0.137	H
HETATM 1724 O	0	-9.385	-12.754	5.253	O
HETATM 1725 H	0	-9.629	-12.833	4.302	H
HETATM 1726 H	0	-9.934	-13.425	5.667	H
HETATM 1727 O	0	-18.639	3.021	8.751	O
HETATM 1728 H	0	-19.536	3.312	8.941	H
HETATM 1729 H	0	-18.772	2.364	8.039	H
HETATM 1730 O	0	-5.600	2.511	7.385	O
HETATM 1731 H	0	-5.286	3.340	7.783	H
HETATM 1732 H	0	-6.573	2.599	7.452	H
HETATM 1733 O	0	-8.270	2.699	7.753	O
HETATM 1734 H	0	-8.434	2.716	8.714	H
HETATM 1735 H	0	-9.180	2.684	7.400	H

HETATM 1736 O	0	-4.868	4.736	8.963	O
HETATM 1737 H	0	-5.455	4.311	9.632	H
HETATM 1738 H	0	-3.993	4.681	9.390	H
HETATM 1739 O	0	-8.125	-0.018	9.705	O
HETATM 1740 H	0	-8.944	-0.529	9.537	H
HETATM 1741 H	0	-7.779	0.110	8.815	H
HETATM 1742 O	0	-5.608	-3.463	10.572	O
HETATM 1743 H	0	-4.838	-4.036	10.389	H
HETATM 1744 H	0	-6.354	-4.080	10.449	H
HETATM 1745 O	0	-11.328	-4.131	11.671	O
HETATM 1746 H	0	-10.471	-3.653	11.601	H
HETATM 1747 H	0	-11.425	-4.264	12.620	H
HETATM 1748 O	0	-2.819	-2.355	-3.732	O
HETATM 1749 H	0	-2.935	-2.595	-4.678	H
HETATM 1750 H	0	-2.632	-1.410	-3.772	H
HETATM 1751 O	0	-12.764	-4.918	8.050	O
HETATM 1752 H	0	-13.120	-5.790	8.313	H
HETATM 1753 H	0	-13.050	-4.856	7.120	H
HETATM 1754 O	0	-13.069	-0.049	9.210	O
HETATM 1755 H	0	-12.584	-0.107	8.360	H
HETATM 1756 H	0	-13.063	-0.970	9.522	H
HETATM 1757 O	0	-7.823	-10.308	2.135	O
HETATM 1758 H	0	-7.602	-9.599	1.508	H
HETATM 1759 H	0	-8.001	-11.067	1.540	H
HETATM 1760 O	0	-13.584	-7.485	8.609	O
HETATM 1761 H	0	-14.373	-7.430	8.021	H
HETATM 1762 H	0	-13.931	-7.960	9.371	H
HETATM 1763 O	0	-11.959	-7.346	5.315	O
HETATM 1764 H	0	-12.533	-6.569	5.406	H
HETATM 1765 H	0	-11.551	-7.430	6.196	H
HETATM 1766 O	0	-18.718	1.186	6.642	O
HETATM 1767 H	0	-18.887	0.548	5.926	H
HETATM 1768 H	0	-17.986	1.721	6.278	H
HETATM 1769 O	0	-8.391	-8.650	6.966	O
HETATM 1770 H	0	-9.290	-8.423	7.267	H
HETATM 1771 H	0	-8.563	-9.107	6.117	H
HETATM 1772 O	0	-17.291	-3.134	8.536	O
HETATM 1773 H	0	-16.554	-2.924	9.158	H
HETATM 1774 H	0	-17.948	-3.528	9.118	H
HETATM 1775 O	0	-5.918	-0.686	11.315	O
HETATM 1776 H	0	-5.892	-1.660	11.348	H
HETATM 1777 H	0	-6.745	-0.514	10.824	H
HETATM 1778 O	0	-15.300	-7.450	4.324	O
HETATM 1779 H	0	-15.975	-7.421	3.639	H
HETATM 1780 H	0	-14.857	-8.308	4.151	H
HETATM 1781 O	0	-14.185	-9.899	3.897	O
HETATM 1782 H	0	-13.216	-9.809	3.999	H
HETATM 1783 H	0	-14.396	-10.651	4.458	H
HETATM 1784 O	0	-15.374	-2.511	10.254	O

HETATM 1785	H	0	-15.466	-1.742	10.856	H
HETATM 1786	H	0	-14.414	-2.588	10.153	H
HETATM 1787	O	0	-12.077	-10.934	1.701	O
HETATM 1788	H	0	-13.034	-10.923	1.813	H
HETATM 1789	H	0	-11.772	-10.408	2.470	H
HETATM 1790	O	0	-11.769	0.096	6.895	O
HETATM 1791	H	0	-12.034	0.017	5.966	H
HETATM 1792	H	0	-11.405	1.000	6.943	H
HETATM 1793	O	0	-15.741	-7.143	7.059	O
HETATM 1794	H	0	-15.667	-7.417	6.129	H
HETATM 1795	H	0	-16.137	-6.260	6.981	H
HETATM 1796	O	0	-10.435	-5.507	9.433	O
HETATM 1797	H	0	-11.114	-5.157	8.826	H
HETATM 1798	H	0	-10.761	-5.205	10.300	H
HETATM 1799	O	0	-16.189	4.301	8.100	O
HETATM 1800	H	0	-16.320	3.878	7.235	H
HETATM 1801	H	0	-17.059	4.174	8.511	H
HETATM 1802	O	0	-17.660	-0.356	8.682	O
HETATM 1803	H	0	-17.607	-1.306	8.480	H
HETATM 1804	H	0	-18.163	0.007	7.932	H
HETATM 1805	O	0	-11.854	2.302	10.038	O
HETATM 1806	H	0	-12.261	1.420	9.940	H
HETATM 1807	H	0	-12.633	2.856	10.243	H
HETATM 1808	O	0	-11.005	2.688	7.467	O
HETATM 1809	H	0	-11.205	2.601	8.421	H
HETATM 1810	H	0	-11.787	3.188	7.154	H
HETATM 1811	O	0	-11.502	-9.607	3.999	O
HETATM 1812	H	0	-10.582	-9.803	4.272	H
HETATM 1813	H	0	-11.648	-8.726	4.417	H
HETATM 1814	O	0	-8.924	-10.078	4.676	O
HETATM 1815	H	0	-8.961	-11.017	4.942	H
HETATM 1816	H	0	-8.474	-10.118	3.808	H
HETATM 1817	O	0	-12.636	-2.761	9.708	O
HETATM 1818	H	0	-12.757	-3.481	9.051	H
HETATM 1819	H	0	-12.285	-3.246	10.483	H
HETATM 1820	O	0	-16.659	1.627	10.111	O
HETATM 1821	H	0	-17.018	0.804	9.699	H
HETATM 1822	H	0	-17.363	2.265	9.891	H
HETATM 1823	O	0	-9.035	2.508	10.375	O
HETATM 1824	H	0	-8.818	1.557	10.381	H
HETATM 1825	H	0	-10.007	2.510	10.461	H
HETATM 1826	O	0	-14.410	3.433	10.260	O
HETATM 1827	H	0	-14.879	3.982	9.615	H
HETATM 1828	H	0	-15.093	2.799	10.525	H
HETATM 1829	O	0	-15.550	-0.288	11.791	O
HETATM 1830	H	0	-15.902	0.448	11.261	H
HETATM 1831	H	0	-15.690	0.002	12.695	H
HETATM 1832	O	0	-13.948	-5.340	5.511	O
HETATM 1833	H	0	-14.748	-4.855	5.791	H

HETATM 1834	H	0	-14.336	-6.056	4.973	H
HETATM 1835	O	0	-10.907	-7.688	7.828	O
HETATM 1836	H	0	-10.562	-7.031	8.461	H
HETATM 1837	H	0	-11.815	-7.832	8.155	H
HETATM 1838	O	0	-6.669	-6.689	7.818	O
HETATM 1839	H	0	-5.780	-7.089	7.912	H
HETATM 1840	H	0	-7.219	-7.443	7.521	H
HETATM 1841	O	0	-5.457	-1.816	8.466	O
HETATM 1842	H	0	-5.552	-2.300	9.313	H
HETATM 1843	H	0	-4.922	-2.445	7.939	H
HETATM 1844	O	0	-0.497	-7.962	10.331	O
HETATM 1845	H	0	-0.798	-8.611	9.678	H
HETATM 1846	H	0	-0.840	-7.119	9.990	H
HETATM 1847	O	0	9.125	-5.083	10.453	O
HETATM 1848	H	0	10.085	-5.119	10.292	H
HETATM 1849	H	0	8.815	-5.948	10.111	H
HETATM 1850	O	0	0.751	-6.136	7.234	O
HETATM 1851	H	0	0.996	-7.077	7.358	H
HETATM 1852	H	0	1.618	-5.694	7.278	H
HETATM 1853	O	0	-2.180	-1.604	7.532	O
HETATM 1854	H	0	-2.791	-0.841	7.538	H
HETATM 1855	H	0	-2.783	-2.357	7.342	H
HETATM 1856	O	0	-1.742	-7.254	6.634	O
HETATM 1857	H	0	-0.916	-6.754	6.749	H
HETATM 1858	H	0	-1.447	-8.050	6.158	H
HETATM 1859	O	0	3.385	-5.297	7.980	O
HETATM 1860	H	0	3.236	-4.572	8.610	H
HETATM 1861	H	0	4.361	-5.366	7.985	H
HETATM 1862	O	0	7.660	0.136	11.395	O
HETATM 1863	H	0	8.115	-0.571	11.890	H
HETATM 1864	H	0	8.225	0.912	11.556	H
HETATM 1865	O	0	-6.482	3.550	10.723	O
HETATM 1866	H	0	-6.124	2.953	11.408	H
HETATM 1867	H	0	-7.422	3.293	10.691	H
HETATM 1868	O	0	-6.185	-10.194	7.713	O
HETATM 1869	H	0	-6.986	-9.668	7.546	H
HETATM 1870	H	0	-6.366	-11.010	7.196	H
HETATM 1871	O	0	5.637	-8.209	10.315	O
HETATM 1872	H	0	5.657	-7.498	10.981	H
HETATM 1873	H	0	4.723	-8.125	9.969	H
HETATM 1874	O	0	1.743	-6.952	11.540	O
HETATM 1875	H	0	0.873	-7.347	11.333	H
HETATM 1876	H	0	2.305	-7.327	10.839	H
HETATM 1877	O	0	-7.719	-5.043	9.731	O
HETATM 1878	H	0	-8.648	-5.330	9.643	H
HETATM 1879	H	0	-7.263	-5.644	9.107	H
HETATM 1880	O	0	3.146	-4.878	12.396	O
HETATM 1881	H	0	2.824	-4.687	13.283	H
HETATM 1882	H	0	2.584	-5.645	12.129	H

HETATM 1883 O	0	-1.046	1.528	0.720	O
HETATM 1884 H	0	-0.694	0.818	0.155	H
HETATM 1885 H	0	-0.671	1.330	1.583	H
HETATM 1886 O	0	-4.053	0.374	7.873	O
HETATM 1887 H	0	-4.576	1.167	7.624	H
HETATM 1888 H	0	-4.743	-0.306	8.018	H
HETATM 1889 O	0	6.165	-10.220	8.519	O
HETATM 1890 H	0	5.876	-9.675	7.763	H
HETATM 1891 H	0	5.951	-9.643	9.278	H
HETATM 1892 O	0	5.572	-5.689	11.451	O
HETATM 1893 H	0	6.217	-5.091	11.877	H
HETATM 1894 H	0	4.731	-5.437	11.881	H
HETATM 1895 O	0	7.445	-3.800	12.043	O
HETATM 1896 H	0	8.155	-4.319	11.606	H
HETATM 1897 H	0	7.944	-3.069	12.454	H
HETATM 1898 O	0	-3.797	-10.070	8.866	O
HETATM 1899 H	0	-4.659	-10.163	8.394	H
HETATM 1900 H	0	-3.967	-10.534	9.692	H
HETATM 1901 O	0	6.005	-5.508	8.752	O
HETATM 1902 H	0	5.829	-5.615	9.707	H
HETATM 1903 H	0	6.771	-6.088	8.618	H
HETATM 1904 O	0	-4.022	-7.437	8.096	O
HETATM 1905 H	0	-3.244	-7.333	7.506	H
HETATM 1906 H	0	-3.926	-8.358	8.404	H
HETATM 1907 O	0	1.317	-8.726	7.720	O
HETATM 1908 H	0	1.808	-9.455	7.286	H
HETATM 1909 H	0	0.492	-9.166	8.008	H
HETATM 1910 O	0	-1.002	-9.615	5.361	O
HETATM 1911 H	0	-0.187	-10.109	5.149	H
HETATM 1912 H	0	-1.494	-9.658	4.534	H
HETATM 1913 O	0	-3.650	-5.109	9.436	O
HETATM 1914 H	0	-3.891	-5.992	9.090	H
HETATM 1915 H	0	-2.679	-5.187	9.527	H
HETATM 1916 O	0	-3.366	0.088	10.485	O
HETATM 1917 H	0	-4.201	-0.281	10.830	H
HETATM 1918 H	0	-3.577	0.244	9.544	H
HETATM 1919 O	0	-10.085	-12.753	2.681	O
HETATM 1920 H	0	-10.809	-12.283	2.240	H
HETATM 1921 H	0	-9.400	-12.796	1.994	H
HETATM 1922 O	0	-1.165	-9.781	8.190	O
HETATM 1923 H	0	-1.243	-9.837	7.223	H
HETATM 1924 H	0	-2.079	-9.969	8.484	H
HETATM 1925 O	0	-6.835	-12.263	6.145	O
HETATM 1926 H	0	-7.747	-12.564	5.995	H
HETATM 1927 H	0	-6.478	-12.251	5.234	H
HETATM 1928 O	0	3.245	-3.450	10.074	O
HETATM 1929 H	0	3.273	-3.909	10.941	H
HETATM 1930 H	0	2.274	-3.360	9.933	H
HETATM 1931 O	0	-2.485	4.801	10.330	O

HETATM 1932 H	0	-2.649	3.980	10.844	H
HETATM 1933 H	0	-1.507	4.866	10.365	H
HETATM 1934 O	0	-0.476	8.354	9.356	O
HETATM 1935 H	0	-0.568	9.200	9.802	H
HETATM 1936 H	0	-1.358	7.958	9.437	H
HETATM 1937 O	0	11.867	-4.999	9.735	O
HETATM 1938 H	0	11.976	-5.883	9.353	H
HETATM 1939 H	0	12.360	-4.447	9.096	H
HETATM 1940 O	0	9.170	-1.770	12.740	O
HETATM 1941 H	0	9.923	-2.122	12.209	H
HETATM 1942 H	0	9.550	-1.704	13.621	H
HETATM 1943 O	0	-0.062	2.312	11.242	O
HETATM 1944 H	0	-0.970	2.305	11.584	H
HETATM 1945 H	0	0.077	3.247	11.017	H
HETATM 1946 O	0	-3.933	-3.586	7.192	O
HETATM 1947 H	0	-3.792	-4.234	7.911	H
HETATM 1948 H	0	-4.618	-4.027	6.641	H
HETATM 1949 O	0	1.344	0.462	9.835	O
HETATM 1950 H	0	0.996	1.129	10.465	H
HETATM 1951 H	0	0.590	-0.160	9.792	H
HETATM 1952 O	0	5.817	0.824	9.560	O
HETATM 1953 H	0	6.304	0.500	10.349	H
HETATM 1954 H	0	5.047	0.224	9.522	H
HETATM 1955 O	0	0.215	-2.763	6.944	O
HETATM 1956 H	0	0.031	-3.416	6.263	H
HETATM 1957 H	0	-0.632	-2.283	7.028	H
HETATM 1958 O	0	9.427	2.282	11.363	O
HETATM 1959 H	0	9.983	1.798	10.718	H
HETATM 1960 H	0	10.068	2.621	11.994	H
HETATM 1961 O	0	-3.098	7.377	9.869	O
HETATM 1962 H	0	-3.342	7.600	10.773	H
HETATM 1963 H	0	-2.875	6.423	9.947	H
HETATM 1964 O	0	8.089	-7.363	9.394	O
HETATM 1965 H	0	8.587	-8.192	9.250	H
HETATM 1966 H	0	7.256	-7.704	9.771	H
HETATM 1967 O	0	12.663	-1.497	9.470	O
HETATM 1968 H	0	12.250	-1.094	8.669	H
HETATM 1969 H	0	13.143	-2.243	9.076	H
HETATM 1970 O	0	0.681	-3.169	9.544	O
HETATM 1971 H	0	0.616	-3.050	8.570	H
HETATM 1972 H	0	0.126	-2.435	9.873	H
HETATM 1973 O	0	-0.927	-1.025	9.844	O
HETATM 1974 H	0	-1.344	-1.248	8.987	H
HETATM 1975 H	0	-1.678	-0.648	10.339	H
HETATM 1976 O	0	5.187	4.986	9.915	O
HETATM 1977 H	0	6.098	4.868	10.257	H
HETATM 1978 H	0	5.158	4.307	9.215	H
HETATM 1979 O	0	-9.049	-2.946	10.950	O
HETATM 1980 H	0	-8.437	-3.591	10.555	H

HETATM 1981	H	0	-9.313	-2.397	10.193	H
HETATM 1982	O	0	0.227	4.921	10.376	O
HETATM 1983	H	0	1.107	5.162	10.730	H
HETATM 1984	H	0	0.384	4.917	9.419	H
HETATM 1985	O	0	13.236	-3.600	7.760	O
HETATM 1986	H	0	12.926	-3.009	7.032	H
HETATM 1987	H	0	14.089	-3.925	7.424	H
HETATM 1988	O	0	3.648	-0.837	9.112	O
HETATM 1989	H	0	2.842	-0.323	9.320	H
HETATM 1990	H	0	3.442	-1.702	9.503	H
HETATM 1991	O	0	8.317	1.252	8.433	O
HETATM 1992	H	0	9.065	1.037	9.016	H
HETATM 1993	H	0	7.539	1.057	8.987	H
HETATM 1994	O	0	8.797	-9.991	9.261	O
HETATM 1995	H	0	7.912	-10.240	8.936	H
HETATM 1996	H	0	9.078	-10.762	9.760	H
HETATM 1997	O	0	-2.890	2.472	11.641	O
HETATM 1998	H	0	-3.708	2.449	12.167	H
HETATM 1999	H	0	-2.928	1.598	11.198	H
HETATM 2000	O	0	-0.931	-5.411	9.288	O
HETATM 2001	H	0	-0.414	-5.661	8.499	H
HETATM 2002	H	0	-0.401	-4.678	9.647	H
HETATM 2003	O	0	-5.481	1.725	12.542	O
HETATM 2004	H	0	-5.751	1.576	13.453	H
HETATM 2005	H	0	-5.619	0.847	12.130	H
HETATM 2006	C	0	11.642	-0.981	6.232	C
HETATM 2007	O	0	11.470	-0.550	7.400	O
HETATM 2008	C	0	10.936	-0.221	5.036	C
HETATM 2009	C	0	9.551	0.386	5.312	C
HETATM 2010	C	0	8.375	-0.352	4.651	C
HETATM 2011	C	0	7.058	0.389	4.849	C
HETATM 2012	O	0	12.387	-1.938	5.900	O
HETATM 2013	C	0	5.819	-0.027	4.011	C
HETATM 2014	C	0	4.725	0.933	4.341	C
HETATM 2015	O	0	6.614	0.435	6.166	O
HETATM 2016	C	0	3.464	0.616	4.631	C
HETATM 2017	C	0	2.393	1.590	4.764	C
HETATM 2018	C	0	1.108	1.227	4.789	C
HETATM 2019	C	0	0.068	2.125	4.818	C
HETATM 2020	C	0	-1.241	1.787	4.909	C
HETATM 2021	C	0	-1.764	0.371	5.038	C
HETATM 2022	C	0	-2.065	-0.268	3.690	C
HETATM 2023	C	0	-3.261	-0.835	3.372	C
HETATM 2024	C	0	-4.431	-0.905	4.344	C
HETATM 2025	C	0	-5.477	-1.940	3.931	C
HETATM 2026	C	0	-6.406	-1.505	2.791	C
HETATM 2027	C	0	-7.465	-2.600	2.609	C
HETATM 2028	C	0	-8.357	-2.337	1.399	C
HETATM 2029	H	0	11.624	0.586	4.755	H

HETATM 2030	H	0	10.903	-0.902	4.178	H
HETATM 2031	H	0	9.427	0.435	6.394	H
HETATM 2032	H	0	9.520	1.432	4.956	H
HETATM 2033	H	0	8.277	-1.365	5.057	H
HETATM 2034	H	0	8.578	-0.457	3.576	H
HETATM 2035	H	0	7.239	1.448	4.572	H
HETATM 2036	H	0	5.556	-1.053	4.269	H
HETATM 2037	H	0	5.012	1.987	4.307	H
HETATM 2038	H	0	3.185	-0.429	4.724	H
HETATM 2039	H	0	2.697	2.636	4.808	H
HETATM 2040	H	0	0.902	0.161	4.797	H
HETATM 2041	H	0	0.312	3.187	4.798	H
HETATM 2042	H	0	-1.964	2.588	4.981	H
HETATM 2043	H	0	-2.663	0.440	5.642	H
HETATM 2044	H	0	-1.061	-0.252	5.586	H
HETATM 2045	H	0	-1.273	-0.282	2.946	H
HETATM 2046	H	0	-3.377	-1.275	2.381	H
HETATM 2047	H	0	-4.899	0.075	4.445	H
HETATM 2048	H	0	-4.058	-1.216	5.320	H
HETATM 2049	H	0	-6.085	-2.166	4.806	H
HETATM 2050	H	0	-4.963	-2.851	3.637	H
HETATM 2051	H	0	-6.893	-0.560	3.042	H
HETATM 2052	H	0	-5.829	-1.381	1.873	H
HETATM 2053	H	0	-8.088	-2.660	3.500	H
HETATM 2054	H	0	-6.978	-3.568	2.486	H
HETATM 2055	H	0	-8.925	-1.418	1.542	H
HETATM 2056	H	0	-7.754	-2.254	0.496	H
HETATM 2057	H	0	-9.043	-3.175	1.290	H